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Klaus Weise

Bayesian-statistical decision threshold, detection limit, and confidence interval in nuclear radiation measurement

When a contribution of a particular nuclear radiation is to be detected, for instance, a spectral line of interest for some purpose of radiation protection, and quantities and their uncertainties must be taken into account which, such as influence quantities, cannot be determined by repeated measurements or by counting nuclear radiation events, then conventional statistics of event frequencies is not sufficient for defining the decision threshold, the detection limit, and the limits of a confidence interval. These characteristic limits are therefore redefined on the basis of Bayesian statistics for a wider applicability and in such a way that the usual practice remains as far as possible unaffected. The principle of maximum entropy is applied to establish probability distributions from available information. Quantiles of these distributions are used for defining the characteristic limits. But such a distribution must not be interpreted as a distribution of event frequencies such as the Poisson distribution. It rather expresses the actual state of incomplete knowledge of a physical quantity. The different definitions and interpretations and their quantitative consequences are presented and discussed with two examples. The new approach provides a theoretical basis for the DIN 25482-10 standard presently in preparation for general applications of the characteristic limits.

Bayes-statistische Erkennungsgrenze, Nachweisgrenze, und Vertrauensbereich bei Kernstrahlungsmessungen. Wenn ein Beitrag einer bestimmten Kernstrahlung nachgewiesen werden soll, z.B. eine fragliche Linie in einem Spektrum zum Zwecke des Strahlenschutzes, und auch Größen und deren Unsicherheiten berücksichtigt werden müssen, die wie Einflußgrößen nicht durch mehrmalige Messung oder durch Zählung von Kernstrahlungsereignissen ermittelt werden können, reicht die konventionelle Statistik von Ereignishäufigkeiten nicht aus, um die Erkennungsgrenze, die Nachweisgrenze und die Grenzen eines Vertrauensbereichs festzulegen. Diese charakteristischen Grenzen werden deshalb auf der Grundlage der Bayesschen Statistik für umfassendere Anwendung neu definiert, und zwar so, daß Auswirkungen auf die bisherige Praxis möglichst gering bleiben. Das Prinzip der maximalen Entropie wird angewendet, um aus vorliegender Information Wahrscheinlichkeitsverteilungen zu gewinnen, deren Quantile für die Definitionen der charakteristischen Grenzen benutzt werden. Eine solche Verteilung darf allerdings nicht wie die Poisson-Verteilung als Verteilung von Ereignishäufigkeiten aufgefaßt werden, sondern sie drückt den aktuellen Stand der unvollständigen Kenntnis über eine physikalische Größe aus. An Hand zweier Beispiele werden die unterschiedlichen Definitionen und Interpretationen und deren quantitative Auswirkungen erläutert und diskutiert. Der neue Zugang bildet die theoretische Grundlage für die z.Z. in Arbeit befindliche Norm DIN 25482-10 für allgemeine Anwendungen der charakteristischen Grenzen.

1 Introduction

The DIN 25482 series of German standards [1–7] (and the corresponding ISO 11929-1 to -6 standards at present in preparation) to be applied in radiation monitoring and protection, provides procedures to stipulate the decision threshold (formerly called the limit of decision), the detection limit, and the limits of a confidence interval in nuclear radiation measurement. DIN 25482-1 [1] is the basic standard of this series. It deals with the important basic case of detecting a potential net radiation contribution of a sample by comparing the results of counting measurements of the zero effect and of the gross effect, the latter being the sum of the sample and zero effects (Sect. 4). In DIN 25482-6 [6], the influence of sample treatment is additionally taken into account. DIN 25482-3 [3] is related to ratemeter measurements, and DIN 25482-2 [2], -4 [4], and -5 [5] to counting spectrometric measurements in simple cases of spectral line detection in a multichannel spectrum of alpha and gamma radiation. DIN 25482-7 [7] deals with counting measurements involving

flowing media and using monitors equipped with filters for the accumulation of radioactive materials during the measurement. It is based on a theory developed in Ref. [8].

