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BAYESIAN DECISION THRESHOLD, DETECTION LIMIT AND CONFIDENCE LIMITS IN IONISING-RADIATION MEASUREMENT

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Based on Bayesian statistics and the Bayesian theory of measurement uncertainty, characteristic limits such as the decision threshold, detection limit and limits of a confidence 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 Guide to the Expression of Uncertainty in Measurement (GUM) and the successive determination of the characteristic limits by using the standard uncertainty obtained from the evaluation. This procedure is elaborated here for several particular models of evaluation. It is, however, so general that it allows for a large variety of applications to similar measurements. It is proposed for the revision of those parts of DIN 25482 and ISO 11929 that are still based on conventional statistics and, therefore, do not allow to take completely into account all the components of measurement uncertainty in the calculation of the characteristic limits.

INTRODUCTION

The recognition and detection of ionising radiation are indispensable basic pre-requisites of radiation protection. For this purpose, the standard series DIN 25482[1–11] and the corresponding standard series ISO 11929[12–19] provide characteristic limits, i.e. decision thresholds, detection limits and confidence limits, for a diversity of application fields. The decision threshold allows a decision to be made for a measurement on whether or not, for instance, radiation of a possibly radioactive sample is present. The detection limit allows a decision on whether or not the measurement procedure intended for application to the measurement meets the requirements to be fulfilled and is, therefore, appropriate for the measurement purpose. Confidence limits enclose with a specified probability the true value of the measurand to be measured.

Because of recent developments in metrology concerning measurement uncertainty, i.e. DIN 1319[20,21] and ISO Guide to the Expression of Uncertainty in Measurement (GUM)[22], the older Parts 1–7 (except Part 4) of DIN 25482[1–7] and the corresponding Parts 1–4 of ISO 11929[12–15] urgently need a revision based on the common, already laid statistical foundation of Part 10 of DIN 25482[8] and Part 7 of ISO 11929[18]. The modern Parts 11–13 of DIN 25482[9–13] and Parts 5–8 of ISO 11929[16–19] are already established on this basis. But since the responsible working group DIN NMP 722 was first suspended and finally disbanded by DIN, the authors, feeling responsible for radiation protection and, being members of the working group 'Detection limits' (AK SIGMA) of the German Radiation Protection Association (Fachverband für Strahlenschutz), elaborated a proposal[23,24] for the revision of DIN 25482 and ISO 11929. This paper outlines the general foundation of the Bayesian characteristic limits and gives exemplarily several particular applications to measurements of ionising radiation.

UNCERTAINTY IN MEASUREMENT

The starting point of any analysis is the definition of the quantity Y to be measured and for which the characteristic limit is to be determined. This measurand [For the proper use of terms of metrology see Ref. (25).] is, for instance, the concentration of an element or an activity of radionuclides in a sample. The measurand is connected to input quantities X_i ($i = 1, \ldots, m$), which originate from measurements or from other sources of information by a model of evaluation. Examples of input quantities are net peak areas from gamma spectra, efficiency data of a detector, sample masses and chemical

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yields. The model of evaluation is a mathematical relationship,

$$Y = G(X_1, X_2, \ldots, X_m). \tag{1}$$

Note, that the model function G need not necessarily be explicitly available. The model may also be given in the form of a computer code.

Measurements yield estimates x_i of the true values of the input quantities X_i. The estimates x_i are associated with the standard uncertainties $u(x_i)$. The evaluation analysis yields an estimate y of the measurand Y using y as an estimate of the true value η of Y in Equation 1 and one obtains

$$y = G(x_1, x_2, \ldots, x_m). \tag{2}$$

If the input quantities X_i are uncorrelated, the standard uncertainty $u(y)$ associated with y is calculated as the positive square root of the variance,

$$u^2(y) = \sum_{i=1}^{m} \left(\frac{\partial G}{\partial x_i} \right)^2 \cdot u^2(x_i). \tag{3}$$

with $c_i \equiv \partial G / \partial x_i$ being the sensitivity coefficients.

If the input quantities X_i are correlated, the standard uncertainty $u(y)$ has to be calculated accordingly using covariances $u(x_i, x_j)$[14].

$$u^2(y) = \sum_{i=1}^{m} \sum_{j=1}^{m} c_i \cdot c_j \cdot u(x_i, x_j), \tag{4}$$

with $u(x_i, x_i) = u^2(x_i)$.

Given n repeated measurements of the input quantities X_i and X_j with the measured values $x_{i,k}$ and $x_{j,k}$ ($k = 1, \ldots, n$) and the respective arithmetic means $\bar{x}_{i,k}$ and $\bar{x}_{j,k}$, then the estimates $x_i = \bar{x}_{i,k}$ and $x_j = \bar{x}_{j,k}$ follow and the covariances $u(x_i, x_j)$ are calculated by

$$u(x_i, x_j) = \frac{1}{n-1} \sum_{k=1}^{n} (x_{i,k} - x_i)(x_{j,k} - x_j). \tag{5}$$

If the partial derivatives are not explicitly available, they can be numerically sufficiently well approximated by using the standard uncertainty $u(x_i)$ as an increment of x_i,

$$\frac{\partial G}{\partial x_i} = \frac{1}{u(x_i)} \cdot (G(x_1, \ldots, x_i + u(x_i)/2, \ldots, x_m) - G(x_1, \ldots, x_i - u(x_i)/2, \ldots, x_m)) \tag{6}$$

The standard uncertainties generally have to be evaluated according to the GUM[22] well in accordance with guidelines of other international bodies[26–28]. In the GUM, uncertainties are evaluated either by 'statistical methods' (Type A) or by 'other means' (Type B). Type A uncertainties can be evaluated from repeated or counting measurements, while Type B uncertainties cannot. They are for instance uncertainties given in certificates of standard reference materials or of calibration radiation sources used in the evaluation of a measurement. The evident contradiction in using different types of statistics in the definitions of the two types of uncertainties was recently overcome by the establishment of a Bayesian theory of measurement uncertainty[29,30]. In this theory, uncertainties of all types are consistently determined. They quantitatively express the actual state of incomplete knowledge about the quantities involved.

