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Determination of the characteristic limits (decision threshold, detection limit and limits of the coverage interval) for measurements of ionizing radiation — Fundamentals and application —

Part 2:
Advanced applications

Détermination des limites caractéristiques (seuil de décision, limite de détection et extrémités de l'intervalle élargi) pour mesurages de rayonnements ionisants — Principes fondamentaux et applications —

Partie 2: Applications avancées

Reference number
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Foreword

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The procedures used to develop this document and those intended for its further maintenance are described in the ISO/IEC Directives, Part 1. In particular, the different approval criteria needed for the different types of ISO documents should be noted. This document was drafted in accordance with the editorial rules of the ISO/IEC Directives, Part 2 (see www.iso.org/directives).

Attention is drawn to the possibility that some of the elements of this document may be the subject of patent rights. ISO shall not be held responsible for identifying any or all such patent rights. Details of any patent rights identified during the development of the document will be in the Introduction and/or on the ISO list of patent declarations received (see www.iso.org/patents).

Any trade name used in this document is information given for the convenience of users and does not constitute an endorsement.

For an explanation of the voluntary nature of standards, the meaning of ISO specific terms and expressions related to conformity assessment, as well as information about ISO's adherence to the World Trade Organization (WTO) principles in the Technical Barriers to Trade (TBT), see www.iso.org/iso/foreword.html.

This document was prepared by This document was prepared by ISO/TC 85, *Nuclear energy, nuclear technologies, and radiological protection*, Subcommittee SC 2, *Radiological protection*.

This second edition of ISO 11929-2 together with ISO 11929-1, ISO 11929-3, cancels and replaces ISO 11929:2010 which have been technically revised, specifically with reference to the type of statistical treatment of the data and extended with respect to the methodology of uncertainty assessment from the ISO/IEC Guide 98-3:2009, to the ISO/IEC Guide 98-3-1:2008.

A list of all the parts in the ISO 11929 series can be found on the ISO website.

Introduction

Measurement uncertainties and characteristic values, such as the decision threshold, the detection limit and limits of the coverage interval for measurements as well as the best estimate and its associated standard measurement uncertainty, are of importance in metrology in general, and for radiological protection in particular. The quantification of the uncertainty associated with a measurement result provides a basis for the trust an individual can have in a measurement result. Conformity with regulatory limits, constraints or reference values can only be demonstrated by taking into account and quantifying all sources of uncertainty. Characteristic limits provide – in the end – the basis for deciding under uncertainty.

The ISO 11929 series provides characteristic values of a non-negative measurand of ionizing radiation. It is also applicable for a wide range of measuring methods extending beyond measurements of ionizing radiation.

The limits to be provided according to the ISO 11929 series for specified probabilities of wrong decisions allow detection possibilities to be assessed for a measurand and for the physical effect quantified by this measurand as follows:

— the "decision threshold" allows a decision to be made on whether or not the physical effect quantified by the measurand is present;

— the "detection limit" indicates the smallest true quantity value of the measurand that can still be detected with the applied measurement procedure; this gives a decision on whether or not the measurement procedure satisfies the requirements and is therefore suitable for the intended measurement purpose;

— the "limits of the coverage interval" enclose, in the case of the physical effect recognized as present, a coverage interval containing the true quantity value of the measurand with a specified probability.

Hereinafter, the limits mentioned are jointly called the "characteristic limits".

NOTE According to ISO/IEC Guide 99:2007 updated by JCGM 200:2012 the term "coverage interval" is used here instead of "confidence interval" in order to distinguish the wording of Bayesian terminology from that of conventional statistics.

All the characteristic values are based on Bayesian statistics and on the ISO/IEC 98-3 Guide to the Expression of Uncertainty in Measurement as well as on the ISO/IEC Guide 98-3-1 and ISO/IEC 98-3-2. As explained in detail in ISO 11929-2, the characteristic values are mathematically defined by means of moments and quantiles of probability distributions of the possible measurand values.

Since measurement uncertainty plays an important part in the ISO 11929 series, the evaluation of measurements and the treatment of measurement uncertainties are carried out by means of the general procedures according to the ISO/IEC Guide 98-3 and to the ISO/IEC Guide 98-3-1; see also References [9 to 13]. This enables the strict separation of the evaluation of the measurements, on the one hand, and the provision and calculation of the characteristic values, on the other hand. The ISO 11929 series makes use of a theory of uncertainty in measurement[14 to 16] based on Bayesian statistics (e.g. References [17 to 22]) in order to allow to take into account also those uncertainties that cannot be derived from repeated or counting measurements. The latter uncertainties cannot be handled by frequentist statistics.

Because of developments in metrology concerning measurement uncertainty laid down in the ISO/IEC Guide 98-3, ISO 11929:2010 was drawn up on the basis of the ISO/IEC Guide 98-3, but using Bayesian statistics and the Bayesian theory of measurement uncertainty. This theory provides a Bayesian foundation for the ISO/IEC Guide 98-3. Moreover, ISO 11929:2010 was based on the definitions of the characteristic values[9], the standard proposal[10], and the introducing article[11]. It unified and replaced all earlier parts of ISO 11929 and was applicable not only to a large variety of particular measurements of ionizing radiation but also, in analogy, to other measurement procedures.

Since the ISO/IEC Guide 98-3-1 has been published, dealing comprehensively with a more general treatment of measurement uncertainty using the Monte Carlo method in complex measurement evaluations. This provided an incentive for writing a corresponding Monte Carlo supplement[12] to ISO 11929:2010 and to revise ISO 11929:2010. The revised ISO 11929 is also essentially founded on Bayesian statistics and can serve as a bridge between ISO 11929:2010 and the ISO/IEC Guide 98-3-1. Moreover, more general definitions of the characteristic values (ISO 11929-2) and the Monte Carlo computation of the characteristic values make it possible to go a step beyond the present state of standardization laid down in ISO 11929:2010 since probability distributions rather than uncertainties can be propagated. It is thus more comprehensive and extending the range of applications.

The ISO 11929 series, moreover, is more explicit on the calculation of the characteristic values. It corrects also a problem in ISO 11929:2010 regarding uncertain quantities and influences, which do not behave randomly in measurements repeated several times. Reference [13] gives a survey on the basis of the revision. Furthermore, in ISO 11929-3, it gives detailed advice how to calculate characteristic values in the case of multivariate measurements using unfolding methods. For such measurements, the ISO/IEC Guide 98-3-2 provides the basis of the uncertainty evaluation.

Formulas are provided for the calculation of the characteristic values of an ionizing radiation measurand via the “standard measurement uncertainty” of the measurand (hereinafter the “standard uncertainty”) derived according to the ISO/IEC Guide 98-3 as well as via probability distributions of the measurand derived in accordance with ISO/IEC Guide 98-3-1. The standard uncertainties or probability distributions take into account the uncertainties of the actual measurement as well as those of sample treatment, calibration of the measuring system and other influences. The latter uncertainties are assumed to be known from previous investigations.

Determination of the characteristic limits (decision threshold, detection limit and limits of the coverage interval) for measurements of ionizing radiation — Fundamentals and application —

Part 2: Advanced applications

1 Scope

The ISO 11929 series specifies a procedure, in the field of ionizing radiation metrology, for the calculation of the “decision threshold”, the “detection limit” and the “limits of the coverage interval” for a non-negative ionizing radiation measurand when counting measurements with preselection of time or counts are carried out. The measurand results from a gross count rate and a background count rate as well as from further quantities on the basis of a model of the evaluation. In particular, the measurand can be the net count rate as the difference of the gross count rate and the background count rate, or the net activity of a sample. It can also be influenced by calibration of the measuring system, by sample treatment and by other factors.

ISO 11929 has been divided into four parts covering elementary applications in ISO 11929-1, advanced applications on the basis of the GUM Supplement 1 in this document, applications to unfolding methods in ISO 11929-3, and guidance to the application in ISO 11929-4.

ISO 11929-1 covers basic applications of counting measurements frequently used in the field of ionizing radiation metrology. It is restricted to applications for which the uncertainties can be evaluated on the basis of the ISO/IEC Guide 98-3 (JCGM 2008). In Annex A of ISO 11929-1:2019 the special case of repeated counting measurements with random influences is covered, while measurements with linear analogous ratemeters are covered in Annex B of ISO 11929-1:2019.

This document extends the former ISO 11929:2010 to the evaluation of measurement uncertainties according to the ISO/IEC Guide 98-3-1. It also presents some explanatory notes regarding general aspects of counting measurements and on Bayesian statistics in measurements.

ISO 11929-3 deals with the evaluation of measurements using unfolding methods and counting spectrometric multi-channel measurements if evaluated by unfolding methods, in particular, for alpha- and gamma-spectrometric measurements. Further, it provides some advice on how to deal with correlations and covariances.

ISO 11929-4 gives guidance to the application of ISO 11929, summarizes shortly the general procedure and then presents a wide range of numerical examples. Information on the statistical roots of ISO 11929 and on its current development may be found elsewhere[30,31].

ISO 11929 also applies analogously to other measurements of any kind especially if a similar model of the evaluation is involved. Further practical examples can be found, for example, in ISO 18589[1], ISO 9696[2], ISO 9697[3], ISO 9698[4], ISO 10703[5], ISO 7503[6], ISO 28218[7], and ISO 11885[8].

NOTE A code system, named UncertRadio, is available for calculations according to ISO 119291 to ISO 11929-3. UncertRadio[27][28] can be downloaded for free from https://www.thuenen.de/en/fi/fields-of-activity/marine-environment/coordination-centre-of-radioactivity/uncertradio/. The download contains a setup installation file which copies all files and folders into a folder specified by the user. After installation one has to add information to the PATH of Windows as indicated by a pop-up window during installation. English language can be chosen and extensive “help” information is available.. Another tool is the package ‘metRology’[32] which is available for programming in R. It contains the two R functions ‘uncert’ and ‘uncertMC’ which perform the GUM conform uncertainty propagation, either analytically or by the Monte Carlo method, respectively. Covariances/correlations of input quantities are included. Applying these two functions within iterations for decision threshold and the detection limit calculations simplifies the programming effort significantly. It is also possible to implement this part of ISO 11929 in a spreadsheet containing a Monte Carlo add-in or into other commercial mathematics software.

2 Normative references

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

ISO 3534-1, *Statistics — Vocabulary and symbols — Part 1: General statistical terms and terms used in probability*

ISO 80000-1, *Quantities and units — Part 1: General*

ISO 80000-10, *Quantities and units — Part 10: Atomic and nuclear physics*

ISO/IEC Guide 98-3, *Uncertainty of measurement — Part 1: Guide to the expression of uncertainty in measurement, JCGM 100:2008*

ISO/IEC Guide 98-3-1, *Evaluation of measurement data — Supplement 1 to the “Guide to the expression of uncertainty in measurement” — a Propagation of distributions using a Monte Carlo method, JCGM 101:2008*

ISO/IEC Guide 98-3-2, *Evaluation of measurement data — Supplement 2 to the “Guide to the expression of uncertainty in measurement” — Models with any number of output quantities, JCGM 102:2011*

ISO/IEC Guide 99, *International vocabulary of metrology — Basic and general concepts and associated terms (VIM), JCGM 200:2012*

3 Terms and definitions

For the purposes of the ISO 11929 series, the terms and definitions given in ISO 80000-1, ISO 80000-10, ISO/IEC Guide 98-3, ISO/IEC Guide 98-3-1, ISO/IEC 98-3-2, ISO/IEC Guide 99 and ISO 3534-1 and the following apply.

— ISO Online browsing platform: available at https://www.iso.org/obp

— IEC Electropedia: available at http://www.electropedia.org/

3.1
quantity value
value of a quantity
value
number and reference together expressing magnitude of a quantity

[SOURCE: JCGM 200:2012, 1.19]

3.2
measurement
process of experimentally obtaining one or more quantity values that can reasonably be attributed to a quantity

[SOURCE: JCGM 200:2012, 2.1]

3.3
measurand
quantity intended to be measured

[SOURCE: JCGM 200:2012, 2.3]

3.4
coverage interval
interval containing the set of true quantity values of a measurand with a stated probability, based on the information available

[SOURCE: JCGM 200:2012, 2.36]

Note 1 to entry: A coverage interval does not need to be centred on the chosen measured quantity value (see JCGM 101:2008).

Note 2 to entry: A coverage interval should not be termed "confidence interval" to avoid confusion with the statistical concept.

3.5
measurement method
method of measurement
generic description of a logical organization of operations used in a measurement

[SOURCE: JCGM 200:2012, 2.4]

3.6
measurement procedure
detailed description of a measurement according to one or more measurement principles and to a given measurement method, based on a measurement model and including any calculation to obtain a measurement result

[SOURCE: JCGM 200:2012, 2.6]

3.7
measurement result
result of measurement
set of quantity values being attributed to a measurand together with any other available relevant information

[SOURCE: JCGM 200:2012, 2.9]

3.8
measured quantity value
value of a measured quantity
measured value
quantity value representing a measurement result

[SOURCE: JCGM 200:2012, 2.10]

3.9
true quantity value
true value of a quantity
true value
quantity value consistent with the definition of a quantity

[SOURCE: JCGM 200:2012, 2.11]

Note 1 to entry: In the Error Approach to describing measurement, a true quantity value is considered unique and, in practice, unknowable. The Uncertainty Approach is to recognize that, owing to the inherently incomplete amount of detail in the definition of a quantity, there is not a single true quantity value but rather a set of true quantity values consistent with the definition. However, this set of values is, in principle and in practice, unknowable. Other approaches dispense altogether with the concept of true quantity value and rely on the concept of metrological compatibility of measurement results for assessing their validity.