The decision threshold and the detection limit serve to assess detection possibilities on the basis of statistical procedures and given error probabilities. The *decision threshold* allows to decide whether or not a „sample" has made a contribution to registered nuclear radiation events or, expressed in other words, whether or not a positive value of the measurand, the physical quantity in question, follows from a measurement. In counting non-spectrometric measurements of nuclear radiation, this measurand is, for instance, an activity which is the net effect following from a gross effect measurement with the sample and a reference or zero effect measurement [1]. In a series of counting measurements on filters during accumulation of radioactive materials, the contribution of the sample, the measurand, consists in a change of the specific activity of the medium flowing through the filter [7, 8]. In spectrometric measurements, for instance, of alpha or gamma radiation, the „sample" may be a spectral

line in a measured spectrum [2, 4, 5]. The *detection limit* is the smallest potential contribution, that is, the smallest positive value of the measurand, which can be detected by a *measurement procedure* intended to be applied. It makes it possible to decide whether or not the measurement procedure complies with present requirements and thus is suitable for the purpose assigned to the measurement in question. To this end, the detection limit is compared with a given *standard value* following from requirements to be met by a measurement procedure on scientific, legal, or other grounds. The measurement procedure will be unsuitable if the detection limit exceeds the standard value. In contrast, a measurement result obtained for a measurand by an evaluation of the measurement data, for instance by a spectrum unfolding, must be compared with the decision threshold. If a contribution of the „sample" is detected, the *confidence interval* will contain the measurand value with a given probability, the *confidence level* [9, 10] (Sect. 3). The confidence interval is enclosed by the *confidence limits*.

All the present standards of the DIN 25482 series are based on conventional statistics because in most cases only counting measurements of nuclear radiation are considered. Accordingly, it is possible and adequate to assume Poisson distributions of the frequencies of radiation events registered. In DIN 25482-6 [6], an influence quantity due to the effect of sample treatment is taken into account and, therefore, a negative binomial distribution of the event frequency can be and is assumed. A more complex distribution of the fluctuating indication of a linear analog ratemeter is used in DIN 25482-3 [3] and derived in Ref. [11]. In general spectrometry, a spectrum unfolding must often be carried out to obtain the measurand in question, for instance, a spectrum parameter such as the net intensity of a spectral line. This problem is dealt with in Ref. [12] to provide a theoretical basis for a future standard of the DIN 25482 series dealing with spectrum unfolding. In treating this problem, incompletely known physical quantities must be considered which in repeated measurements do not behave randomly – these might be, for example, influence quantities – or for which distributions of values encountered in measurements many times repeated are unknown and cannot be assumed or obtained. An approach to this problem has recently been attempted by the author [12], applying DIN 1319-4 [14] and the *Guide to the expression of uncertainty in measurement* [9] and using estimates and associated uncertainties of those quantities. In this Guide, uncertainties are evaluated either by „statistical methods" (type A) or by „other means" (type B), i.e. by methods of either conventional statistics or Bayesian statistics. The uncertainties are then combined regardless of their origin. This is common practice and can be accepted as an adequate first approximation, but is not satisfactory from the theoretical point of view. This was the incentive to establish a Bayesian theory of measurement uncertainty [10] in which the type A and type B methods are unified and identified with the methods of Bayesian statistics. In addition, the principle of maximum entropy is used to establish probability distributions of estimators assigned to the physical quantities. But such a distribution must not be interpreted as that of values which occur or are assumed to occur in repeated or counting measurements. Instead, based on the information actually available, it quantitatively expresses the actual state of incomplete knowledge of the physical quantities involved. It is a degree of belief in the sense of the probability $1/2$ assigned to each of the two sides of a coin *before* tossing it.

For the purpose of including information which cannot be regarded as obtained from repeated or counting measure-

ments, we redefine the decision threshold, the detection limit, and the confidence limits in a general way on the basis of Bayesian statistics (Sect. 3) using also the Bayesian theory of measurement uncertainty [10] (Sect. 5). In this paper, we summarily call them the *characteristic limits* and define them in as close agreement with the usual definitions as possible so that no essential changes will be necessary in practice. The new approach however has a wider applicability and is more satisfying from the theoretical point of view. The different definitions and interpretations and their quantitative consequences are demonstrated and discussed with two examples. One of these is the important basic, but not easy to handle case of counting measurements dealt with in DIN 25482-1 [1]. In Sect. 4, we apply both statistics to it. The characteristic limits are also redefined to provide a theoretical foundation for the new, basic DIN 25482-10 standard presently in preparation. This standard is intended for the general application to a large variety of problems and procedures dealing with the characteristic limits in nuclear radiation measurement so that no need remains to establish an own standard for each of those cases.