BAYESIAN STATISTICS IN MEASUREMENT

The basic difference between conventional and Bayesian statistics lies in the different use of the term probability. Considering measurements, conventional statistics describes the probability distribution $f(y \mid \eta)$, i.e. the conditional distribution of estimates y given the true value η of the measurand Y. Since the true value of a measurand is principally unknown, it is the basic task of an experiment to make statements about it. Bayesian statistics allows the calculation of the probability distribution $f(\eta \mid y)$ of the true value η of a measurand Y given the measured estimate y. The measurement uncertainty and the characteristic limits are based on the distributions $f(y \mid \eta)$ and $f(\eta \mid y)$. These implicitly depend on further conditions and information such as the model, measurement data and associated uncertainties.

In order to establish $f(\eta \mid y)$, one uses an approach, which separates the information about the measurand obtained from the actual experiment from other information available about the measurand by

$$f(\eta \mid y) = C \cdot f_0(\eta \mid y) \cdot f(\eta). \tag{7}$$

$f_0(\eta \mid y)$ is the probability distribution that the measurand Y has the true value η if only the measured value y and the associated uncertainty $u(y)$ are given. It only accounts for the measured values and neglects any other information about the measurand. $f(\eta)$ represents all the information about the measurand available before the experiment is performed. Therefore, it does not depend on y. C is a normalisation constant.

If, for instance, an activity of a radiation source or a concentration of an element is the measurand, there exists the meaningful information that the measurand is non-negative ($\eta \geq 0$) before the measurement is carried out. This yields for $f(\eta)$:

$$f(\eta) = \begin{cases} \text{const} & (\eta \geq 0) \\ 0 & (\eta < 0). \end{cases} \tag{8}$$

Note, that 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 η is non-negative. All non-negative values of the measurand have the same *a priori* probability if there is no other information about the true value of the measurand before the measurement has been performed.

Since $f_0(\eta \mid y)$ in essence considers the experimental information, the expectation $E_0(\eta) = y$ and the variance $\mathrm{Var}_0(\eta) = u^2(y)$ should hold true for the probability distribution $f_0(\eta \mid y)$.

According to Weise and Wöger[29,30], the probability distribution $f(\eta \mid y)$ can be determined by applying the principle of maximum (information) entropy S[31],

$$S = -\int f(\eta \mid y) \cdot \ln(f_0(\eta \mid y))\mathrm{d}\eta = \max. \tag{9}$$

Equation 9 can be solved with the constraints $E_0(\eta) = y$ and $\mathrm{Var}_0(\eta) = u^2(y)$ by the method of Lagrangian multiplicators and one obtains the result

$$f(\eta \mid y) = C \cdot f(\eta) \cdot \exp\left(-(\eta - y)^2/(2 \cdot u^2(y))\right). \tag{10}$$

Accordingly, the distribution $f(\eta \mid y)$ is a product of the model prior $f(\eta)$ and a gaussian $N(y, u(y))$, i.e. a truncated gaussian (Figure 1). Note, that the gaussian in Equation 10 is not an approximation as in conventional statistics or a distribution of measured values from repeated or counting measurements. It is instead the explicit result of maximising the information entropy and expresses the state of knowledge about the measurand Y.

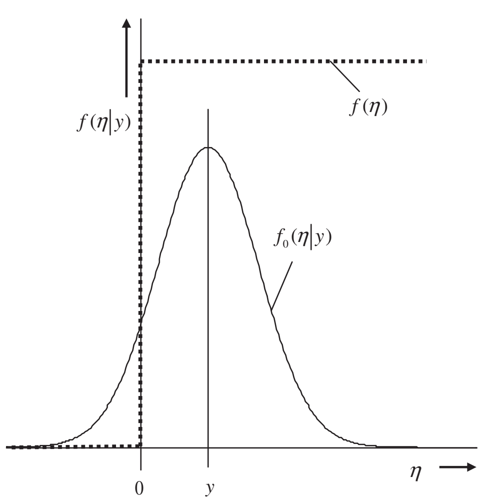

Figure 1. Illustration of the probability distribution given in Equation 10 for a non-negative measurand Y.

After $f(\eta \mid y)$ is obtained, the Bayes theorem also allows the calculation of the probability distribution $f(y \mid \eta)$ of an estimate y given the true value η of the measurand Y,

$$f(y \mid \eta) \cdot f(\eta) = f(\eta \mid y) \cdot f(y). \tag{11}$$

The distribution $f(y)$ is uniform for all possible measurement results y, and $f(\eta)$ is uniform for all $\eta \geq 0$ according to Equation 8. Thus, $f(y \mid \eta)$ is obtained from Equations 10 and 11 by approximating the now not available $u(y)$ by a function $\tilde{u}(\eta)$.

$$f(y \mid \eta) = C \cdot \exp(-(y - \eta)^2/(2 \cdot \tilde{u}^2(\eta))) \quad (\eta \geq 0). \tag{12}$$

The probability distribution $f(y \mid \eta)$ is a gaussian for a given true value η of the measurand with the standard uncertainty $\tilde{u}(\eta)$. Note, that the true value η of the measurand Y is now a parameter in Equation 12 and that the variance $u^2(y)$ of the probability distribution $f(\eta \mid y)$ equals the variance $\tilde{u}^2(\eta)$ of the probability distribution $f(y \mid \eta)$,

$$u^2(y) = \tilde{u}^2(\eta). \tag{13}$$

CALCULATION OF THE STANDARD UNCERTAINTY AS A FUNCTION OF THE TRUE VALUE OF THE MEASURAND

For the provision and numerical calculation of the decision threshold and detection limit, the standard uncertainty of the measurand is needed as a function $\bar{u}(\eta)$ of the true value $\eta \geq 0$ of the measurand. This function has to be determined in a way similar to $u(y)$ within the framework of the evaluation of the measurements by application of DIN 1319-3[20], DIN 1319-4[21], GUM[22] or DIN V ENV 13005[26]. In most cases, $\tilde{u}(\eta)$ has to be formed as a positive square root of a variance function $\tilde{u}^2(\eta)$ calculated first. This function must be defined, unique and continuous for all $\eta \geq 0$ and must not assume negative values.