Note 2 to entry: When the definitional uncertainty associated with the measurand is considered to be negligible compared to the other components of the measurement uncertainty, the measurand may be considered to have an "essentially unique" true quantity value. This is the approach taken by the ISO/IEC Guide 98-3 and associated documents, where the word "true" is considered to be redundant.

3.10
measurement uncertainty
uncertainty of measurement
uncertainty
non-negative parameter characterizing the dispersion of the quantity values being attributed to a measurand, based on the information used

[SOURCE: JCGM 200:2012, 2.26]

Note 1 to entry: Measurement uncertainty includes components arising from systematic effects, such as components associated with corrections and the assigned quantity values of measurement standards, as well as the definitional uncertainty. Sometimes estimated systematic effects are not corrected for but, instead, associated measurement uncertainty components are incorporated.

Note 2 to entry: The parameter may be, for example, a standard deviation called standard measurement uncertainty (or a specified multiple of it), or the half-width of an interval, having a stated coverage probability.

Note 3 to entry: Measurement uncertainty comprises, in general, many components. Some of these may be evaluated by Type A evaluation of measurement uncertainty from the statistical distribution of the quantity values from series of measurements and can be characterized by standard deviations. The other components, which may be evaluated by Type B evaluation of measurement uncertainty, can also be characterized by standard deviations, evaluated from probability distribution based on experience or other information.

Note 4 to entry: In general, for a given set of information, it is understood that the measurement uncertainty is associated with a stated quantity value attributed to the measurand. A modification of this value results in a modification of the associated uncertainty.

3.11
model of evaluation
set of mathematical relationships between all measured and other quantities involved in the evaluation of measurements

Note 1 to entry: The model of evaluation does not need to be an explicit function; it can also be an algorithm realized by a computer code.

3.12
decision threshold
value of the estimator of the measurand, which when exceeded by the result of an actual measurement using a given measurement procedure of a measurand quantifying a physical effect, is used to decide that the physical effect is present

Note 1 to entry: The decision threshold is defined such that in cases where the measurement result, y, exceeds the decision threshold, y^*, the probability that the true value of the measurand is zero is less or equal to a chosen probability for a wrong decision, α.

Note 2 to entry: If the result, y, is below the decision threshold, y^*, it is decided to conclude that the result cannot be attributed to the physical effect; nevertheless it cannot be concluded that it is absent.

3.13
detection limit
smallest true value of the measurand which ensures a specified probability of being detectable by the measurement procedure

Note 1 to entry: With the decision threshold according to 4.13, the detection limit is the smallest true value of the measurand for which the probability of wrongly deciding that the true value of the measurand is zero is equal to a specified value, β, when, in fact, the true value of the measurand is not zero. The probability of being detectable is consequently $(1-\beta)$.

Note 2 to entry: The terms detection limit and decision threshold are used in an ambiguous way in different standards (e.g. standards related to chemical analysis or quality assurance). If these terms are referred to one has to state according to which standard they are used.

3.14
probabilistically symmetric coverage interval
coverage interval for a quantity such that the probability that the quantity is less than the smallest value in the interval is equal to the probability that the quantity is greater than the largest value in the interval

[SOURCE: JCGM 101:2008, 3.15]

3.15
shortest coverage interval
coverage interval for a quantity with the shortest length among all coverage intervals for that quantity having the same coverage probability

[SOURCE: JCGM 101:2008, 3.16]

3.16
limits of the coverage interval
values which define a coverage interval

Note 1 to entry: The limits are calculated in the ISO 11929 series to contain the true value of the measurand with a specified probability $(1-\gamma)$.

Note 2 to entry: The definition of a coverage interval is ambiguous without further stipulations. In this standard two alternatives, namely the probabilistically symmetric and the shortest coverage interval are used.

3.17
best estimate of the true quantity value of the measurand
expectation value of the probability distribution of the true quantity value of the measurand, given the experimental result and all prior information on the measurand

Note 1 to entry: The best estimate is the one among all possible estimates of the measurand on the basis of given information, which is associated with the minimum uncertainty.

3.18
guideline value
value which corresponds to scientific, legal or other requirements with regard to the detection capability and which is intended to be assessed by the measurement procedure by comparison with the detection limit

Note 1 to entry: The guideline value can be given, for example, as an activity, a specific activity or an activity concentration, a surface activity or a dose rate.

Note 2 to entry: The comparison of the detection limit with a guideline value allows a decision on whether or not the measurement procedure satisfies the requirements set forth by the guideline value and is therefore suitable for the intended measurement purpose. The measurement procedure satisfies the requirement if the detection limit is smaller than the guideline value.

Note 3 to entry: The guideline value shall not be confused with other values stipulated as conformity requests or as regulatory limits.

3.19
background effect
measurement effect caused by radiation other than that caused by the object of the measurement itself

Note 1 to entry: The background effect can be due to natural radiation sources or radioactive materials in or around the measuring instrumentation and also to the sample itself (for instance, from other lines in a spectrum).

3.20
background effect in spectrometric measurement
number of events of no interest in the region of a specific line in the spectrum

3.21
net effect
contribution of the possible radiation of a measurement object (for instance, of a radiation source or radiation field) to the measurement effect

3.22
gross effect
measurement effect caused by the background effect and the net effect

3.23
shielding factor
factor describing the reduction of the background count rate by the effect of shielding caused by the measurement object

3.24
relaxation time constant
duration in which the output signal of a linear-scale ratemeter decreases to 1/e times the starting value after stopping the sequence of the input pulses

4 Quantities and symbols

The symbols for auxiliary quantities and the symbols only used in the annexes are not listed. Physical quantities are denoted by upper-case letters but shall be carefully distinguished from their values, denoted by the corresponding lower-case letters.

m	number of input quantities
n_{M}	number of Monte Carlo trials performed
X_i	input quantity $(i=1,\ldots,m)$
x_i	estimate of the input quantity X_i

$\tilde{x}_i$	possible true quantity values of the input quantity X_i
$x_{1,i},\ldots,x_{n,i}$	drawing set of $x_1,\ldots,x_n$ from the i-th Monte Carlo trial
ξ_i	integration variable of possible true quantity values of the input quantity X_i
$u(x_i)$	standard uncertainty of the input quantity X_i associated with the estimate x_i
Δx_i	width of the region of the possible values of the input quantity X_i
$u_{\mathrm{rel}}(w)$	relative standard uncertainty of a quantity W associated with the estimate w
G	model function
Y	non-negative measurand, which quantifies the physical effect of interest; also used as the symbol for a random variable as an estimator of the measurand
Y_0	random variable used as an estimator of the measurand which does not take into account that the measurand is non-negative
$\tilde{y}$	possible or assumed true values of the measurand; if the physical effect of interest is not present, then $\tilde{y}=0$; otherwise, $\tilde{y}>0$
η	integration variable of possible true quantity values of the output quantity Y
y	determined value of the estimator Y, estimate of the measurand, primary measurement result of the measurand
y'	variable describing possible measurement results (estimates)
y_j	values y from different measurements $(j=0,1,2,\ldots)$
$\mathbf{\bar{y}}_{\mathrm{M}}=\left\{y_1,\ldots,y_{n_{\mathrm{M}}}\right\}$	vector of results from n_{M} Monte Carlo trials
$u(y)$	standard uncertainty of the measurand associated with the primary measurement result y
$\tilde{u}(\tilde{y})$	standard uncertainty of the estimator Y as a function of an assumed true value $\tilde{y}$ of the measurand
$f_Y(y\|\tilde{y})$	probability distribution; i.e. the conditional probability distribution of estimates, y, given an assumed true value, $\tilde{y}$, of the measurand, Y
$f_Y(\tilde{y}\|y)$	probability distributions of the possible true values, $\tilde{y}$, of the measurand, Y, given the measured estimate, y (Bayesian statistics)
$f_Y(\tilde{y}\|\mathbf{a})$	probability distribution of the possible true value, $\tilde{y}$, of the measurand, Y, given a set of information $\mathbf{a}$ about the input quantities and their values and relations to the output quantity
$f_Y(\tilde{y})$	model prior; it represents all the information about the measurand available before the experiment is performed
$F_Y(\tilde{y}\|\mathbf{a})$	distribution function of the probability distribution $f_Y(\tilde{y}\|\mathbf{a})$

$\mathrm{H}(x)$	Heaviside step function: $f_{\mathrm{H}}(x)=\begin{cases}0\\1\end{cases}$ for $\begin{cases}x<0\\x\geq 0\end{cases}$
$\mathrm{Ga}(\tilde{r};n,1/t)$	Gamma function as the probability density function (PDF) of the true value $\tilde{r}$ of a count rate R given n counts obtained during a counting time t
$\mathrm{N}(x,u(x))$	Normal or Gaussian distribution with the parameters x and $u(x)$
$\mathrm{R}(x_{\mathrm{L}},x_{\mathrm{U}})$	Rectangular distribution with the lower and upper limits x_{L} and x_{U}
$\mathrm{E}(f_X(x))$	expectation of $f_X(x)$
$\mathrm{Var}(f_X(x))$	variance of $f_X(x)$
$\mathbf{a}$	sets of information regarding the input quantities, respectively, including their values and relations
$\mathbf{a}'$	modified sets of information regarding the input quantities, respectively, including their values and relations
$\hat{y}$	best estimate of the measurand
$u(\hat{y})$	standard uncertainty of the measurand associated with the best estimate $\hat{y}$
y^*	decision threshold of the measurand
$y^\#$	detection limit of the measurand
y_{r}	guideline value of the measurand
$y^{\triangleleft}$, $y^{\triangleright}$	lower and upper limit of the symmetric coverage interval, respectively, of the measurand
$y^{<}$, $y^{>}$	lower and upper limit of the shortest coverage interval, respectively, of the measurand
R_i	count rate as an input quantity X_i
R_{n}	count rate of the net effect (net count rate)
R_{g}	count rate of the gross effect (gross count rate)
R_0	count rate of the background effect (background count rate)
r_{g}, r_0	estimate of the gross count rate and of the background count rate, respectively
ρ_{g},ρ_0	integration variables of possible true quantity values of the gross and background count rates R_{g},R_0
n_i	number of counted pulses obtained from the measurement of the count rate R_i
n_{g}, n_0	number of counted pulses of the gross effect and of the background effect, respectively
t_i	measurement duration of the measurement of the count rate R_i

t_g, t_0	measurement duration of the measurement of the gross effect and of the background effect, respectively
r_i	estimate of the count rate ρ_i
τ_g, τ_0	relaxation time constant of a ratemeter used for the measurement of the gross effect and of the background effect, respectively
α, β	probability of a false positive and false negative decision, respectively
$1-\gamma$	probability for the coverage interval of the measurand
q_p	quantile of a distribution for the probability p

5 Summary of procedures for evaluating and reporting uncertainty and characteristic limits

This clause gives in a concise form the procedure to be followed for evaluating a measurement of a single measurand on the basis of the ISO/IEC Guide 98-3-1 and calculating the characteristic limits, i.e. the decision threshold, the detection limit and the limits of a coverage interval. This procedure is universally suitable, also in cases when the ISO/IEC Guide 98-3 approximation cannot be used or if the latter method does not provide a result for the detection limit.

It is assumed that the measurand is non-negative. This information is only used when calculating a coverage interval and the best estimate and its associated uncertainty. It is a further characteristic of measurements of ionizing radiation that they have to be performed in the presence of a radiation background which has to be subtracted from a gross measurement quantity. The procedures described in this Standard likewise are applicable to any measurements where a background or blank contribution has to be subtracted from a gross quantity.

The procedures stipulated in of the ISO 11929 series and the ISO/IEC Guide 98-3-1 are exclusively based on Bayesian statistics. The probability distribution, $f_Y(\tilde{y}|\mathbf{a})$, which completely describe the uncertainties are to be derived by the Principle of Maximum Information Entropy (PME) or Bayes Theorem based on the available information $\mathbf{a}$. The original ISO/IEC Guide 98-3 is contained in the ISO/IEC Guide 98-3-1 as a special case, namely that the available information is $\mathbf{a}=\{\mathbf{x},\mathbf{u}(\mathbf{x})\}$ only. But also in this case the ISO/IEC Guide 98-3-1 has not the restriction regarding linearization of the model and is no longer an approximation.

It is assumed in this document that the user has considered beforehand the applicability of the ISO/IEC GUIDE 98-3 and has decided that it is necessary and suitable to proceed according to the ISO/IEC Guide 98-3-1 and ISO 11929 Part 2. See Clause 2 of ISO 11929-1 for guidance.

The application of this document is structured into 8 consecutive steps. A detailed workflow of this document is given in Figure 1. Guidance for practically applying Monte Carlo methods is given for each step of the calculations in Clauses 6 to 10.

The steps are as follows:

— Step 1: Modelling the measurement starts with the definition of the non-negative measurand, Y, and of its representation as a function, $Y=G(X_1,...,X_m)$, of the input quantities; X_1 is the gross effect.