Bayesian statistics has already been used by Miller et al. [15] to define the decision threshold (they call it the „critical level"). They do not use the principle of maximum entropy to establish probability distributions but make reasonable assumptions on these. As the authors themselves point out, their definition is essentially different from the conventional-statistical definition and thus gives quite different numerical values for the decision threshold (Sect. 3).

2 Elements of probability theory

A short overview of the needed basic elements of probability theory is given here. For more details of the concepts and fundamentals of probability theory and statistics, see the standards or a textbook on these subjects, for instance, Refs. [16–18].

Conventional statistics and *Bayesian statistics* [19, 20] are both based on probability theory, but they differ in their understanding of the *probability* $\Pr(A)$ of a *(random) event* A which may or may not occur in an experiment carried out under well-defined conditions $(0 \leq \Pr(A) \leq 1)$. The experiment could, for example, simply consist in tossing a coin. In conventional (frequency) statistics, $\Pr(A)$ is interpreted as the relative frequency with which A will occur or is assumed to occur if the experiment is or was many times repeated independently under the same nominal conditions. In Bayesian (sometimes also called subjective) statistics, $\Pr(A)$ expresses the degree of belief, based on information actually available, that A will happen in the experiment *before* the experiment is carried out or its outcome is noticed. In fact, this is the classical meaning of probability introduced by Bernoulli and Laplace [21]. $\Pr(A)$ must be understood as, for instance, the probability $1/2$ assigned to the event $A = \{„head"\}$ before tossing a coin. We also introduce the *conditional probability* $\Pr(A \mid B)$, the probability of the random event A under the additional condition that event B has already occurred or will occur or is assumed to occur. The relationship

$$\Pr(A \mid B) \Pr(B) = \Pr(B \mid A) \Pr(A) = \Pr(AB) \tag{1}$$

is called the *Bayes theorem*. AB denotes the event „A and B". Events A and B are *independent* if $\Pr(A \mid B) = \Pr(A)$. If A and B of AB are explicitly described by formulae, e.g. $A =$

$\{X < 1\}$, we seperate these by a semicolon and omit the brackets: e.g. $\Pr(X < 1; Y = 0)$. The *expansion theorem*

$$\Pr(A) = \sum_i \Pr(A \mid B_j) \Pr(B_j) \tag{2}$$

is valid if exactly one of the events B_j occurs in the experiment. The sum may also be an integral if $\Pr(B_j)$ is proportional to a differential increment dz of any integration variable z replacing j as in Eqs. (3) and (4) below.

When the experiment is carried out, a real *random variable* X (or $\hat{x}$) assumes one of its potential *values*, a real number (times an appropriate unit). $F_X(x) = \Pr(X \le x)$ is the *(cumulative) distribution function* of X, the variable x representing an arbitrary value. The probability of the random event $A = \{X \le x\}$ may be a conditional one: the conditional distribution function is then denoted by $F_X(x \mid B)$ with a particular event B. A distribution function is single-valued and non-decreasing. At every abscissa x, it is either continuous, or it has a step there and is continuous from the right. i.e. from values larger than x. The number of steps is either finite or countably infinite. The random variable X is *discrete* if it can assume only discrete values x_j with $p_X(x_j) = \Pr(X = x_j) > 0$, in which $p_X(x_j)$ is the *probability function* of X. Then, $F_X(x) = \sum_j p_X(x_j)$ for $x_j \le x$. For example, the random variable assigned to the number of counted nuclear events of a particular kind is discrete. X is *continuous* if there is a non-negative function $f_X(x)$, the *probability density* of X, with the property $F_X(x) = \int_{-\infty}^{x} f_X(z)\,dz$. Then, $f_X(x)\,dx = dF_X(x) = \Pr(x - \frac{1}{2}dx < X \le x + \frac{1}{2}dx)$. Either of a distribution function, a probability function or density is also briefly referred to as a *distribution*.