In some cases, $\tilde{u}(\eta)$ can be explicitly specified, provided that $u(x_1)$ is given as a function $h_1(x_1)$ of x_1. In such cases, y has to be replaced by η and Equation 2 must be solved for the estimate x_1 of the input quantity X_1, which in the following is always taken as the gross effect quantity. With a specified η, the value x_1 can also be calculated numerically from Equation 2, for instance, by means of an iteration procedure, which results in x_1 as a function of η and $x_2, \ldots, x_m$. This function has to replace x_1 in Equation 3 and in $u(x_1) = h_1(x_1)$, which finally yields $\tilde{u}(\eta)$ instead of $u(y)$. In most cases of the models dealt with in this paper, one has to proceed in this way. Otherwise, $\tilde{u}(\eta)$ can be obtained as an

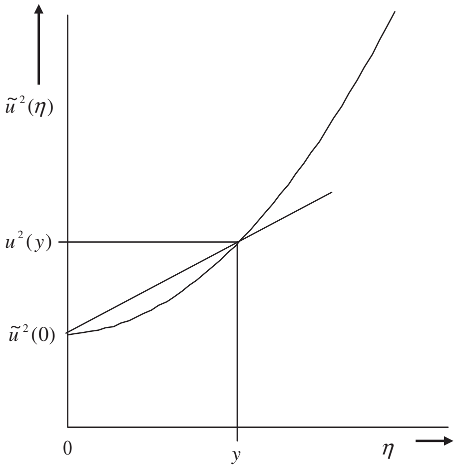

Figure 2. Illustration of the function $\tilde{u}^2(\eta)$ and the interpolation formula of Equation 18.

approximation by interpolation from the data y_j and $u(y_j)$ of several measurements (Figure 2).

DECISION THRESHOLD AND DETECTION LIMIT

Without a detailed mathematical foundation of Bayesian characteristic limits, which may be found elsewhere[(32)], we can now define the characteristic limits for a non-negative measurand Y, which is, for instance, a concentration of an element or an activity of a radionuclide in a sample. The true value η is zero if the element or the radionuclide is not present. The decision threshold and the detection limit are defined[(32)] on the basis of statistically testing the null hypothesis H_0: $\eta = 0$ against the alternative hypothesis H_1: $\eta > 0$.

A decision quantity Y has to be attributed to the measurand, which being a random variable, is likewise an estimator of the measurand. It is postulated that the expectation E(Y) of the decision quantity Y is equal to the true value η of the measurand. A value y of the estimator Y derived from measurements is an estimate of the measurand. As a result of the measurement, y and the associated standard uncertainty $u(y)$ are derived according to the GUM[(22)] as a complete result of the measurement. y and $u(y)$ have to be derived by evaluation of measured quantities and of other information by way of the mathematical model, which takes into account all relevant quantities. Generally, it will not be explicitly made use of the fact that the measurand is non-negative. Therefore, y may become negative, in particular, if the true value of the measurand is close to zero.

For the determination of the decision threshold and the detection limit, the standard uncertainty of

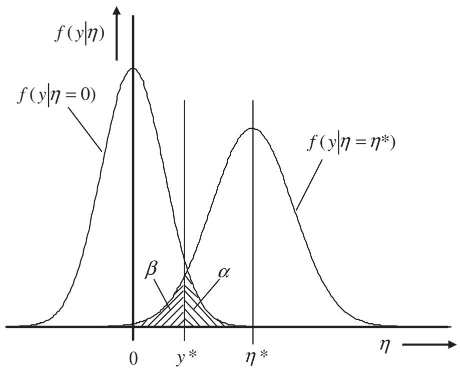

Figure 3. Illustration of the decision threshold y^* and the detection limit η^*.

the decision quantity has to be calculated, if possible, as a function $\tilde{u}(\eta)$ of the true value η of the measurand. In case this is not possible, approximate solutions are described below.

Then, the decision threshold y^* (Figure 3) is a characteristic limit, which, when exceeded by a result y of a measurement, helps one to decide that the element or radionuclide is present in the sample. If $y \le y^*$, the null hypothesis, H_0: $\eta = 0$, cannot be rejected and one decides that the element or radionuclide is not found in this sample. If this decision rule $P(y > y^* \mid \eta = 0) = \alpha$ is observed, a wrong acceptance of the alternative hypothesis, H_1: $\eta > 0$, occurs with the probability α, which is the probability of the error of the first kind of the statistical test used.

The decision threshold is given by

$$y^* = k_{1-\alpha} \cdot \tilde{u}(0), \tag{14}$$

with $k_{1-\alpha}$ being the $(1-\alpha)$-quantile of the standardised normal distribution. $\tilde{u}(0)$ is the uncertainty of the measurand if its true value equals zero. If the approximation $\tilde{u}(\eta = 0) = u(y)$ is sufficient, one obtains

$$y^* = k_{1-\alpha} \cdot u(y). \tag{15}$$

The detection limit η^* (Figure 4) is the smallest true value of the measurand detectable with the measuring method. It is defined by $P(y < y^* \mid \eta = \eta^*) = \beta$. The detection limit η^* is sufficiently larger than the decision threshold y^* such that the probability of $y < y^*$ equals the probability β of the error of the second kind in the case of $\eta = \eta^*$. The detection limit is given by

$$\eta^* = y^* + k_{1-\beta} \cdot \tilde{u}(\eta^*), \tag{16}$$

with $k_{1-\beta}$ being the $(1-\beta)$-quantile of the standardised normal distribution.

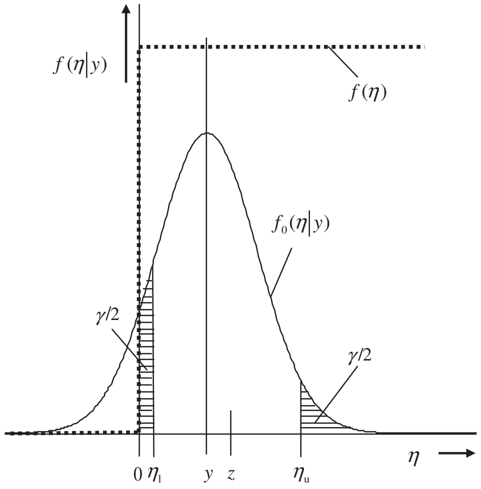

Figure 4. Illustration of the confidence limits η_l and η_u and of the best estimate z of the true value η of a non-negative measurand Y.