— Step 2: Establishing the joint probability distribution $f_{\mathbf{X}}(\tilde{\mathbf{x}}|\mathbf{a})$ of the input quantities $\mathbf{X}$ and propagation to obtain the probability distribution $f_Y(\tilde{y}|\mathbf{a})$ of the output quantity Y.

— Step 3: The evaluation of the measurement by calculating the primary measurement result as the expectation of $f_Y(\tilde{y}|\mathbf{a})$ and its associated standard uncertainty as the square root of the variance of $f_Y(\tilde{y}|\mathbf{a})$.

— Step 4: Calculating by iteration the decision threshold y^* as the $(1-\alpha)-$ quantile of the probability distribution $f_Y(y|\mathbf{a}', \tilde{y}=0)$ and decisions to be made.

— Step 5: Calculating by iteration the detection limit as the $\beta-$quantile of the probability distribution $f_Y(y|\mathbf{a}', \tilde{y}=y^\#)$ and assessment of the measurement method.

— Step 6: Calculating a coverage interval for the measurand based on $f_Y(\tilde{y}|\mathbf{a}, Y \geq 0)$ taking, however, into account that the measurand is non-negative.

— Step 7: Calculating the best estimate of the measurand and its associated standard uncertainty based on $f_Y(\tilde{y}|\mathbf{a}, Y \geq 0)$ taking, however, into account that the measurand is non-negative.

— Step 8: Reporting the results.

NOTE The terms probability distribution, probability density and probability density function (PDF) are used synonymuously for the probability density $f_X(x)$ of a random variable X. The distribution function $F_X(x)$ describes the integral probability $F_X(x)=\int_{-\infty}^{x} f_X(\xi)\mathrm{d}\xi$.

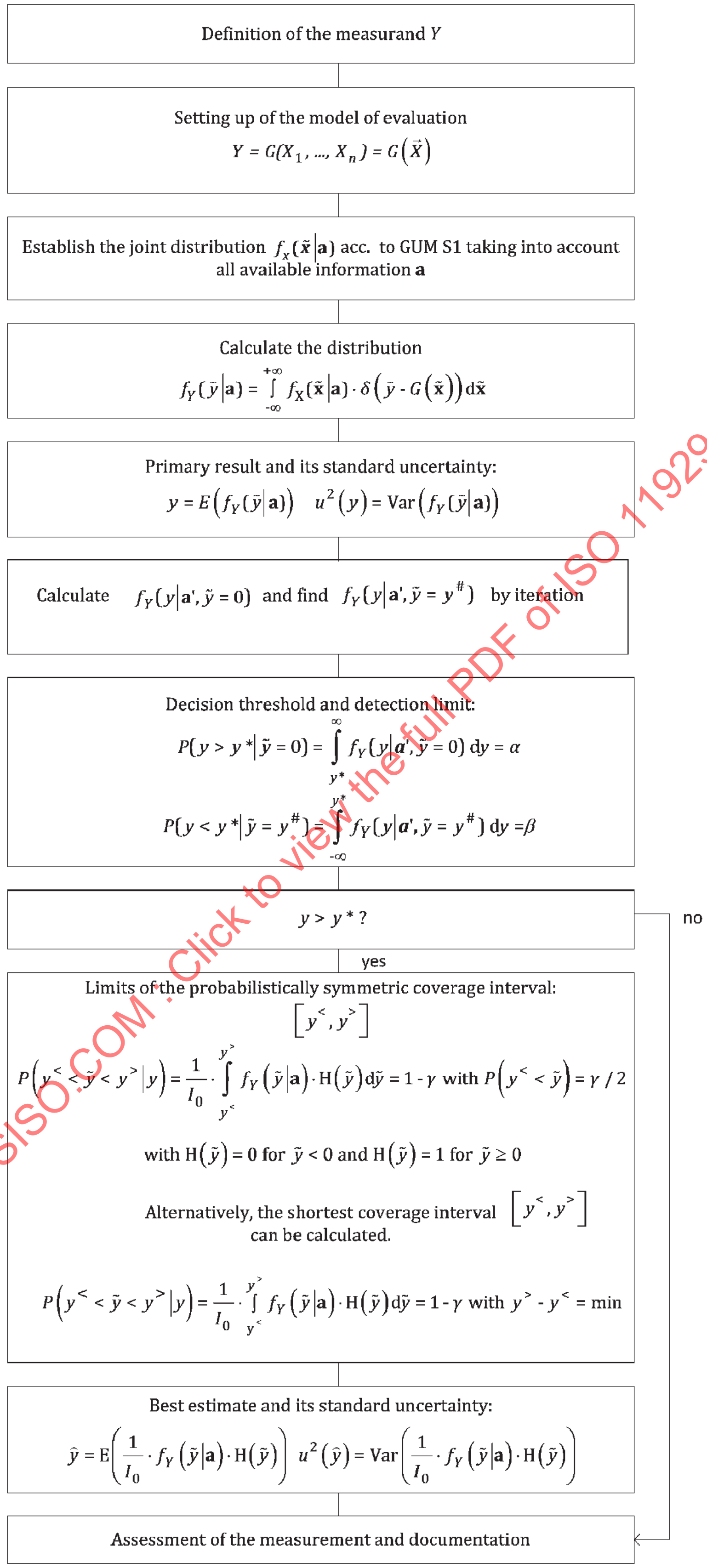


Figure 1 — Flow diagramm of ISO 11929-2 when applying ISO/IEC Guide 98-3-1

6 Evaluation of a measurement on the basis of ISO/IEC Guide 98-3-1

6.1 Introduction and decisions to be made

In this document, the evaluation of a measurement is strictly based on procedures stipulated in the ISO/IEC Guide 98-3 and the ISO/IEC Guide 98-3-1. The procedures according to the ISO/IEC Guide 98-3 and the ISO/IEC Guide 98-3-1 have different historical roots and fields of application. The ISO/IEC Guide 98-3 was developed with a still unclear statistical basis having mixed frequentistic and Bayesian argumentations. Moreover, the application of the ISO/IEC Guide 98-3 was and is limited to models of evaluation which can – at least locally – be linearized and it represents an approximation using a first order Taylor expansion. Independent of these limitations, the ISO/IEC Guide 98-3 was successful for a wide range of applications, which frequently also did exceed the limits of its declared requirements.

A clear statement of the statistical roots and statistical methodology as well as provisions for the lacking generality of the ISO/IEC Guide 98-3 were made only in the ISO/IEC Guide 98-3-1. The ISO/IEC Guide 98-3-1 states that its framework is exclusively based on Bayesian statistics and that the probability distributions which completely describe the uncertainties are to be derived by the Bayes Theorem or the Principle of Maximum Information Entropy (PME)[23] based on the available information **a**.

NOTE 1 The original ISO/IEC Guide 98-3 is contained in ISO/IEC Guide 98-3-1 as a special case, namely that the available information is $\mathbf{a}=\{\mathbf{x},\mathbf{u}(\mathbf{x})\}$ only. But also if this is the case, the ISO/IEC Guide 98-3-1 has not the restriction regarding linearization of the model and is no longer an approximation.

NOTE 2 An actual (2015) draft of a revised ISO/IEC Guide 98-3 also points out that Bayesian Statistics is the sole basis of the ISO/IEC Guide 98-3 framework.

Therefore the following decisions have to be made beforehand by the user:

— depending on the available information the user has to decide whether to proceed according to the ISO/IEC Guide 98-3 or the ISO/IEC Guide 98-3-1. If the available information is only $\mathbf{a}=\{\mathbf{x},\mathbf{u}(\mathbf{x})\}$, the ISO/IEC Guide 98-3 has to be applied provided that its requirements are met;

— the user has to decide whether the model of evaluation fulfils the conditions of the ISO/IEC Guide 98-3 approach or not;

— if the ISO/IEC Guide 98-3 approach is used and the primary measurement result and its associated standard uncertainty are calculated and if it turns out that a detection limit does not exist, the user has to decide whether this lack of knowledge is acceptable or not. If this is not the case, the user has to use the ISO/IEC Guide 98-3-1 approach which also allows handling large relative uncertainties.

6.2 General aspects concerning the measurand and the model of evaluation

A non-negative measurand shall be assigned to the physical effect to be investigated as the output quantity according to a given measurement task. The measurand shall quantify the effect. It assumes the true value zero if the effect is not present in a particular case.

A random variable Y, an estimator, shall be assigned to the measurand. The symbol Y is also used in this clause for the measurand itself. Then the model of the evaluation has to be set up which mathematically connects the output quantity with all the input quantities $\mathbf{X}$ involved. The vector $\mathbf{X}=\{X_1,X_2,...,X_m\}$ denotes also the random variables X_i serving as estimators of the input quantities X_i. Formula (1) is the model of the evaluation.

$$Y=G(X_1,...,X_m)=G(\mathbf{X}) \tag{1}$$

NOTE In the general model of Formula (1), X_1 is the gross quantity of the measurement.

A quite general model of evaluation in measurements of ionizing radiation, treated in detail in this document, is given by

$$Y = G(X_1, ..., X_m) = (X_1 - X_2 X_3 - X_4) \cdot \frac{X_6 X_8 \cdots}{X_5 X_7 \cdots} = (X_1 - X_2 X_3 - X_4) \cdot W \qquad (2)$$

with

$$W = \frac{X_6 X_8 \cdots}{X_5 X_7 \cdots} \qquad (3)$$

where $X_1 = R_g = N_g / t_g$ is the gross count rate and $X_2 = R_0 = N_0 / t_0$ is the background count rate. The other input quantities, X_i , are calibration, correction or influence quantities, or conversion factors, for instance the emission or response probability or, in particular, X_3 is a shielding factor and X_4 an additional background correction quantity expressed as a count rate. If some of the input quantities are not involved, $x_i = 1$ $(i = 3; i > 4)$, $x_4 = 0$ and $u(x_i) = 0$ shall be set for them.

6.3 Establishing probability distributions for the input quantities

On the basis of the available information **a** probability distributions, $f_X(\tilde{\mathbf{x}}|\mathbf{a})$, have to be assigned to the X_i according to the stipulations laid down in ISO/IEC Guide 98-3-1 based on the Bayes' Theorem or the Principle of Maximum Entropy (PME)[23] or the Bayes Theorem; see also References [12][13]. It may happen, that the available information is not sufficient to establish a meaningful probability distribution $f_X(\tilde{\mathbf{x}}|\mathbf{a})$. Then, eventually further information has to be obtained, either experimentally or by other means in order to justify the probability distribution chosen for an estimator of a quantity.

NOTE 1 The set of information **a** contains the information **x** of the estimates of the input quantities as well as any other prior information about the possible quantity values $\tilde{\mathbf{x}}$ of **X**.

NOTE 2 ISO/IEC Guide 98-3-1 allows for more and other information about the X_i than the ISO/IEC Guide 98-3 and gives guidance to set up the proper probability distributions $f_{\mathbf{X}}(\tilde{\mathbf{x}}|\mathbf{a})$ applying the PME to the available information **a**.

Frequently occurring probability distributions in measurements of ionizing radiation are the normal or Gaussian distribution, the Gamma distribution, the rectangular distribution and the logarithmic normal distribution ("log-normal distribution" for short).

The **normal or Gaussian distribution** is the exact solution of the PME if the available information consists only of a measured value x and its associated standard uncertainty $u(x)$ (ISO/IEC Guide 98-3-1; 6.4.7).

$$f_{\mathbf{X}}(\tilde{x}|x, u(x)) = \mathrm{N}(x, u(x)) = \frac{1}{\sqrt{2\pi} \cdot u(x)} \cdot \exp\left(\frac{-(\tilde{x} - x)^2}{2 \cdot u^2(x)}\right) \qquad (4)$$

This probability distribution has the expectation x and the variance $u^2(x)$.

NOTE 3 If only an estimate x and its associated standard uncertainty $u(x)$ is available for an input quantity X_i, then the probability distribution is a Gaussian (normal) distribution $f_{X_i}(\tilde{x}_i|x_i, u(x_i)) = \mathrm{N}(x_i, u(x_i))$.

In ISO 11929-1 only use is made of the expectation and variance of the count rate distribution. Consequently, a Gaussian distribution is then used for the rate which is a sufficient approximation of the Gamma distribution for large count numbers. If small count numbers are dealt with, this ISO 11929-2 has to be applied as described in detail in Annex A.

The **Gamma distribution** is the solution of the Bayes Theorem using a Jeffrey's prior $f_R(\tilde{r})=1/\tilde{r}$ if the measurand is a count rate R and the available information is the number of counts n measured during a measuring time t. See Annex A and ISO/IEC Guide 98-3-1; 6.4.11 for details.

$$f_R(\tilde{r}|n,t)=\frac{t^n\cdot\tilde{r}^{n-1}}{(n-1)!}\cdot\exp(-\tilde{r}\cdot t) \tag{5}$$

This Gamma distribution has the expectation

$$r=\mathrm{E}(f_R(\tilde{r}|n,t))=\int_0^\infty \rho\cdot f_R(\rho|n,t)\,\mathrm{d}\rho=n/t \tag{6}$$

and the variance

$$u^2(r)=\mathrm{Var}(f_R(\tilde{r}|n,t))=\int_0^\infty(\rho-r)^2\cdot f_R(\rho|n,t)\,\mathrm{d}\rho=n/t^2. \tag{7}$$

NOTE 4 The probability distribution of a count rate, $X_i=R_i$, is obtained from counts, n_i, drawn from a Poisson process during a measurement of duration, t_i, is a Gamma distribution; see Annex A and References [12][13]. This Gamma distribution has to be used, in particular, in the case of low count numbers where the deviations of the Gaussian distribution from the Gamma distribution are relevant. For larger count numbers, the information used in ISO 11929-1, i.e. $x_i=n_i/t_i$ and $u^2(x_i)=n_i\big/t_i^2$ and the resulting Gaussian distribution are sufficient.

The **rectangular distribution** is the exact solution of the PME if the only available information is that x is constraint to a lower bound a and an upper bound b and behaves randomly in-between (ISO/IEC Guide 98-3-1, 6.4.2).

$$f_X(\tilde{x}|a,b)=\frac{1}{(b-a)} \tag{8}$$

This rectangular distribution has the expectation

$$x=\mathrm{E}(f_X(\tilde{x}|a,b))=\int_a^b \xi\cdot f_X(\xi|a,b)\,\mathrm{d}\xi=\frac{(a+b)}{2} \tag{9}$$

and the variance

$$u^2(x)=\mathrm{Var}(f_X(\tilde{x}|a,b))=\int_a^b(\xi-x)^2\cdot f_X(\xi|a,b)\,\mathrm{d}\xi=\frac{(b-a)^2}{12} \tag{10}$$

If only the range of possible values of a quantity, X_i, is known and meaningful, the probability distribution resulting from the PME is a rectangular distribution as the probability distribution. This probability distribution also follows from Laplace' Principle of Indifference. If this quantity,X_i, appears in the denominator of the model function and has a range of possible values $[x_\mathrm{L},x_\mathrm{U}]$, it shall not be replaced by a quantity $1/X_i$ in the numerator with a range of possible values $[1/x_\mathrm{U},1/x_\mathrm{L}]$ because the rectangular probability distribution in the denominator does not result in a rectangular distribution of $1/X_i$ in the nominator.

The **log-normal distribution** is the exact solution of the PME if the measurand is a multi-factorial quantity and the available information consists of a mean value $m(\ln(\mathbf{x}))$ of the logarithms of measured values $\mathbf{x}$ and their standard deviation $s(\ln(\mathbf{x}))$.

$$f_X(\tilde{x}|m(\ln(\mathbf{x})),s(\ln(\mathbf{x}))) = \frac{1}{\sqrt{2\pi}\cdot\tilde{x}\cdot s(\ln(\mathbf{x}))}\cdot\exp\left(\frac{-(\ln(\tilde{x})-m(\ln(x))^2}{2\cdot s^2(\ln(\mathbf{x}))}\right) \tag{11}$$

This log-normal distribution has the expectation

$$\begin{aligned} x &= \mathrm{E}\left(f_X(\tilde{x}|m(\ln(\mathbf{x})),s(\ln(\mathbf{x}))\right) = \int_0^\infty \xi\cdot f_X(\xi|m(\ln(\mathbf{x})),s(\ln(\mathbf{x}))\,\mathrm{d}\xi \\ &= \exp\left(m(\ln(\mathbf{x}))+\frac{s^2(\ln(\mathbf{x}))}{2}\right) \end{aligned} \tag{12}$$

and the variance

$$\begin{aligned} u^2(x) &= \mathrm{Var}\left(f_X(\tilde{x}|m(\ln(\mathbf{x})),s(\ln(\mathbf{x})))\right) = \int_a^b (\xi-x)^2\cdot f_X(\xi|m(\ln(\mathbf{x})),s(\ln(\mathbf{x}))\,\mathrm{d}\xi \\ &= \exp\left(2\cdot m(\ln(\mathbf{x}))+s^2(\ln(\mathbf{x}))\right)\cdot\left(\exp(s^2(\ln(\mathbf{x})))-1\right) \end{aligned} \tag{13}$$

NOTE 5 Alternatively the PME, the Bayes' Theorem or the expansion theorem of the probability theory can be applied to include known frequency or parameter distributions, respectively. If more information about the input quantity involved is available than assumed in this document, it can be used in form of suitable model priors considered in the Bayes theorem.

6.4 Propagating probability distributions

After establishing the probability distributions of all input quantities, a joint probability distribution, $f_{\mathbf{X}}(\tilde{\mathbf{x}}|\mathbf{a})$, has to be formed which in case of independent input quantities is given as

$$f_{\mathbf{X}}(\tilde{\mathbf{x}}|\mathbf{a}) = \prod_1^m f_{X_i}(\tilde{x}_i|\mathbf{a}_i) \tag{14}$$

with a_i being the subset of information available for X_i. A joint probability distribution has to be assigned to those X_i that are not independent and inserted in Formula (14) for the respective input quantities; see ISO/IEC Guide 98-3-1 or Reference [26] for details.

The posterior probability distribution $f_Y(\tilde{y}|\mathbf{a})$ is calculated from the joint probability distribution $f_X(\tilde{\mathrm{x}}|\mathbf{a})$ using the model Formula $Y = G(\mathrm{X})$ by the so-called Markov formula

$$f_Y(\tilde{y}|\mathbf{a}) = \int_{-\infty}^{+\infty} f_{\mathbf{X}}(\xi|\mathbf{a})\cdot\delta(\tilde{y}-G(\xi))\,\mathrm{d}\xi \tag{15}$$

The ISO/IEC Guide 98-3-1 recommends the application of Monte Carlo techniques to solve Formula (15) and to derive $f_Y(\tilde{y}|\mathbf{a})$. Suitable numeric is described in detail elsewhere[12].

Using the Monte Carlo approach, $i = 1,\ldots,n_\mathrm{M}$ Monte Carlo trials are performed for propagating the probability distributions by drawing sets $x_{1,i},\ldots,x_{n,i}$ from the probability distributions $f_{X_i}(\tilde{x}_i|\mathbf{a})$. For each of these sets, one calculates $y_i = G(x_{1,i},\ldots,x_{n,i})$. The vector $\tilde{\mathbf{y}}_\mathrm{M} = \{y_1,\ldots,y_{n_\mathrm{M}}\}$ ordered ascendingly and afterwards assigning cumulative probabilities i / n_M to the y_i of $\tilde{\mathbf{y}}_M$ is a discrete representation of the distribution function $F_Y(\tilde{y}|\mathbf{a}) = \int_{-\infty}^{\tilde{y}} f_Y(\eta|\mathbf{a})\mathrm{d}\eta$ of Y.

NOTE In establishing $f_{\mathbf{X}}(\tilde{\mathbf{x}}|\mathbf{a})$, in performing the Monte Carlo trials and in calculating $F_Y(\tilde{y}|\mathbf{a})$ one does not take into account that the input quantities, X_i, and the measurand, Y, are non-negative. The fact that the measurand, Y, is non-negative is only taking into account when calculating the limits of the coverage interval, $y^{\triangleleft}, y^{\triangleright}$ or $y^{<}, y^{>}$, and the best estimate, $\hat{y}$, and its associated standard uncertainty, $u(\hat{y})$.

If the probability distribution $f_X(\tilde{\mathbf{x}}|\mathbf{a})$ is explicitly available, the integral of Formula (15) can also have an explicit solution.

6.5 Evaluation of the primary measurement result

The primary measurement result y is calculated as the expectation of $f_Y(\tilde{y}|\mathbf{a})$ by

$$y = \mathrm{E}(f_Y(\tilde{y}|\mathbf{a})) = \int_{-\infty}^{+\infty} \eta \cdot f_Y(\eta|\mathbf{a})\,\mathrm{d}\eta \tag{16}$$

NOTE 1 The primary measurement result does not take into account that the measurand is non-negative. This is only be taken into account in Clauses 9 and 10 when calculating coverage intervals and the best estimate and its associated standard uncertainty.

Using the Monte Carlo approach, the primary measurement result y is calculated from the vector $\tilde{\mathbf{y}}_M = \{y_1, ..., y_{n_M}\}$ as the arithmetic mean $y = \frac{1}{n_M} \cdot \sum_{i=1}^{n_M} y_i$.

NOTE 2 Quantiles q_p for the probability p of the probability distribution $f_Y(\tilde{y}|\mathbf{a})$ can be conveniently calculated from the vector $\tilde{\mathbf{y}}_M = \{y_1, ..., y_{n_M}\}$ by searching the value y_k with $k / n_M = p$.

6.6 Standard uncertainty associated with the primary measurement result

The standard uncertainty $u(y)$ associated with the primary result y of the measurement is calculated as the square root of the variance of $f_Y(\tilde{y}|\mathbf{a})$ by

$$u^2(y) = \mathrm{Var}(f_Y(\tilde{y}|\mathbf{a})) = \int_{-\infty}^{+\infty} (\eta - y)^2 \cdot f_Y(\eta|\mathbf{a})\,\mathrm{d}\eta \tag{17}$$

In general, the fact that the measurand is non-negative is not explicitly taken into account in the evaluation. Therefore, the primary result, y, may be negative, especially when the measurand nearly assumes the true value zero. The primary measurement result, y, differs from the best estimate, $\hat{y}$, of the measurand calculated in Clause 10. With $\hat{y}$, the knowledge that the measurand is non-negative is taken into account. The standard uncertainty, $u(\hat{y})$, associated with $\hat{y}$ is smaller than $u(y)$.

Using the Monte Carlo approach, the standard uncertainty $u(y)$ associated with the primary measurement result y is are calculated from the vector $\tilde{\mathbf{y}}_M = \{y_1, ..., y_{n_M}\}$ as the standard deviation

$u(y) = \sqrt{\frac{1}{n_M - 1} \cdot \sum_{i=1}^{n_M} (y_i - y)^2}$.

The fact that the measurand is non-negative is taken into account later; see 9.1.

7 PDF for an assumed true value of the measurand

For the provision and numerical calculation of the decision threshold in 8.2 and of the detection limit in 8.3, the standard uncertainty of the measurand is needed for assumed true values of the measurand. In ISO 11929-1, in which the ISO/IEC Guide 98-3 methodology is used, the standard uncertainty as a function of assumed true values of the measurand could be explicitly given. This is not possible if the ISO/IEC Guide 98-3-1 is used, but standard uncertainties for individual assumed true values of the measurand can be determined in a way similar to $u(y)$ within the framework of the evaluation of the measurements by application of the ISO/IEC Guide 98-3-1; see also References [9][10].

In the approach according to ISO/IEC Guide 98-3-1 the standard uncertainty as a function of assumed values of the measurand can be derived as approximation by repeated numerical calculations for an assumed values $\tilde{y}$ of the measurand resulting in probability distribution $f_Y(y|\mathbf{a}')$ with a modified set of information $\mathbf{a}'$ which takes into account the remaining information of **a**. To this end, the value of the gross input quantity x_1 has to be modified. The standard uncertainty for an assumed true value of the measurand is derived from the variance of the probability distribution $f_Y(y|\mathbf{a}')$.

For the calculation of the decision threshold and the detection limit iterative methods have to be used. For each iteration step, a new probability distribution $f_{X_1}(\tilde{x}_1|\mathbf{a}',x_1)$ shall be established with a modified value x_1 of the gross quantity X_1. Then, $i=1,...,n_\mathrm{M}$ new Monte Carlo trials are performed by drawing sets $x_{1,i},...,x_{n,i}$ from the probability distributions $f_{X_1}(\tilde{x}_1|\mathbf{a}',x_1), f_{X_i}(\tilde{x}_i|\mathbf{a}'), i=2,...,n)$. For each of these sets one again calculates $y_i=G(x_{1,i},...,x_{n,i})$. The new vector $\mathbf{y}_\mathrm{M}(\mathbf{a}')=\{y_1,...,y_{n_\mathrm{M}}\}$ ordered ascendingly and afterwards assigning probabilities i/n_M to the y_i of $\tilde{\mathbf{y}}_\mathrm{M}(\mathbf{a}')$ is a discrete representation of the distribution function $F_Y(\tilde{y}|\mathbf{a}',x_1)=\int_{-\infty}^{\tilde{y}} f_Y(\eta|\mathbf{a}',x_1)\mathrm{d}\eta$ of Y.

NOTE Due to Monte Carlo uncertainties of means and quantiles, the functions underlying the iteration become “noisy”. Therefore, root finding methods being more robust than e.g. the bisection method are to be applied, such as the secant method or Ridders’ method. The convergence of such an iteration procedure is not as precise as in the case of Part 1.

8 Decision threshold, detection limit and assessments

8.1 Specifications

The probability, α, of a false positive decision, the probability, β, of a false negative decision and the probability, $1-\gamma$, for the coverage interval shall be specified. The choice depends on the application. A frequently cited choice is $\alpha=\beta$ and the value 0,05 for α and β. For the coverage interval the probability $\gamma=0{,}05$ is frequently chosen.

If it is to be assessed whether or not a measurement procedure for the measurand satisfies the requirements to be fulfilled for scientific, legal or other reasons, a guideline value, y_r, as a value of the measurand, for instance, an activity, shall also be specified.

8.2 Decision threshold

The decision threshold, y^*, of the non-negative measurand according to 6.2, quantifying the physical effect of interest, is the value of the estimator, Y, which allows the conclusion that the physical effect is present, if the primary measurement result, y, exceeds the decision threshold, y^*. If the result, y, is below the decision threshold, y^*, the result cannot be attributed to the physical effect, nevertheless it cannot be concluded that it is absent. If the physical effect is really absent, the probability of taking the wrong decision, that the effect is present, is equal to the specified probability, α (probability of the wrong decision that it is not absent if it actually is).