Equation 16 is an implicit one. The detection limit can be calculated from it by iteration using, for example, the starting approximation $\eta^* = 2 \cdot y^*$.

For the numerical calculation of the decision threshold and the detection limit, the function $\tilde{u}(\eta)$ is needed, which gives the standard uncertainty of the decision quantity as a function of the true value η of the measurand. This function generally has to be determined in the course of the evaluation of the measurement according to the GUM[22]. Often this function is only slowly increasing. Therefore, it is justified in many cases to use the approximation $\tilde{u}(\eta) = u(y)$. If the approximation $\tilde{u}(\eta) = u(y)$ is sufficient for all true values η, then

$$\eta^* = (k_{1-\alpha} + k_{1-\beta}) \cdot u(y), \tag{17}$$

is valid.

This applies in particular if the primary estimate y of the measurand is not much larger than its standard uncertainty $u(y)$. Frequently, the value of y is calculated as the difference (net effect) of two quantity values of approximately equal size with x_1 being the gross effect and x_0 being the background or blank effect, both obtained from independent measurements. In this case of $y = x_1 - x_0$ one gets $u^2(y) = u^2(x_1) + u^2(x_0)$ with the standard uncertainties $u(x_1)$ and $u(x_0)$ associated with x_1 and x_0, respectively. From this, one obtains $\tilde{u}(0) = 2 \cdot u^2(x_0)$, since for $\eta = 0$ one expects $x_1 = x_0$.

If only $\tilde{u}(0)$ and $u(y)$ are known, the approximation by linear interpolation according to Equation 18 is often sufficient for $y > 0$:

$$\tilde{u}^2(\eta) = \tilde{u}^2(0) \cdot (1 - \eta/y) + u^2(y) \cdot \eta/y. \tag{18}$$

In many practical cases $\tilde{u}^2(\eta)$ is a slowly increasing linear function of η. This justifies the approximations above, in particular, the linear interpolation of $\tilde{u}^2(\eta)$ instead of $\tilde{u}(\eta)$ itself.

With the interpolation formula according to Equation 18 one gets the approximation

$$\eta^* = a + \sqrt{a^2 + (k_{1-\beta}^2 - k_{1-\alpha}^2) \cdot \tilde{u}^2(0)}, \tag{19}$$

with

$$a = k_{1-\alpha} \cdot \tilde{u}(0) + \frac{1}{2}(k_{1-\beta}^2/y) \cdot (u^2(y) - \tilde{u}^2(0)). \tag{20}$$

For $\alpha = \beta$, one receives $\eta^* = 2 \cdot a$.

CONFIDENCE LIMITS

The confidence interval (Figure 4) 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 confidence interval, η_l and η_u, respectively, according to

$$\eta_l = y - k_p \cdot u(y) \text{ with } p = \omega \cdot (1 - \gamma/2); \tag{21}$$

$$\eta_u = y + k_q \cdot u(y) \text{ with } q = 1 - \omega \cdot \gamma/2. \tag{22}$$

The parameter ω is given by

$$\omega = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{y/u(y)} \exp(-z^2/2)\mathrm{d}z = \Phi(y/u(y)). \tag{23}$$

Values of the function $\Phi(t)$, which is the distribution function of the standardised normal distribution, and the quantiles k_p of the standardised normal distribution are tabulated[34].

The limits of the confidence interval to be determined refer to η taken as another estimator of the measurand Y. The confidence limits are not symmetrical around the expectation $z = \mathrm{E}(\eta)$. The probabilities of $\eta < \eta_l$ and $\eta > \eta_u$, however, are both equal to $\gamma/2$ and the relationship $0 < \eta_l < \eta_u$ is valid. If y and $u(y)$ are of similar size, this asymmetry of the confidence interval is clearly visible. But for $y \gg u(y)$, the well-known formula

$$\eta_{l,u} = y \pm k_{1-\gamma/2} \cdot u(y) \tag{24}$$

is valid as an approximation. Equation 24 is applicable if

$$y >\approx 2 \cdot k_{1-\gamma/2} \cdot u(y) \tag{25}$$

ASSESSMENT OF AN ANALYTICAL TECHNIQUE

Having performed a measurement and an evaluation of the measurement according to the GUM[14], the performance of the analytical technique can be assessed in the following way.

A measured result has to be compared with the decision threshold calculated by means of Equation 15. If a result of the measurement y is larger than the decision threshold y^*, one decides that a non-zero effect quantified by the measurand is observed and that the element or activity is present in the sample.

To check whether a measurement procedure is suitable for measuring the measurand, the calculated detection limit has to be compared with a specified guideline value, e.g. according to specified requirements on the sensitivity of the measurement procedure from scientific, legal or other reasons. The detection limit has to be calculated by means of Equation 16. If the detection limit thus determined is smaller than the guideline value, the procedure is suitable for the measurement, otherwise it is not.

If a non-zero effect is observed, i.e. $y > y^*$, the best estimate z of the measurand (Figure 4) can be calculated as the expectation of the probability distribution $f(\eta \mid y)$ and the standard deviation of η is the standard uncertainty $u(z)$ associated with the best estimate z of the measurand Y.

$$u(z) = \sqrt{Var(\eta).(26)}$$

Using ω from Equation 23, the best estimate z is calculated by

$$z = \mathrm{E}(\eta) = y + \frac{u(y) \cdot \exp(-y^2/(2 \cdot u^2(y)))}{\omega \cdot \sqrt{2\pi}}, \quad (27)$$

with the associated standard uncertainty $u(z)$

$$u(z) = \sqrt{u^2(y) - (z - y) \cdot z}. \quad (28)$$

The following relationships $z \geq y$ and $z \geq 0$ as well as $u(z) \leq u(y)$ are valid. For $y \gg u(y)$ the approximations $z = y$ and $u(z) = u(y)$ are valid. See Figure 4 for an illustration of the confidence interval and the best estimate of the measurand.