A determined primary measurement result, y, for the non-negative measurand is only significant for the true value of the measurand to differ from zero ($\tilde{y} > 0$), if it is larger than the decision threshold

$$P(y > y^* | \tilde{y} = 0) = \int_{y^*}^{\infty} f_Y(y' | \mathbf{a}', \tilde{y} = 0)\, \mathrm{d}y' = \alpha \tag{18}$$

The integral according to Formula (18) has to be evaluated using Monte Carlo techniques. See Reference [12] for details of the suitable numeric.

An asymmetric shape of $f_Y(y' | \mathbf{a}', \tilde{y} = 0)$ may result in a mean value deviating from $\tilde{y} = 0$. Using the Monte Carlo approach, the decision threshold y^* is therefore calculated by iteration to minimize this deviation. Root-finding methods can be applied, such as bisection, *regula falsi* or interpolation. For each iteration step, new probability distributions $f_{X_1}(\tilde{x}_1 | \mathbf{a}', x_1)$ have to be established with a modified value x_1 of the gross quantity X_1. Then, $i = 1, \ldots, n_\mathrm{M}$ new Monte Carlo trials are performed by drawing sets $x_{1,i}, \ldots, x_{n,i}$ from the probability distributions $f_{X_1}(\tilde{x}_1 | \mathbf{a}', x_1), f_{X_i}(\tilde{x}_i | \mathbf{a}'), i = 2, \ldots, n$. For each of these sets, one again calculates $y_i = G(x_{1,i}, \ldots, x_{n,i})$. The new vector $\bar{\mathbf{y}}_\mathrm{M}(\mathbf{a}') = \{y_1, \ldots, y_{n_\mathrm{M}}\}$ ordered ascendingly and afterwards assigning cumulative probabilities i / n_M to the y_i of $\bar{\mathbf{y}}_\mathrm{M}(\mathbf{a}')$ is a discrete representation of the distribution function $F_Y(\tilde{y} | \mathbf{a}', x_1) = \int_{-\infty}^{\tilde{y}} f_Y(\eta | \mathbf{a}', x_1)\, \mathrm{d}\eta$ of Y. By iteration one searches for the function $F_Y(\tilde{y} | \mathbf{a}', x_1) = \int_{-\infty}^{\tilde{y}} f_Y(\eta | \mathbf{a}', x_1)\, \mathrm{d}\eta$ with $\mathrm{E}\left(f_Y(\tilde{y} | \mathbf{a}', x_1)\right) = 0$. From the respective $\bar{\mathbf{y}}_\mathrm{M}(\mathbf{a}') = \{y_1, \ldots, y_{n_\mathrm{M}}\}$ of the probability distribution, one calculates the probability $P(y^* < y_k) = k / n_\mathrm{M}$ by searching the largest index k with $y_k > y^*$. The (1-α)-quantile of this vector $\bar{\mathbf{y}}_\mathrm{M}(\mathbf{a}') = \{y_1, \ldots, y_{n_\mathrm{M}}\}$ is the decision threshold y^*.

If the probability distribution $f(y' | \mathbf{a}', \tilde{y} = 0)$ is explicitly available, the integral according to Formula (18) can be evaluated by any suitable means.

8.3 Detection limit

The detection limit, $y^\#$, is the smallest true value of the measurand, for which, by applying the decision rule according to 8.2, the probability of the wrong decision, that the physical effect is absent if it is not, does not exceed the specified probability, β.

In order to find out whether a measurement procedure is suitable for the measurement purpose, the detection limit, $y^\#$, is compared with the specified guideline value, y_r, of the measurand. The detection limit, $y^\#$, is the smallest true value of the measurand which can be detected with the measurement procedure used. It is high enough compared to the decision threshold, y^*, that the probability of a false negative decision does not exceed β. The detection limit, $y^\#$, is obtained as the smallest solution of Formula (19):

$$P(y < y^* | \tilde{y} = y^\#) = \int_{-\infty}^{y^*} f_Y(y' | \mathbf{a}', \tilde{y} = y^\#)\, \mathrm{d}y' = \beta \tag{19}$$

Using the Monte Carlo approach, the detection limit $y^\#$ is calculated by iteration by applying root-finding methods such as bisection methods, *regula falsi* or interpolation. For each iteration step, new probability distributions $f_{X_1}(\tilde{x}_1 | \mathbf{a}', x_1)$ have to be established with a modified value x_1 of the gross quantity X_1. Then, $i = 1, \ldots, n_\mathrm{M}$ new Monte Carlo trials are performed by drawing sets $x_{1,i}, \ldots, x_{n,i}$ from the probability distributions $f_{X_1}(\tilde{x}_1 | \mathbf{a}', x_1), f_{X_i}(\tilde{x}_i | \mathbf{a}'), i = 2, \ldots, n$. For each of these sets, one again calculates $y_i = G(x_{1,i}, \ldots, x_{n,i})$. The new vector $\bar{\mathbf{y}}_\mathrm{M}(\mathbf{a}') = \{y_1, \ldots, y_{n_\mathrm{M}}\}$ ordered ascendingly is a discrete representation of the distribution function $F_Y(\tilde{y} | \mathbf{a}', x_1) = \int_{-\infty}^{\tilde{y}} f_Y(\eta | \mathbf{a}', x_1)\, \mathrm{d}\eta$ of Y. From this new $\bar{\mathbf{y}}_\mathrm{M}(\mathbf{a}') = \{y_1, \ldots, y_{n_\mathrm{M}}\}$, one calculates the probability $P(y_i < y^*) = k / n_M$ by searching the largest index k with $y_k < y^*$. This procedure is repeated until the condition $P(y_i < y^*) - \beta = 0$ is met and one obtains a vector $\bar{\mathbf{y}}_M(\mathbf{a}') = \{y_1, ..., y_{n_M}\}$ which fulfills this condition. The arithmetic mean of this vector $\bar{\mathbf{y}}_M(\mathbf{a}') = \{y_1, ..., y_{n_M}\}$ is the detection limit $y^\#$.

If the probability distribution $f_Y(y' | \tilde{y})$ is explicitly available, the integral according to Formula (19) can be evaluated by any suitable mathematical means.

8.4 Assessments

The primary measurement result, y, has to be compared with the decision threshold, y^*. If the primary measurement result, y, exceeds the decision threshold, y^*, it is decided to conclude that the physical effect provided by the measurand is present, i.e. that a contribution from the sample has been recognized.

If the result, y, is below the decision threshold, y^*, it is decided to conclude that the result cannot be attributed to the physical effect. Nevertheless, it cannot be concluded that it is absent. If the physical effect is really absent, the probability of taking the wrong decision, that the effect is present, is equal to the specified probability, α.

The decision on whether or not a measurement procedure to be applied sufficiently satisfies the requirements regarding the detection of the physical effect quantified by the measurand is made by comparing the detection limit, $y^\#$, with the specified guideline value, y_r. If $y^\# > y_r$, the measurement procedure is not suitable for the intended measurement purpose with respect to the requirements.

To improve the situation in the case of $y^\# > y_r$, it can often be sufficient to choose longer measurement durations or to preselect more counts of the measurement procedure. This reduces the detection limit.

NOTE Occasionally, it can happen that a primary measurement result is larger than the decision threshold, i.e. $y > y^*$, is obtained and thus an effect of the sample is recognized, but the detection limit is larger than the specified guideline, i.e. $y^\# > y_r$. This is, for instance, the case if due to particular circumstances the background counting rate is too high and at the same time the contribution from the sample is also high. If the primary measurement result, y, and its associated standard uncertainty, $u(y)$, conform with the measurement objective the result can be accepted though formally the criterion of the detection limit in comparison with the guideline value is not fulfilled.

9 Limits of the coverage interval

9.1 General Aspects

The limits of the coverage interval are provided for a physical effect, recognized as present according to 8.2. Limits of the coverage interval are defined in such a way that the coverage interval contains the true value of the measurand with the specified probability $1-\gamma$ (see 8.1). The limits of the coverage interval as well as the best estimate and its associated standard uncertainty (Clause 10) take into account the fact that the measurand is non-negative.

There is no unique definition for the coverage interval if only the condition $1-\gamma$ is given. Further conditions are required which lead among others to the definitions of the probabilistically symmetric coverage interval and the shortest coverage interval. For the calculation of the limits of both types of coverage intervals, this document provides formulas.

If the information that the measurand is non-negative is taken into account the posterior probability distribution is given by

$$f_Y(\tilde{y}|\mathbf{a},Y\geq 0)=\frac{1}{I_0}\cdot f_Y(\tilde{y}|\mathbf{a})\cdot \mathrm{H}(\tilde{y}) \tag{20}$$

with

$$I_0=\int_0^{+\infty} f_Y(\eta|\mathbf{a})\,\mathrm{d}\eta \tag{21}$$

and $1/I_0$ being a normalisation factor.

9.2 The probabilistically symmetric coverage interval

The probabilistically symmetric coverage interval (Figure B.2) includes for a result, y, of a measurement which exceeds the decision threshold, y^*, the true value of the measurand with a probability $1-\gamma$. It is enclosed by the lower and upper limit of the symmetric coverage interval, respectively $y^{\triangleleft}$ and $y^{\triangleright}$, derived as $(1-\gamma/2)$-quantiles of the probability distribution, $f_Y(\tilde{y}|\mathbf{a})$, of the true value given the experimental result and the prior knowledge that the measurand is non-negative. They are calculated as the upper and lower $\gamma/2$ quantile of the posterior probability distribution which takes into account that the measurand is non-negative [Formula (20)]:

$$\int_{-\infty}^{y^{\triangleleft}} f_Y(\eta|\mathbf{a},Y\geq 0)\,\mathrm{d}\eta=\gamma/2 \tag{22}$$

$$\int_{y^{\triangleright}}^{\infty} f_Y(\eta|\mathbf{a},Y\geq 0)\,\mathrm{d}\eta=\gamma/2\,. \tag{23}$$

Using the Monte Carlo approach, the limits of the probabilistically symmetric coverage interval $y^{\triangleleft}$ and $y^{\triangleright}$ are the $q_{\gamma/2}$ and $q_{1-\gamma/2}$ quantiles of the probability distribution $f_Y(\tilde{y}|\mathbf{a})$ represented by the vector $\bar{\mathbf{y}}_\mathrm{M}=\{y_1,...,y_{n_\mathrm{M}}\}$ and taking into account that the measurand is non-negative. These quantiles can be conveniently calculated from the vector $\bar{\mathbf{y}}_\mathrm{M}=\{y_1,...,y_{n_\mathrm{M}}\}$ by searching the values $y_{k_1}=y^{\triangleleft}$ and $y_{k_2}=y^{\triangleright}$ with the conditions $y_i\geq 0$, $k_1/n_{\mathrm{M},1}=\gamma/2$ and $k_2/n_{\mathrm{M},1}=1-\gamma/2$; $n_{\mathrm{M},1}$ is the number of $y_i\geq 0$.

If the probability distribution $f_Y(\tilde{y}|\mathbf{a})$ is explicitly available the quantiles according to Formula (20) can be evaluated by any suitable means.

9.3 The shortest coverage interval

The shortest coverage interval $[y^<,y^>]$ (Figure B.2) includes for a primary result, y, of a measurement which exceeds the decision threshold, y^*, the true value of the measurand with a probability $1-\gamma$. It is enclosed by the lower and upper limit of the shortest coverage interval, respectively $y^<$ and $y^>$, of the posterior probability distribution which takes into account that the measurand is non-negative according to Formula (20):

$$\int_{y^<}^{y^>} f_Y(\eta|\mathbf{a},Y\geq 0)\,\mathrm{d}\eta=1-\gamma \text{ with } y^>-y^<=\min\,. \tag{24}$$

Using the Monte Carlo approach, the limits of the shortest coverage interval $y^<$ and $y^>$ are the q_{p_1} and q_{p_2} quantiles of the probability distribution $f_Y(\tilde{y}|\mathbf{a})$ represented by the vector $\bar{y}_\mathrm{M}=\{y_1,...,y_{n_\mathrm{M}}\}$ under the conditions $y_i \geq 0$, $p_1 + p_2 = 1 - \gamma$ and $\left| q_{p_1} - q_{p_2} \right| = \min$. These quantiles can be calculated from the vector $\tilde{\mathbf{y}}_\mathrm{M} = \left\{ y_1, ..., y_{n_\mathrm{M}} \right\}$ by iteration with the aforesaid conditions.

NOTE In the case of a large number n_M of trials a simple loop can be applied after having sorted the vector $\tilde{\mathbf{y}}_\mathrm{M}$ ascendingly: For $i = 1, ..., (\gamma n_M)$ calculate the difference $(y_k - y_i)$ with $k = (1-\gamma) n_M + i$. The minimum difference defines i_min, k_min yielding $q_{p_1} = y_{i_\mathrm{min}}$ and $q_{p_2} = y_{k_\mathrm{min}}$.

10 The best estimate and its associated standard uncertainty

The determined primary measurement result, y, of the measurand shall be compared with the decision threshold, y^*. If $y > y^*$, the physical effect quantified by the measurand is recognized as present. Otherwise, it is decided to conclude that the effect is absent.

If $y \geq y^*$ the best estimate $\hat{y}$ of the measurand and its associated standard uncertainty $u(\hat{y})$ are given by

$$\hat{y} = \mathrm{E}(f_Y(\tilde{y} | \mathbf{a}, Y \geq 0)) = \int_{-\infty}^{+\infty} \eta \cdot f_Y(\eta | \mathbf{a}, Y \geq 0) \,\mathrm{d}\eta \tag{25}$$

$$u^2(\hat{y}) = \mathrm{Var}(f_Y(\tilde{y} | \mathbf{a}, Y \geq 0) = \int_{-\infty}^{+\infty} (\eta - \hat{y})^2 \cdot f_Y(\eta | \mathbf{a}, Y \geq 0) \,\mathrm{d}\eta \tag{26}$$

If the uncertainties were evaluated according to the ISO/IEC Guide 98-3-1, the best estimate and its associated standard uncertainty have to be determined from Monte Carlo calculations and to be calculated by explicitly solving the integrals of Formulas (25) and (26).

If the probability distribution $f_Y(\tilde{y} | \mathbf{a})$ is explicitly available the integrals according to Formulas (25) and (26) can be evaluated by any suitable means.

NOTE 1 The best estimate and its associated standard uncertainty are independent of the type of coverage interval used.

NOTE 2 If the best estimate, $\hat{y}$, and its standard uncertainty, $u(\hat{y})$, are calculated, the recording of the primary measurement result, y, and its standard uncertainty, $u(y)$, can be omitted.

Using the Monte Carlo approach, for the calculation of the best estimate and its associated uncertainty, as well as for the limits of the coverage intervals, the original set $\tilde{\mathbf{y}}_\mathrm{M} = \left\{ y_1, ..., y_{n_\mathrm{M}} \right\}$ representing the distribution function $F_Y(\tilde{y} | \mathbf{a}) = \int_{-\infty}^{\tilde{y}} f_Y(\eta | \mathbf{a}) \mathrm{d}\eta$ according to 6.4, is used considering the condition that the measurand is non-negative. The best estimate and its associated standard uncertainty are then calculated as the arithmetic mean and the standard deviation of the $y_i \geq 0$.

11 Documentation

The content of the test report depends on the specific application as well as on demands of the customer or regulator.

Independently of this, information shall be retained in order to justify the data of the test report and to guarantee traceability. This applies in particular to:

a) a reference to this document, i.e. ISO 11929-2;

b) the physical effect of interest, measurand and model of the evaluation;

c) the probabilities α and β of a false positive and a false negative decision, respectively, as well as the coverage probability γ and, if necessary, the guideline value, y_r;

d) the primary measurement result, y, and the standard uncertainty, $u(y)$, associated with y;

e) the decision threshold, y^*;

f) detection limit $y^\#$;

g) a statement, if necessary, as to whether or not the measurement procedure is suitable for the intended measurement purpose;

h) a statement as to whether or not the physical effect is recognized as being present;

NOTE 1 If the physical effect is not recognized as being present given the probability α, i.e. if $y < y^*$ (see 8.4), it is occasionally demanded by the regulator to document $< y^\#$ instead of the measured result, y. Such documentation can be meaningful since it allows, by comparison with the guideline value, to demonstrate that the measurement procedure is suitable for the intended measurement purpose. It is, however, misleading because the mathematical meaning is not correct.

NOTE 2 Occasionally, it is requested by the customer or regulator to compare the primary measurement result, y, with the detection limit, $y^\#$, in order to decide whether the physical effect is recognized or not. Such stipulations are not in accordance with the ISO 11929 series. They have the consequence that it is decided to conclude too frequently that there the physical effect is absent when in fact it is not absent.

i) the physical effect, if recognized as being present, the lower limit of the symmetric coverage interval, $y^\triangleleft$, and the upper limit of the symmetric coverage interval, $y^\triangleright$, with the probability, $1-\gamma$, for the coverage interval, best estimate, $\hat{y}$, of the measurand, and standard uncertainty, $u(\hat{y})$ associated with $\hat{y}$.

NOTE 3 Alternatively, the lower limit of the shortest coverage interval, $y^<$, and the upper limit of the shortest coverage interval, $y^>$, with the probability, $1-\gamma$, for the coverage interval, the best estimate, $\hat{y}$, of the measurand, and the standard uncertainty, $u(\hat{y})$ associated with $\hat{y}$ can be documented.

Annex A
(normative)

Measurements with low count numbers

Measurements with low count numbers have to be dealt with separately since the ISO/IEC Guide 98-3 approximation of a Gaussian probability distribution is in principle no longer valid. The procedure to derive the respective probability distributions for two cases of reasonably large and small count numbers are explained in this Annex.

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: $\tilde{r}\cdot t$.

Here, $\tilde{r}$ is the (true) value of the count rate $Y=R$ of interest, the measurand. For N, a Poisson probability function

$$p_N(n|\tilde{r},t)=\frac{e^{-\tilde{r}\cdot t}(\tilde{r}\cdot t)^n}{n!};\quad n=0,1,2,... \tag{A.1}$$

In most cases $\mathrm{E}(N)=\mathrm{Var}(N)=\tilde{r}\cdot t$ can be assumed for physical reasons because nuclear events are physically independent and mean-life, dead-time effects, pileup 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 probability distribution of the count rate measurand R, the Bayes theorem is applied:

$$f_R(\tilde{r}|n,t)=C\cdot p_N(n|\tilde{r},t)\cdot f_R(\tilde{r}|t) \tag{A.2}$$

where $p_N(n|\tilde{r},t)$ is the likelihood, i.e. the probability to record n counts given the parameter $\tilde{r}\cdot t$ of the probability distribution of R. $f_R(\tilde{r}|t)$ is a prior, i.e. the probability distribution of R before the measurement is performed. According to Jaynes[23] a suitable prior is $f_R(\tilde{r}|t)=C/\tilde{r}$. Inserting it into the Bayes theorem considered above and normalizing yields with Formula (A.3) the gamma distribution

$$f_R(\tilde{r}|n,t)=\frac{t\cdot e^{-\tilde{r}\cdot t}(\tilde{r}\cdot t)^{n-1}}{(n-1)!}\quad \tilde{r}\geq 0 \tag{A.3}$$

which is set to zero for $\tilde{r}<0$. The expectation $\mathrm{E}\left(f_R(\tilde{r}|n,t)\right)=r=n/t$ is the measurement result. The variance $\mathrm{Var}\left(f_R(\tilde{r}|n,t)\right)=r/t=n/t^2$ leads to the associated standard uncertainty $u(r)=\sqrt{r/t}=\sqrt{n/t^2}$. This information about $u(r)$ is used in ISO 11929-1 for reasonably large count numbers.

The particular case $n=0$ shall be treated separately: $\mathrm{E}\left(f_R(\tilde{r}|n,t)\right)$ and $\mathrm{Var}\left(f_R(\tilde{r}|n,t)\right)$ vanish, and $f_R(\tilde{r}|n,t)=\delta(\tilde{r})$ and a zero uncertainty follows. 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 $f_R(\tilde{r}|t)$, one should always obtain $\mathrm{E}\left(f_R(\tilde{r}|n,t)\right)>0$ and $\mathrm{Var}\left(f_R(\tilde{r}|n,t)\right)>0$.

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 $\tilde{r}>0$ at least a few counts can be expected.

The duration t is therefore no longer arbitrary. This knowledge can justify a prior $f_R(\tilde{r}|t) = C/\tilde{r}^{\nu}$ with $0 \leq \nu < 1$ (e.g. the Jeffreys prior with $f_R(\tilde{r}|t) = C/\sqrt{\tilde{r}}$ [25]). This reduces the prior for small $\tilde{r}$ 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 $f_R(\tilde{r}|t) = C$ - i.e. $\nu = 0$ - similar to other physical quantities in practice. The Bayes theorem and normalization then yield the gamma probability distribution

$$f_R(\tilde{r}|n,t) = t \cdot e^{-\tilde{r} \cdot t} (\tilde{r} \cdot t)^n / n! \quad \tilde{r} \geq 0 \tag{A.4}$$

The expectation $\mathrm{E}\left(f_R(\tilde{r}|n,t)\right) = r = (n+1)/t$ is the measurement result and the variance $\mathrm{Var}\left(f_R(\tilde{r}|n,t)\right) = u^2(r) = (n+1)/t^2$ leads to the associated standard uncertainty. In particular, this holds for the case that a n is zero.

NOTE 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 ISO/IEC Guide 98-3 turns out to also contain the estimate $\tilde{r} = 0$. Asymptotically for large n, both approaches discussed lead to the same results. The main differences only occur for very small n.

When applying this document, Formula (A.3) shall be used if $n > 0$ and Formula (A.4) if $n = 0$. When ISO 11929-1 is used $r = n/t$ and $u^2(r) = r/t = n/t^2$ shall be set if $n > 0$ and $r = 1/t$ and $u^2(r) = 1/t^2$ shall be set if $n = 0$.

Annex B
(informative)

Explanatory notes

B.1 General aspects of counting measurements

A measurement of ionizing radiation consists in general at least partially, in counting electronic pulses induced by ionizing radiation events. Such a measurement comprises several individual countings, but can also comprise sequences of individual countings. Examples are the countings on samples of radioactive material or on blanks, countings for the determination of the background effect or the countings in the individual channels of a multi-channel spectrum or in a temporal sequence in the same measurement situation. With each of the countings, either the measurement duration (time preselection) or the counting result (preselection of counts) can be fixed. On the basis of Bayesian statistics, all countings are treated in the same way as follows (see Reference [16]).

The pulse number, N, of each of the countings is taken as a separate random variable. n is the counting result and t is the counting duration (measurement duration). N has the expectation value $\tilde{r} \cdot t$, where $\tilde{r}$ is the count rate or, with spectrum measurements, the spectral density. In the latter case, t is the channel width with respect to the assigned quantity, for instance, the particle energy. Either $\tilde{r}$ or $\tilde{r} \cdot t$ is the measurand. It is assumed that dead-time and mean-life effects, pile-up of the pulses, and instrumental instabilities can be neglected during counting and that all the counted pulses are induced by different ionizing radiation events which are physically independent. The pulse number, N, follows a Poisson distribution and the pulse numbers of all the countings are independent of each another.

Irrespective of whether n pulses are recorded in a measurement of a preselected duration (or of a fixed channel width), t (time preselection), or whether the measurement duration, t, needed for the counting of a preselected pulse number, n, is measured (preselection of counts), $\tilde{r} \cdot t$ follows a gamma distribution (see Reference [13]), where $\tilde{r}$ is taken as a random variable. Then the best estimate, r, of the count rate (or spectral density) and the standard uncertainty, $u(r)$, associated with r follow from

$$r = \mathrm{E}(\tilde{r}) = n/t \; ; \quad u^2(r) = \mathrm{Var}(\tilde{r}) = n/t^2 = r/t \tag{B.1}$$

The case n = 0 results in $u(r)$ = 0. This disappearing uncertainty of $\tilde{r}$ means that $\tilde{r} = 0$ is exactly valid. But $u(r)$ = 0 is an unrealistic result because, with a finite measurement duration, one can never be sure that exactly $\tilde{r} = 0$ if no pulse happens to be recorded. This case can also lead to a zero denominator when the least-squares method according to ISO/IEC Guide 98-5 (see References [9][10]) is applied and a division by $u^2(r)$ shall be made. This shortcoming, i.e. in low-level measurements, can be avoided by replacing all of the counting results n by n + 1 or, with a multi-channel spectrum, by a suitable combination of channels. Here, the measurement duration (or channel width) is assumed to be chosen from experience such that at least a few pulses can be expected if $\tilde{r} > 0$.

B.2 Bayesian statistics in measurement and probability distributions

B.2.1 General Aspects

Based on Bayesian statistics (see Reference [17][21]) and the Bayesian theory of measurement uncertainty (see references [14][16]), characteristic values such as the decision threshold, detection limit and limits of a coverage interval can be calculated taking into account all sources of uncertainty. This approach consists of the complete evaluation of a measurement according to the ISO/IEC Guide 98-3 or ISO/IEC Guide 98-3-1 and the succeeding determination of the characteristic values taking into account all sources of uncertainty. Bayesian statistics allows a consistent foundation of the ISO/IEC Guide 98-3 or ISO/IEC Guide 98-3-1 for both type A and type B uncertainties. This is in contrast to conventional (frequentistic) statistics in which type B uncertainties cannot be accounted for.

The objective of the evaluation of a measurement is to obtain an estimate (measurement result), y, of the true value, $\tilde{y}$, of a measurand, Y, and the standard uncertainty, $u(y)$, associated with y. Since the true value, $\tilde{y}$, is unknown and unknowable it is uncertain and only probability statements can be made about it. Such a probability statement can be established in form of a probability density functions (PDF), $f_Y(\tilde{y}|y,I)$, of a random variable serving as an estimator of the measurand. The PDF quantifies the conditional probability that the true value is $\tilde{y}$ given a measurement result y and any other available information I. The PDF $f_Y(\tilde{y}|y,I)$ completely describes the uncertainty about the true value $\tilde{y}$ associated with the measurement result y.