APPLICATIONS

Frequently used models

Many applications, in fields other than measurements of ionising radiation, use models of evaluation of the general mathematical form:

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

$$\text{with } W = \frac{X_6 \cdot X_8 \cdots}{X_5 \cdot X_7 \cdots}. \quad (29)$$

In measurements of ionising radiation, $X_1 = \rho_g$ and $X_2 = \rho_0$ frequently are the counting rates of a gross and a background measurement, respectively. X_3 can, for instance, be a shielding correction[11,17] and X_4 an additional general background correction. X_5, X_6,... are calibration and correction factors. If X_3 or X_4 are not needed, $x_3 = 1$ and $u(x_3) = 0$ or $x_4 = 0$ and $u(x_4) = 0$ have to be set.

By replacing the quantities in Equation 29 by their actual estimates x_i and w for W one obtains with $x_1 = r_g = n_g/t_g$ and $x_2 = r_0 = n_0/t_0$:

$$y = G(x_1, \ldots, x_m) = (x_1 - x_2 \cdot x_3 - x_4) \cdot w = (r_g - r_0 \cdot x_3 - x_4) \cdot w = \left(\frac{n_g}{t_g} - \frac{n_0}{t_0} x_3 - x_4\right) \cdot w \quad (30)$$

n_g and n_0 are the numbers of counted events in the gross and the background measurement of duration t_g and t_0, respectively.

With the partial derivatives

$$\frac{\partial G}{\partial X_1} = W; \; \frac{\partial G}{\partial X_2} = -X_3 \cdot W; \; \frac{\partial G}{\partial X_3} = -X_2 \cdot W; \; \frac{\partial G}{\partial X_4} = -W; \; \frac{\partial G}{\partial X_i} = \pm \frac{Y}{X_i} (i \geq 5), \quad (31)$$

and by substituting the estimates x_i, w and y, Equation 3 yields the standard uncertainty $u(y)$ of the measurand Y associated with y:

$$u^2(y) = w^2 \cdot (u^2(x_1) + x_3^2 \cdot u^2(x_2) + x_2^2 \cdot u^2(x_3) + u^2(x_4)) + y^2 \cdot u_{rel}^2(w) = w^2 \cdot (r_g/t_g + x_3^2 r_0/t_0 + r_0^2 \cdot u^2(x_3) + u^2(x_4)) + y^2 \cdot u_{rel}^2(w) \quad (32)$$

where

$$u_{rel}^2(w) = \sum_{i=5}^{m} \frac{u^2(x_i)}{x_i^2}$$

is the sum of the squared relative standard uncertainties of the quantities X_5 to X_m. For $m < 5$, the values $w = 1$ and $u_{rel}^2(w) = 0$ apply.

For a true value η one expects

$$n_g = \eta/w + r_0 \cdot x_3 + x_4 \quad (33)$$

and with Equation 32 one obtains

$$\tilde{u}^2(\eta) = w^2 \cdot \left[(\eta/w + r_0 \cdot x_3 + x_4)/t_g + x_3^2 \cdot r_0/t_0 + r_0^2 \cdot u^2(x_3) + u^2(x_4)\right] + \eta^2 \cdot u_{rel}^2(w) \quad (34)$$

This yields for $\eta = 0$ the decision threshold

$$y^* = k_{1-\alpha} \cdot \tilde{u}(0) = k_{1-\alpha} \cdot w \cdot \sqrt{(r_0 \cdot x_3 + x_4)/t_g + x_3^2 \cdot r_0/t_0 + r_0^2 \cdot u^2(x_3) + u^2(x_4)} \quad (35)$$

Note that in this class of models the decision threshold does not depend on the uncertainty of W.

For the detection limit one obtains the equation

$$\eta^* = y^* + k_{1-\beta} \cdot \tilde{u}(\eta^*) = y^* + k_{1-\beta} \cdot \sqrt{\begin{aligned} & w^2 \cdot \left[(\eta^*/w + r_0 \cdot x_3 + x_4)/t_g + x_3^2 \cdot r_0/t_0 \right. \\ & \left. + r_0^2 \cdot u^2(x_3) + u^2(x_4) \right] + \eta^{*2} \cdot u_{rel}^2(w) \end{aligned}} \quad (36)$$

which has to be solved for η^*. Equation 36 has a solution if $k_{1-\beta}^2 \cdot u_{rel}^2(w) < 1$.

Determination of an activity

In ionising-radiation measurements, often the activity is determined from a measurement of a net count rate value ($r_g - r_0$) as the difference of a gross count rate value $r_g = n_g/t_g$ and a background count rate value $r_0 = n_0/t_0$ with time pre-selection multiplied by a calibration factor w with the standard uncertainties $u(r_g) = r_g/t_g$, $u(r_0) = r_0/t_0$ and $u(w)$, respectively. This yields the simple model

$$y = (r_g - r_0) \cdot w = (n_g/t_g - n_0/t_0) \cdot w \quad (37)$$

which is just a special case of Equation 30 with $x_1 = r_g$, $x_2 = r_0$, $x_3 = 1$, $u(x_3) = 0$, $x_4 = 0$ and $u(x_4) = 0$. However, because it is used so frequently, it shall be explicitly dealt with here. Equation 3 yields the standard uncertainty $u(y)$ of the measurand Y associated with y

$$u^2(y) = w^2 \cdot (r_g/t_g + r_0/t_0) + y^2 \cdot u_{rel}^2(w) \quad (38)$$

with $u_{rel}(w) = u(w)/w$.