In most cases the measurand Y is not measured directly, but is determined from other quantities $X_1, ..., X_m$ through a functional relationship G:

$$Y = G(X_1, ..., X_m) \quad \text{(B.2)}$$

where G is called the model of evaluation. In the model of evaluation, the measurand is the output quantity and the quantities on which it depends are the input quantities.

Given that the model of evaluation is sufficiently correct Formula (B.2) can be assumed to hold also for the true values of the quantities involved.

$$\tilde{y} = G(\tilde{x}_1, ..., \tilde{x}_m) \quad \text{(B.3)}$$

The uncertainties about the true values, $\tilde{x}_1, ..., \tilde{x}_m$, of the input quantities, $X_1, ..., X_m$, associated with measurement results, $x_1, ..., x_m$, are also described by PDFs $f_{X_i}(\tilde{x}_i|x_i, I)(i = 1,...,m)$ as explained above for an arbitrary quantity Y.

Tools for establishing the PDFs are the Principle of Maximum Entropy (PME)[23,24], the Bayes Theorem and the Product Rule. Bayesian statistics provides the basis for the ISO/IEC Guide 98-3-1 which is more generally applicable than the ISO/IEC Guide 98-3 and contains the ISO/IEC Guide 98-3 as a special case. If no further information is available non-informative Jeffreys priors should be applied when using the Bayes theorem in order to establish $f_{\mathbf{X}}(\tilde{\mathbf{x}}|\mathbf{a})$; see Annex A for examples.

The probability distribution $f_{\mathbf{Z}}(\tilde{\mathbf{z}}|\mathbf{a})$ of any random variables $\mathbf{Z}$ can in general be obtained from actually available information $\mathbf{a}$ by using the PME. The PME is a fundamental, first principle in Bayesian Statistics and in the uncertainty theory. It plays a part similar to other variational principles in physics like that of external action. The Bayes and expansion theorems can be applied if possible and suitable, alternatively, in combination, or in succession. If two of these alternatives are applicable to a particular case their results need to be identical, provided that the same information is in analogy and correctly taken into account.

The basic difference between conventional and Bayesian statistics lies in the different use of the term probability, conventional statistics defining probability as a limit of frequencies while Bayesian statistics defines it as a degree of belief in an uncertain proposition; see (References [23][24] for a detailed discussion.

Considering measurements, conventional statistics describes the probability distribution, $f_Y(y|\tilde{y})$, i.e. the conditional probability distribution of estimates, y, given the true value, $\tilde{y}$, of the measurand, Y. Since the true value of a measurand is principally unknown and unknowable, it is the basic task of an experiment to make probability statements about it. Bayesian statistics allows the calculation of the probability distribution, $f_Y(\tilde{y}|y,I)$, of the true value, $\tilde{y}$, of the measurand, Y, given the measured estimate, y, and any other relevant information, I.

The measurement uncertainty and the characteristic values are based on the probability distributions, $f_Y(y|\tilde{y})$ and $f_Y(\tilde{y}|y)$ as well as on $f_Y(\tilde{y}|y,I)$ using Bayesian statistics and the Bayesian definition of probability. These PDFs implicitly depend on further conditions and information such as the model, measurement data and associated uncertainties.

After $f_Y(\tilde{y}|y)$ is obtained, the Bayes theorem also allows the calculation of the probability distribution, $f_Y(y|\tilde{y})$, of an estimate, y, given an assumed true value, $\tilde{y}$, of the measurand, Y:

$$f_Y(y|\tilde{y})\cdot f_Y(\tilde{y}) = f_Y(\tilde{y}|y)\cdot f_Y(y) \tag{B.4}$$

The probability distribution, $f_Y(y)$, is uniform for all possible measurement results, y, before the measurement is carried out and $f_Y(\tilde{y})$ is uniform for all $\tilde{y}\geq 0$. Thus, $f_Y(y|\tilde{y})$ is obtained by approximating the now not available $u(y)$ by a function $\tilde{u}(\tilde{y})$.

B.2.2 The ISO/IEC Guide 98-3-1 approach

The ISO/IEC Guide 98-3-1 approach is generally applicable and can handle any set of available information. To apply it, first the PDFs $f_{X_i}(\tilde{x}_i|x_i,I)\,(i=1,...,m)$ have to be established given the $x_1,...,x_m$ and any other available information I. Detailed guidance for the establishment of the PDFs is given in the ISO/IEC Guide 98-3-1; see also 6.3 and Annex A of this document. After establishing the PDFs of all input quantities the joint PDF $f_{\mathbf{X}}(\tilde{\mathbf{x}}|\mathbf{x},I)$ of the input quantities has to be set up. In 6.3 the symbol $\mathbf{a}$ is used summarily to denote the sets of information $\mathbf{x}$ and I. This symbol $\mathbf{a}$ is also used with the same meaning in the following parts of this Appendix.

NOTE 1 The set of information $\mathbf{a}$ contains the information $\mathbf{x}$ of the estimates of the input quantities as well as any other prior information about $\tilde{\mathbf{x}}$ and $\mathbf{X}$ except that the measurand Y is non-negative.

In case of independent input quantities the joint PDF $f_{\mathbf{X}}(\tilde{\mathbf{x}}|\mathbf{a})$ is given as

$$f_{\mathbf{X}}(\tilde{\mathbf{x}}|\mathbf{a}) = \prod\nolimits_1^m f_{X_i}(\tilde{x}_i|\mathbf{a}) \tag{B.5}$$

A joint PDF has to be assigned to those X_i that are not independent and inserted in Formula (B.5) for the respective input quantities. See also 6.4 for establishing the joint distribution.

The normalized posterior probability distribution, $f_Y(\tilde{y}|\mathbf{a})$, of a more general form is calculated from the joint probability distribution $f_{\mathbf{X}}(\tilde{\mathbf{x}}|\mathbf{a})$ using the model Formula $Y = G(\mathrm{X})$ by the so-called Markov formula:

$$f_Y(\tilde{y}|\mathbf{a}) = \int_{-\infty}^{+\infty} f_{\mathbf{X}}(\xi|\mathbf{a})\cdot\delta(\tilde{y} - G(\xi))\,\mathrm{d}\xi \tag{B.6}$$

Then the primary measurement result, y, of the measurand is calculated as the expectation of the PDF $f_Y(\tilde{y}|\mathbf{a})$:

$$y = \mathrm{E}(f_Y(\tilde{y}|\mathbf{a})) = \int_{-\infty}^{+\infty} \eta\cdot f_Y(\eta|\mathbf{a})\,\mathrm{d}\eta \tag{B.7}$$

and the standard uncertainty, $u(y)$, associated with the primary measurement result, y, as the square root of the variance of $f_Y(\tilde{y}|\mathbf{a})$:

$$u^2(y) = \mathrm{Var}(f_Y(\tilde{y}|\mathbf{a})) = \int_{-\infty}^{+\infty} (\eta - y)^2\cdot f_Y(\eta|\mathbf{a})\,\mathrm{d}\eta \tag{B.8}$$

NOTE 2 The calculations according to Formulas (B.7) and (B.8) require $f_Y(\tilde{y}|\mathbf{a})$ to be normalized.

B.2.3 The ISO/IEC Guide 98-3 approach

In the ISO/IEC Guide 98-3 approach the available information is only $\mathbf{a}=\{\mathbf{x},\mathbf{u}(\mathbf{x})\}$. That means that the underlying distributions are Gaussian ones, as described below. Then, an estimate, y, of the true value, $\tilde{y}$, of the measurand, Y, is obtained by inserting the estimates $x_1,...,x_m$ into the model Formula. The model of evaluation constitutes a mathematical expression or computer algorithm that gives an estimate, y, of the measurand, Y, corresponding to any plausible estimates of the input quantities, $x_1,...,x_m$, via the relationship

$$y=G(x_1,...,x_m) \quad \text{(B.9)}$$

The standard uncertainty about Y associated with the estimate y is calculated by

$$\begin{aligned} u^2(y) &= \sum_{i,j=1}^{m} \frac{\partial G}{\partial X_i}\frac{\partial G}{\partial X_j} u(x_i,x_j) \\ &= \sum_{i=1}^{m} c_i^2 \cdot u^2(x_i) + 2\cdot\sum_{i=1}^{m-1}\sum_{j=i+1}^{m} c_i\cdot c_j\cdot u(x_i)\cdot u(x_j)\cdot r(x_i,x_j) \end{aligned} \quad \text{(B.10)}$$

with $u(x_i,x_j)$ being the covariances of x_i and x_j, $c_i \equiv \left.\frac{\partial G}{\partial X_i}\right|_{x_1,...,x_m}$ the sensitivity coefficients and $r(x_i,x_j)$ the correlation coefficient.

According to References [2 to 5], the probability distribution, $f_Y(\tilde{y}|y)$, can be determined by applying the Principle of Maximum (information) Entropy (see reference [23][24]):

$$S=-\int f_Y(\tilde{y}|y)\cdot\ln\left[f_Y(\tilde{y}|y)\right]\mathrm{d}\tilde{y}=\max \quad \text{(B.11)}$$

Formula (B.11) can be solved with the constraints $\mathrm{E}(f_Y(\tilde{y}|y))=y$ and $\mathrm{Var}(f_Y(\tilde{y}|y))=u^2(y)$ using the method of Lagrangian multiplicators which yields the result that the probability distribution $f_Y(\tilde{y}|\mathbf{a})$ generally is a non-normalized Gaussian distribution. With this one obtains the final result for $f_Y(\tilde{y}|y)$:

$$f_Y(\tilde{y}|y)=C\cdot\exp\left\{-(\tilde{y}-y)^2/(2\cdot u^2(y))\right\} \quad \text{(B.12)}$$

Formula (B.12) is not an approximation, but the exact solution of Formula (B.11) given the constraints mentioned above. In this Gaussian distribution y and $u(y)$ are fixed and given values while $\tilde{y}$ is the independent variable. These arguments around Formulas (B.11) and (B.12) are valid as well for the PDFs $f_X(\tilde{\mathrm{x}}|\mathbf{a})$ of the input quantities. All the PDFs are Gaussian distributions.

When applying the ISO/IEC Guide 98-3 it has to be taken into account that the ISO/IEC Guide 98-3 uses an approximation, namely a Taylor expansion truncated after the linear term. If this approximation is not sufficient for a model of evaluation the ISO/IEC Guide 98-3-1 approach has to be used. To apply the ISO/IEC Guide 98-3 approach the model of evaluation should be linear or at least can be locally linearized.

With $f_Y(\tilde{y}|y)$ according to Formula (B.12) the Bayes theorem also allows calculating the probability distribution, $f_Y(y|\tilde{y})$, of an estimate, y, given an assumed true value, $\tilde{y}$, of the measurand, Y. $f_Y(y|\tilde{y})$ is obtained from Formulas (B.10) and (B.11) by approximating the now not available $u(y)$ by a function $\tilde{u}(\tilde{y})$.

$$f_Y(y|\tilde{y})=C\cdot\exp\left\{-(y-\tilde{y})^2/(2\cdot\tilde{u}^2(\tilde{y}))\right\} \quad (\tilde{y}\geq 0) \quad \text{(B.13)}$$

The probability distribution, $f_Y(y|\tilde{y})$, is a non-normalized Gaussian distribution for an assumed true value, $\tilde{y}$, of the measurand, Y, with the associated standard uncertainty, $\tilde{u}(\tilde{y})$. The true value, $\tilde{y}$, is now a parameter in Formula (B.13) and that the variance, $u^2(y)$, of the probability distribution, $f_Y(\tilde{y}|y)$, is expressed by the variance, $\tilde{u}^2(\tilde{y})$, of the probability distribution, $f_Y(y|\tilde{y})$, is expressed by

$$u^2(y) = \tilde{u}^2(\tilde{y}) \tag{B.14}$$

In spite of the facts that the ISO/IEC Guide 98-3 is just a special case of the general approach of the ISO/IEC Guide 98-3-1 and that it is an approximation for models of evaluation which are linear or can be locally linearized it is applicable and sufficient for a wide range of applications. In those cases, the results obtained by applying the ISO/IEC Guide 98-3 or ISO/IEC Guide 98-3-1 are practically identical. There are, however, cases where to PDFs according to the ISO/IEC Guide 98-3-1 are strongly deviating from Gaussian distributions. This is, for instance, the case if there are quantities with large or dominating uncertainties occurring in the denominator of the model of evaluation or if large uncertainties of a calibration factor do not allow deriving a detection limit. In such cases, the application of the ISO/IEC Guide 98-3-1 overcomes these problems; see also ISO 11929-1:2019, Clause 2.

B.3 Limits of the coverage interval and best estimate

B.3.1 General aspects

Neither the information $\mathbf{a}$ nor the establishment and calculation of $f_X(\tilde{x}|\mathbf{a})$, $f_Y(\tilde{y}|\mathbf{a})$, y, and $u(y)$ take into account that the measurand Y and the input quantities $X_1, ..., X_m$ are non-negative. Thus, the primary measurement result y according to Formula (B.7) may be negative.