With this information, $\tilde{u}(\eta)$ can be explicitly calculated since one expects for a true value η of the measurand a number of counts n_g in the gross measurement

$$n_g = \eta/w + r_0 \cdot t_g. \quad (39)$$

Since $u^2(n_g) = n_g$ is valid for a poisson process, one can calculate $\bar{u}(\eta)$ using Equation 38 as

$$\tilde{u}^2(\eta) = w^2 \cdot ((\eta/w + r_0)/t_g + r_0/t_0) + \eta^2 \cdot u_{rel}^2(w) \quad (40)$$

and obtains for $\eta = 0$ the decision threshold

$$y^* = k_{1-\alpha} \cdot \tilde{u}(0) = k_{1-\alpha} \cdot w \cdot \sqrt{r_0 \cdot \left(\frac{1}{t_g} + \frac{1}{t_0}\right)} \quad (41)$$

and for the detection limit

$$\eta^* = y^* + k_{1-\beta} \cdot \tilde{u}(\eta^*) = y^* + k_{1-\beta} \cdot \sqrt{w^2 \cdot ((\eta^*/w + r_0)/t_g + r_0/t_0) + \eta^{*2} \cdot u_{rel}^2(w)} \quad (42)$$

which can conveniently be solved by iteration with the starting value $\eta^* = 2y^*$. For $\alpha = \beta$, i.e. $k_{1-\alpha} = k_{1-\beta}$, Equation 42 has the simple explicit solution;

$$\eta^* = \frac{2 \cdot y^* + (k_{1-\alpha}^2 \cdot w)/t_g}{1 - k_{1-\alpha}^2 \cdot u_{rel}^2(w)}. \quad (43)$$

General measurement of a net quantity with calibration

The simple model of Equation 37 can also be used to demonstrate that the approach described here is not limited to measurements of ionising radiation. A model in the form of Equation 44 describes an evaluation of any measurand derived from a gross or sample measurement and a background or blank measurement. The value y of the measurand Y is the difference of the gross signal x_g and the blank signal x_0 multiplied by a calibration factor w with their respective standard uncertainties $u(x_g)$, $u(x_0)$ and $u(w)$.

$$y = (x_g - x_0) \cdot w \quad (44)$$

Then the standard uncertainty $u(y)$ associated with y is given by

$$u^2(y) = w^2 \cdot (u^2(x_g) + u^2(x_0)) + y^2 \cdot u_{rel}^2(w) \quad (45)$$

with $u_{rel}(w) = u(w)/w$.

The minimum information requirement to allow for the calculation of the decision threshold and the detection limit is that the experiment was successfully performed at least one time each for the gross and the background measurements. This means that x_g, $u(x_g)$, x_0, $u(x_0)$, w and $u(w)$ are available. In particular, it is not needed for the following that x_g and x_0 result from a Poisson process.

For $\eta = 0$, one expects $x_g = x_0$ and obtains with Equation 45 $\tilde{u}(0) = 2 \cdot u(x_0)$. Then, the decision threshold is calculated by;

$$y^* = k_{1-\alpha} \cdot w \cdot \sqrt{2} \cdot u(x_0). \quad (46)$$

If no further information on the measurement procedure and on $\tilde{u}(\eta)$ is given, the detection limit can only be calculated using the interpolation formula (Equation 18) and obtains an explicit formula for the detection limit (Equations 19 and 20). Note, however, that the explicit formula for the detection limit is only an approximation, which works best if $y \approx\geq 2y^*$.

A special case of the model of Equation 44 is that of ratemeter measurements where a net count rate value ($r_g - r_0$) as the difference of a gross count rate value r_g and a background count rate value r_0 multiplied by a calibration factor w is used, but where the standard uncertainties cannot be calculated as $u(x_g) = x_g/t_g$ and $u(x_0) = x_0/t_0$.

Ratemeter measurments

A ratemeter is understood, here, as an analogue/digital working count rate measuring instrument where the output signal increases sharply (with a negligible rise time constant) upon the arrival of an input pulse and then decreases exponentially with a relaxation time constant τ until the next input pulse arrives. The signal increase must be the same for all pulses and the relaxation time constant must be independent of the count rate. A digitally working count rate measuring instrument simulating the one just described is also taken as a ratemeter that has to be considered here.

Each particular measurement using a ratemeter must be carried out in the stationary state of the ratemeter. This requires at least a sufficiently fixed time span between the start of measurement and reading the ratemeter indication. This applies to each sample and to each background effect measurement. According to Ref. (33), fixed time spans of 3τ or 7τ correspond to deviations of the indication by 5% or 0.1% of the magnitude of the difference between the indication at the start of measurement and that at the end of the time span. If further uncertain influences have to be taken into account, then a time span of, at least, 7τ should be chosen, if possible.

The expectation values ρ_g and ρ_0 of the output signals of the ratemeter in the cases of measuring the gross and background effects, respectively, are taken as the input quantities X_1 and X_2 for the calculation of the characteristic limits; $X_1 = \rho_g$ and $X_2 = \rho_0$. With the values r_g and r_0 of the output signals determined at the respective moments of measurement, the following approaches result for the values of the input quantities and the associated standard uncertainties:

$$y = (x_g - x_0) \cdot w \quad (47)$$

with

$$x_1 = r_g;\ x_2 = r_0;\ u^2(x_1) = \frac{r_g}{2\tau_g};\ u^2(x_2) = \frac{r_0}{2\tau_0}. \quad (48)$$

In Equation 48, approximations with a maximum relative deviation of 5% for $r_g\tau_g \geq 0.65$ and of 1% for $r_g\tau_g \geq 1.32$ are specified according to Ref. (33). The same applies to $r_0\tau_0$. The relaxation time constants τ_g and τ_0 have to be adjusted accordingly.

The ratemeter measurement is equivalent to a counting measurement with time pre-selection as given (Equation 37) and with the measurement durations $t_g = 2\tau_g$ and $t_0 = 2\tau_0$. The quotients n_g/t_g and n_0/t_0 of the counting measurement have to be replaced here by the measured count rate values r_g and r_0, respectively, of the ratemeter measurement. This applies, in particular, to Equation 39. The standard uncertainties of the relaxation time constants do not appear in the equations and are, therefore, not needed.

For the model specified in the form of Equation 47, Equation 48 leads to

$$u^2(y) = w^2 \cdot \left(\frac{r_g}{2\tau_g} + \frac{r_0}{2\tau_0}\right) + (r_g - r_0)^2 \cdot u^2(w). \quad (49)$$

Replacing y by η and eliminating $r_g = \eta/w + r_0$ yields

$$\tilde{u}^2(\eta) = w^2 \cdot \left[\frac{\eta}{2\tau_g \cdot w} + r_0 \cdot \left(\frac{1}{2\tau_g} + \frac{1}{2\tau_0}\right)\right] + \eta^2 \cdot u^2_{rel}(w) \quad (50)$$

and one obtains the decision threshold

$$y^* = k_{1-\alpha} \cdot w \cdot \sqrt{r_0 \cdot \left(\frac{1}{2\tau_g} + \frac{1}{2\tau_0}\right)} \quad (51)$$

and the detection limit

$$\eta^* = y^* + k_{1-\beta} \cdot \sqrt{\begin{array}{c} w^2 \cdot \left[\frac{\eta^*}{2\tau_g \cdot w} + r_0 \cdot \left(\frac{1}{2\tau_g} + \frac{1}{2\tau_0}\right)\right] \\ + \eta^{*2} \cdot u^2_{rel}(w) \end{array}} \quad (52)$$

Spectrometric measurements

This procedure can also be applied to counting spectrometric measurements when a particular line in a measured multi-channel spectrum has to be considered and no adjustment calculations, for instance an unfolding, have to be carried out. The net intensity of the line is first determined by separating the background. Then, if another measurand, for instance an activity, has to be calculated, one has to proceed as described for the models according to Equation 29, in particular, to calculate $\tilde{u}(\eta)$ according to Equation 34.

Independent Poisson-distributed random variables N_i ($i = 1, \ldots, m$ as well as $i =$ g) are assigned to selected channels of a measured multi-channel spectrum—if necessary, the channels of a channel region of the spectrum can be combined to form a single channel—with the contents n_i of the channels (or channel regions), and the expectation values of the N_i are taken as input quantities X_i. In the following, ϑ_i is the lower and ϑ'_i is the upper limit of channel i; ϑ is, for instance, the energy or time or another continuous scaling variable assigned to the channel number. The channel widths $t_i = \vartheta'_i - \vartheta_i$ correspond to t. Thus, $X_i = \rho_i t_i$ with the mean spectral density ρ_i in channel i and $x_i = n_i$ is an estimate of X_i with the squared standard uncertainty $u^2(x_i) = n_i$ associated with x_i. For $i =$ g, the quantities n_g and $X_g = \rho_g \cdot t_g$ represent the combined channels of a line of interest

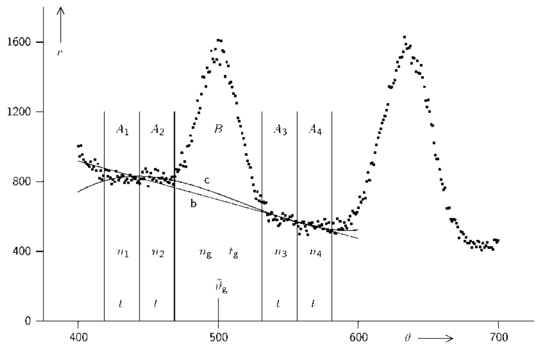

Figure 5. Section of a multi-channel spectrum, recorded using a NaI detector, with the background shapes calculated according to cases (b) and (c).

in the spectrum. The measurand Y with the true value η is the net intensity of the line, i.e. the expectation of the net content of channel i = g (region B, Figure 5).

At first, the background of the line of interest must be determined, which also includes the contributions of the tails of disturbing lines. A suitable function $H(\vartheta, a_1,\ldots,a_m)$, representing the spectral density of the line background with the parameters a_k, is introduced so that

$$n_i = \int_{\vartheta_i}^{\vartheta_i'} H(\vartheta; a_l, \ldots, a_m)\mathrm{d}\vartheta; \; (i = l, \ldots, m) \quad (53)$$

from which the a_k have to be calculated as functions of the n_i. The background contribution to the line is then

$$z_0 = \int_{\vartheta_g}^{\vartheta_g'} H(\vartheta; a_l, \ldots, a_m)\mathrm{d}\vartheta. \quad (54)$$

The random variable Z_0, associated with the background contribution z_0, implicitly is a function of the input quantities X_i because z_0 is calculated from the $x_i = n_i$. The model approach for the measurand Y reads

$$y = G(X_g, X_l, \ldots, X_m) = X_g - Z_0 \quad (55)$$

from which

$$y = n_g - z_0; \; u^2(y) = n_g + u^2(z_0);$$
$$u^2(z_0) = \sum_{i=1}^{m} \left(\sum_{k=1}^{m} \frac{\partial z_0}{\partial a_k} \frac{\partial a_k}{\partial n_i} \right)^2 n_i \quad (56)$$

follow. The bracketed sum equals $\partial z_0/\partial n_i$. For the calculation of the function $\tilde{u}(\eta)$, the net content η of channel g is first specified. Then, y in Equation 56 is replaced by η. This allows n_g to be eliminated, which is not available if η is specified. This results in $n_g = \eta + z_0$ and

$$\tilde{u}^2(\eta) = \eta + z_0 + u^2(z_0). \quad (57)$$

The characteristic limits according to Section 6 then follow from Equations 56 and 57.

If the approach

$$H(\vartheta) = \sum_{k=1}^{m} \alpha_k \cdot \psi_k(\vartheta). \quad (58)$$

linear in the a_k is applied with given functions $\psi_k(\vartheta)$, then Equation 53 represents a system of linear equations for the a_k. Thus, the a_k depend linearly on the n_i and the partial derivatives in Equation 56 do not depend on the n_i. Then,

$$u^2(z_0) = \sum_{i=1}^{m} b_i^2 \cdot n_i \quad (59)$$

with quantities b_i not depending on the n_i. Equation 59 also follows when the background contribution z_0 to the line is calculated linearly from the channel contents n_i with suitably specified coefficients b_i:

$$z_0 = \sum_{i=1}^{m} b_i \cdot n_i. \quad (60)$$

Depending on the background shapes, the approach given in Equations 56–60 has different applications. If events of a single line with a known location in the spectrum are to be detected, then the following cases of the background shape as a function of ϑ and the associated approaches have to be distinguished;

(a) Constant background: approach $H(\vartheta) = a_1$ (constant, $m = 1$)
(b) Linear background, which can often be assumed with gamma radiation: approach $H(\vartheta) = a_1 + a_2\vartheta$ (straight line, $m = 2$)
(c) Weakly curved background with disturbing neighbouring lines: approach $H(\vartheta) = a_1 + a_2\vartheta + a_3\vartheta^2 + a_4\vartheta^3$ (cubic parabola, $m = 4$)
(d) Strongly curved background, which can be present with strongly overlapping lines, for instance, with alpha radiation: approach according to Equation 58.