The fact that the measurand Y is non-negative is taken into account after calculating the PDF $f_Y(\tilde{y}|\mathbf{a})$ by means of the Product Rule:

$$f_Y(\tilde{y}|\mathbf{a}, Y \geq 0) = C \cdot f_Y(\tilde{y}|\mathbf{a}) \cdot f_Y(\tilde{y}|Y \geq 0) \tag{B.15}$$

The non-negativity can be taken into account by a model prior

$$f_Y(\tilde{y}|Y \geq 0) = \mathrm{H}(\tilde{y}) = \begin{cases} 1 & (\tilde{y} \geq 0) \\ 0 & (\tilde{y} < 0) \end{cases} \tag{B.16}$$

which deletes the non-physical parts of the PDF $f_Y(\tilde{y}|\mathbf{a})$ and after renormalization with the normalization constant, $C = \dfrac{1}{I_0} = \left[\int_0^{+\infty} f_Y(\tilde{y}|\mathbf{a})\,\mathrm{d}\tilde{y}\right]^{-1}$, yields the posterior PDF $f_Y(\tilde{y}|\mathbf{a}, Y \geq 0) = C \cdot f_Y(\tilde{y}|\mathbf{a}) \cdot \mathrm{H}(\tilde{y})$.

NOTE 1 The actual result, y, of a measurement, for instance a net count rate, can be negative. But the experimentalist knows a priori without performing an experiment that the true value, $\tilde{y}$, is non-negative. All non-negative values of the measurand have the same a priori probability, if there is no other information available about the true value before the measurement has been performed.

NOTE 2 Without reducing the generality of the approach of this document also in the approach according to ISO/IEC Guide 98-3-1 the factorisation according to Formula (B.15) and the only model prior that the measurand is non-negative according to Formula (B.16) are maintained. If a user has more prior information and desires to consider it in a suitable model prior the user is free to do so.

If required the probabilistically symmetric coverage interval or the shortest coverage interval have to be calculated on the basis of the posterior PDF $f_Y(\tilde{y}|\mathbf{a}, Y \geq 0)$.

The definition of a coverage interval $[y^{\mathrm{L}}, y^{\mathrm{U}}]$, which satisfies the condition

$$P(y^{\mathrm{L}} < \tilde{y} < y^{\mathrm{U}} | y) = \frac{1}{I_0} \int_{y^{\mathrm{L}}}^{y^{\mathrm{U}}} f_Y(\tilde{y}|\mathbf{a}) \cdot \mathrm{H}(\tilde{y})\,\mathrm{d}\tilde{y} \;\text{ with }\; I_0 = \int_0^{+\infty} f_Y(\tilde{y}|\mathbf{a})\,\mathrm{d}\tilde{y} \tag{B.17}$$

that it contains the true value of the measurand with a preselected probability $1-\gamma$, is not unique unless further conditions are added. In this document, two possible definitions are alternatively used, the symmetric coverage interval and the shortest coverage interval.

The limits of the coverage interval are derived as $(1-\gamma/2)$-quantiles of the probability distribution, $f_Y(\tilde{y}|\mathbf{a}, Y \geq 0)$, of the true value given the experimental result and the a priori knowledge that the measurand is non-negative. The best estimate is the expectation value of this probability distribution, $f_Y(\tilde{y}|\mathbf{a}, Y \geq 0)$.

The probabilistically symmetric coverage interval (Figure B.2) includes for a result, y, of a measurement which exceeds the decision threshold, y^*, the true value of the measurand with a probability $1-\gamma$. It is enclosed by the lower and upper limit of the symmetric coverage interval, respectively $y^{\triangleleft}$ and $y^{\triangleright}$, derived as $(1-\gamma/2)$-quantiles of the probability distribution, $f_Y(\tilde{y}|\mathbf{a}, Y \geq 0)$, of the true value given the experimental result and the prior knowledge that the measurand is non-negative. They are calculated via the conditions

$$P(\tilde{y} < y^{\triangleleft} | y) = \frac{1}{I_0} \int_0^{y^{\triangleleft}} f_Y(\tilde{y}|\mathbf{a}) \cdot \mathrm{H}(\tilde{y})\,\mathrm{d}\tilde{y} = \gamma/2 \tag{B.18}$$

$$P(\tilde{y} > y^{\triangleright} | y) = \frac{1}{I_0} \int_{y^{\triangleright}}^{\infty} f_Y(\tilde{y}|\mathbf{a}) \cdot \mathrm{H}(\tilde{y})\,\mathrm{d}\tilde{y} = \gamma/2 \tag{B.19}$$

The shortest coverage interval $[y^{<}, y^{>}]$ (Figure B.2) includes for a result, y, of a measurement which exceeds the decision threshold, y^*, the true value of the measurand with a probability $1-\gamma$. It is enclosed by the lower and upper limit of the shortest coverage interval, respectively $y^{<}$ and $y^{>}$, derived from the probability distribution, $f_Y(\tilde{y}|\mathbf{a}, Y \geq 0)$, of the true value given the experimental result and the prior knowledge that the measurand is non-negative, i.e.

$$P(y^{<} < \tilde{y} < y^{>} | y) = \frac{1}{I_0} \int_{y^{<}}^{y^{>}} f_Y(\tilde{y}|\mathbf{a}) \cdot \mathrm{H}(\tilde{y})\,\mathrm{d}\tilde{y} = 1-\gamma \;\text{ with }\; y^{>} - y^{<} = \min \tag{B.20}$$

If a non-zero effect is observed, i.e. $y > y^*$, the best estimate $\hat{y}$ of the measurand Y is calculated as the expectation of $f_Y(\tilde{y}|\mathbf{a}, Y \geq 0)$

$$\hat{y} = \mathrm{E}(f_Y(\tilde{y}|\mathbf{a}, Y \geq 0)) = \int_{-\infty}^{+\infty} \eta \cdot f_Y(\eta|\mathbf{a}, Y \geq 0)\,\mathrm{d}\eta \tag{B.21}$$

and the standard uncertainty $u(\hat{y})$ associated with the best estimate $\hat{y}$ as the square root of the variance of $f_Y(\tilde{y}|\mathbf{a}, Y \geq 0)$

$$u^2(\hat{y}) = \mathrm{Var}(f_Y(\tilde{y}|\mathbf{a}, Y \geq 0)) = \int_{-\infty}^{+\infty} (\eta - \hat{y})^2 \cdot f_Y(\eta|\mathbf{a}, Y \geq 0)\,\mathrm{d}\eta \tag{B.22}$$

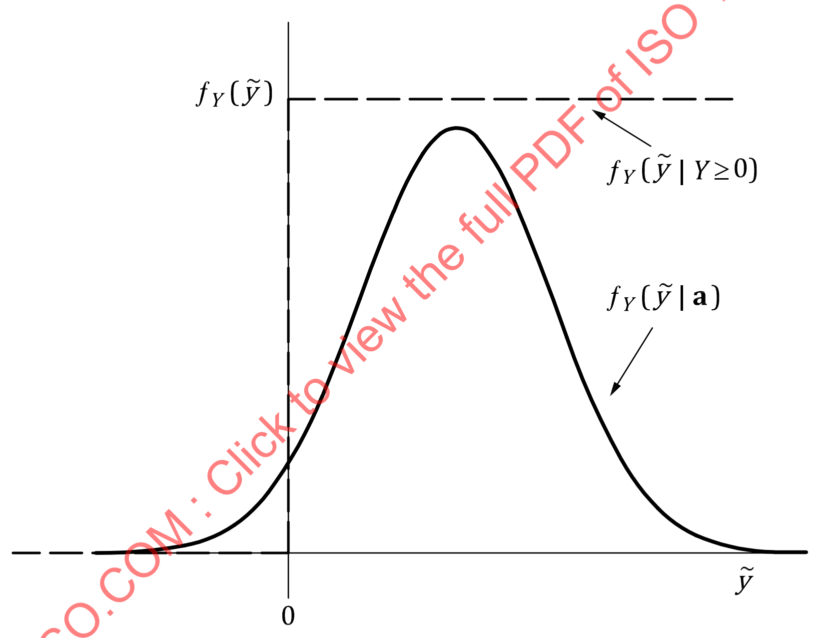
B.3.2 The ISO/IEC Guide 98-3-1 approach

In this document, Monte Carlo Methods are applied when using the ISO/IEC Guide 98-3-1 approach. As described in (6.4) to (6.6) thereby directly the distribution function $F_Y(\tilde{y}|\mathbf{a}, Y \geq 0) = \int_0^{\tilde{y}} C \cdot f_Y(\eta|\mathbf{a}) \cdot \mathrm{H}(\eta)\,\mathrm{d}\eta$ of the PDF $f_Y(\tilde{y}|\mathbf{a}, Y \geq 0) = C \cdot f_Y(\tilde{y}|\mathbf{a}) \cdot \mathrm{H}(\tilde{y})$ is obtained. The calculation of the limits of the probabilistically symmetric coverage interval can be calculated from $F_Y(\tilde{y}|\mathbf{a},Y\geq 0)$ by searching the quantiles for the probabilities $\gamma/2$ and $1-\gamma/2$. The limits of the shortest coverage interval are obtained from $F_Y(\tilde{y}|\mathbf{a},Y\geq 0)$ by searching for the shortest interval $[y^{<},y^{>}]$ with the condition $F_Y(y^{>}|\mathbf{a},Y\geq 0)-F_Y(y^{<}|\mathbf{a},Y\geq 0)=1-\gamma$.

The best estimate $\hat{y}$ and its associated standard uncertainty $u(\hat{y})$ are calculated as the expectation of $F_Y(\tilde{y}|\mathbf{a},Y\geq 0)$, respectively, as the square root of the variance of $F_Y(\tilde{y}|\mathbf{a},Y\geq 0)$.

B.3.3 The ISO/IEC Guide 98-3 approach

In the case of applying the ISO/IEC Guide 98-3 the normalized probability distribution $f_Y(\tilde{y}|\mathbf{a},Y\geq 0)$ is a product of the model prior according to Formula (B.16) and a Gaussian distribution $\mathrm{N}\left[y,u(y)\right]$, i.e. a truncated Gaussian exemplified in Figure B.1. The Gaussian in Formula (B.12) is not an approximation as in conventional statistics or a distribution of measured values from repeated or counting measurements. It is instead the exact result of maximizing the information entropy and expresses the state of knowledge about the measurand, *Y*.



Key

$\tilde{y}$	possible true values of the measurand, *Y*
$f_Y(\tilde{y})$	probability distribution of the possible true value, $\tilde{y}$, of the measurand, *Y*
$f_Y(\tilde{y}\|\mathbf{a})$	probability distribution of the possible true value, $\tilde{y}$, of the measurand, *Y*, given only the measured estimate, *y*, respectively the information **a**
$f_Y(\tilde{y}\|Y\geq 0)$	prior probability distribution of the possible true value, $\tilde{y}$, of the measurand, *Y*, taking into account that the measurand is non-negative

Figure B.1 — Illustration of the probability distribution given in Formula (B.14) for a non-negative measurand *Y*

This leads in the case of the probabilistically symmetric coverage interval (Figure B.2) to the explicit formulas:

$$y^{\triangleleft} = y - k_p\, u(y) \text{ with } p=\omega\cdot(1-\gamma/2) \tag{B.23}$$

$$y^{\triangleright} = y + k_q u(y) \text{ with } q = 1 - \omega\gamma/2 \tag{B.24}$$

The parameter ω is given by

$$\omega = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{y/u(y)} \exp\left(-\frac{v^2}{2}\right) \mathrm{d}v = \Phi\left[y/u(y)\right] \tag{B.25}$$

The limits of the shortest coverage interval (Figure B.2) are calculated either by

$$y^{<}, y^{>} = y \pm k_p u(y) \; ; p = (1 + \omega(1 - \gamma))/2 \tag{B.26}$$

or for $y^{<} < 0$ by

$$y^{<} = 0; \quad y^{>} = y \pm k_q u(y); \quad q = 1 - \varpi\gamma \tag{B.27}$$

with ω according to Formula (B.25).

The best estimate, $\hat{y}$, of the measurand (Figure B.2, B.3) can be calculated as the expectation of the probability distribution, $f_Y(\tilde{y}|\mathbf{a}, Y \geq 0) = C \cdot f_Y(\tilde{y}|\mathbf{a}) \cdot \mathrm{H}(\tilde{y})$, and the standard deviation of $\tilde{y}$ is the standard uncertainty, $u(\hat{y})$, associated with the best estimate, $\hat{y}$, of the measurand, Y,

$$u^2(\hat{y}) = \mathrm{Var}\left(\frac{1}{I_0} \cdot f_Y(\tilde{y}|\mathbf{a}) f_{\mathrm{H}}(\tilde{y})\right) \tag{B.28}$$

Using ω from Formula (B.25), the best estimate $\hat{y}$ is calculated by

$$\hat{y} = \mathrm{E}\left(\frac{1}{I_0} \cdot f_Y(\tilde{y}|\mathbf{a}) f_{\mathrm{H}}(\tilde{y})\right) = y + \frac{u(y) \cdot \exp\left\{-y^2 / \left[2 \cdot u^2(y)\right]\right\}}{\omega\sqrt{2\pi}} \tag{B.29}$$

with the associated standard uncertainty, $u(\hat{y})$,

$$u(\hat{y}) = \sqrt{u^2(y) - (\hat{y} - y) \cdot \hat{y}} \tag{B.30}$$

The following relationships $\hat{y} > y$ and $\hat{y} > 0$, as well as $u(\hat{y}) < u(y)$ are valid. For $y >> u(y)$ the approximations $\hat{y} = y$ and $u(\hat{y}) = u(y)$ are valid.

NOTE The calculation of the best estimate and its associated standard uncertainty are independent from the type of coverage interval used.