In cases (a), (b) and (c), the scaling variable ϑ is required to be linearly assigned to the channel number.

In cases (a) and (b), it is suitable for the background determination to introduce three adjacent channel regions A_1, B and A_2 in the following way.

Region B comprises all the channels belonging to the line and has the total content n_g and the width t_g.

If the line shape can be assumed as a gaussian curve with the full width h at half maximum, then region B has to be placed as symmetrically as possible over the line. The following should be chosen;

$$t_g \approx 2,5h \tag{61}$$

if fluctuations of the channel assignment cannot be excluded or the background does not dominate, for instance, with pronounced lines. In case of a dominant background, the most favourable width

$$t_g \approx 1,2h \tag{62}$$

has to be specified for region B. This region then covers approximately the portion $f = 0.84$ of the line area. In general, $f = 2 \cdot \Phi(v\sqrt{2\ln 2}) - 1$, if $t_g = v \cdot h$ with a chosen factor v.

In principle, the full width h at half maximum has to be determined from the resolution of the measuring system or under the same measurement conditions by means of a reference sample emitting the line to be investigated strongly enough, or from neighbouring lines with comparable shapes and widths. Region B must comprise an integer number of channels, so that t_g has to be rounded up accordingly.

Regions A_1 and A_2, bordering region B below and above, have to be specified with the same widths $t = t_1 = t_2$ in case (b) only. The total width $t_0 = t_1 + t_2 = 2t$ has to be chosen as large as possible but at most so large that the background shape over all regions can still be taken as approximately constant [case (a)] or linear [case(b)]. n_1 and n_2 are the total contents of all channels of regions A_1 and A_2, respectively. Moreover, $n_0 = n_1 + n_2$.

Hence follows for cases (a) and (b):

$$z_0 = c_0 \cdot n_0;\; u^2(z_0) = c_0^2 = c_0^2 \cdot n_0;\; c_0 = t_g/t_0. \tag{63}$$

$\tilde{u}^2(\eta)$ follows from Equation 57.

Instead, in case (c), five adjacent channel regions A_1, A_2, B, A_3 and A_4 have to be introduced in the way described above with the same widths t of the regions A_i (Figure 5). With the sum $n_0 = n_1 + n_2 + n_3 + n_4$, i.e. the total content of all channels of regions A_i, with their total width $t_0 = 4t$ and with the auxiliary quantity $n_0' = n_1 - n_2 - n_3 + n_4$, the following is then valid:

$$\begin{aligned} z_0 &= c_0 \cdot n_0 - c_1 \cdot n_0'; \\ u^2(z_0) &= (c_0^2 + c_1^2) \cdot n_0 - 2c_0 \cdot c_1 \cdot n_0'; \\ c_0 &= t_g/t_0; \\ c_1 &= c_0 \cdot (4/3 + 4c_0 + 8c_0^2/3)/(1 + 2c_0) \end{aligned} \tag{64}$$

and $\tilde{u}^2(\eta)$ follows from Equation 57. Two numerical examples of case (c) are treated in Refs (23) and (24).

In case (d), m adjacent regions A_i have to be introduced in the same way, with approximately half of them arranged below and above region B. The regions A_i need not have the same widths. The power functions ϑ^{k-1} have to be chosen to some extent as above as the functions $\psi_k(\vartheta)$. For the same purpose, the functional shapes of the disturbing neighbouring lines that have to be considered should also be chosen as far as possible and known. Then, $\tilde{u}^2(\eta)$ again follows from Equation 57. Detailed advice on obtaining the regions for determining the background may be found elsewhere[23,24].

After $\tilde{u}^2(\eta)$ has been calculated in all cases according to Equation 57, the characteristic limits result with Equations 14 and 16.

FURTHER APPLICATIONS

The procedure described here is so general that it allows a large variety of applications to similar measurements. Some important cases were treated above in detail. Many other applications do not differ in their models from those explicitly given here, but merely in the interpretation of the input quantities X_1 and X_2 and in setting up the corresponding estimates x_1 and x_2 and standard uncertainties $u(x_1)$ and $u(x_2)$.

Independent of the application, the main task consists of determining the primary measurement result y of the measurand and the associated standard uncertainty $u(y)$ as well as the standard uncertainty $\tilde{u}(\eta)$ as a function of the measurand. Subsequently, with all applications, the decision threshold y^*, the detection limit η^*, the confidence limits η_l and η_u and the best estimate z of the measurand with the associated standard uncertainty $u(z)$ can be calculated according to Equations 14, 16, 21–23.

Numerical examples are given in Refs (18, 23, 24, 35, 36). Further applications of the approach presented in this paper are described elsewhere:

- Albedo dosemeters[9];
- Counting measurements on moving objects[11,17];
- Repeated counting measurements with random influences[23,24];
- Counting measurements on filters during accumulation of radioactive materials[16];
- Alpha spectrometry[23,24];
- Unfolding in spectrometric measurements[10,19,37].

CONCLUSIONS

With the GUM there exists an internationally accepted, standardised procedure for the determination of measurement uncertainties.

With standard uncertainties according to the GUM, characteristic limits can be calculated for any measurement procedure according to DIN 25482-10 and ISO 11929-7.

The procedures described in this paper and in Refs (23, 24) provide a basis for the revision of DIN 25481 Parts 1–7 (except Part 4) and ISO 11929 Parts 1–4. With revised standards DIN 25482 and ISO 11929, a consistent standardisation of the calculation of characteristic limits will be provided, covering an extremely wide range of models.

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