The *expectation value* $\mathrm{E}G(X)$ of a function $G(X)$ of a random variable X is defined by

$$\mathrm{E}G(X) = \int G(x)\,dF_X(x). \tag{3}$$

In particular for discrete or continuous X we only deal with,

$$\mathrm{E}G(X) = \sum_j G(x_j)\,p_X(x_j) \text{ or } \mathrm{E}G(X) = \int G(x) f_X(x)\,dx. \tag{4}$$

respectively. The *non-central second-order moment* $\mathrm{E}(X - x_0)^2$ of X with respect to a particular value x_0 assumes for $x_0 = \mathrm{E}X$ its minimum value $\mathrm{Var}\,X = \mathrm{E}(X - \mathrm{E}X)^2$, the *variance* of X, the square root of which is called the *standard deviation* $\sigma(X)$. $\varphi_X(\omega) = \mathrm{E}\exp(i\omega X)$ is the *characteristic function* of X. The random variable X or its distribution is *standardized* if $\mathrm{E}X = 0$ and $\mathrm{Var}\,X = 1$.

A value x_η is a *quantile* of X for a given probability η if $\Pr(X < x_\eta) \le \eta$ and $\Pr(X \le x_\eta) = F_X(x_\eta) \ge \eta$. The two conditions are needed if $F_X(x)$ has a step at the abscissa $x = x_\eta$. Otherwise, $F_X(x_\eta) = \eta$. It can happen that $F_X(x) = \eta$ for all x of an interval. Then we choose as x_η either the lower or the upper interval limit. With the latter choice, we denote the quantile by $\bar{x}_\eta$. In all other cases, this quantile is identical to x_η. The particular quantile of the standardized normal distribution $f_X(x) = \exp(-\frac{1}{2}x^2)/\sqrt{2\pi}$ is denoted by k_η and obeys the relationship $k_{1-\eta} = -k_\eta$.

We always use a lower case letter to denote a value of a random variable, and we denote this random variable either by the same letter with a hat ($\hat{\ }$) or by the corresponding upper case letter. For brevity and convenience, we then can in many cases omit the symbol of the random variable, briefly describe random events such as $\{X = x\}$ or $\{x - \frac{1}{2}dx < X \le x + \frac{1}{2}dx\}$ by x, and use abbreviations such as

$$f(x \mid \xi) = p_X(x \mid \hat{\xi} = \xi) = \Pr(X = x \mid \hat{\xi} = \xi);$$

$$f(x \mid \xi) = f_X(x \mid \hat{\xi} = \xi) = \Pr\left(x - \frac{1}{2}dx < x \le x + \frac{1}{2}dx \mid \hat{\xi} = \xi\right) / dx \tag{5}$$

for probability functions and densities. f acts more as an operator than as a function: f(x) and f(y) are in general different functions! Therefore f is written *upright*. Using f, the Bayes and expansion theorems according to Eqs. (1) and (2) read

$$f(x \mid \xi)\, f(\xi) = f(\xi \mid x)\, f(x) = f(x; \xi); \tag{6}$$

$$f(x) = \int f(x \mid \xi)\, f(\xi)\, d\xi. \tag{7}$$

Here, the integral must be replaced by a sum if $\hat{\xi}$ is discrete.

To derive the probability density $f(y)$ of a function $Y = G(X_1, X_2, \ldots)$ of several continuous random variables X_i with their joint probability density $f(x_1; x_2; \ldots)$ and using the Dirac delta function $\delta(y - z)$ with $\delta(y - z) = 0$ for $y \ne z$ and $\int(y - z)\,dy = 1$, the *Markov formula* can be applied:

$$f(y) = \int \delta(y - G(x_1, x_2, \ldots))\, f(x_1; x_2; \ldots)\, dx_1\, dx_2 \cdots. \tag{8}$$

This equation is a special case of Eq. (7) with x replaced by y, ξ by the x_i, and $f(x \mid \xi)$ by the delta function according to the functional relationship involved. A formula similar to Eq. (8) is valid for discrete random variables X_i and Y with the Kronecker symbol $\delta_{y,z}$ with $\delta_{y,z} = 0$ for $y \ne z$ and $\delta_{y,z} = 1$ for $y = z$:

$$f(y) = \sum_{x_1, x_2, \ldots} \delta_{y, G(x_1, x_2, \ldots)}\, f(x_1; x_2; \ldots). \tag{9}$$

In this sum, every summation variable x_i is understood to assume all the potential values x_{ij} of the random variable X_i, and $f(x_1; x_2; \ldots)$ is the joint probability function of the variables X_i. The random variables X_i are *independent* if $f(x_1; x_2; \ldots) = f(x_1) f(x_2) \cdots$. We call an operation according to Eqs. (8) or (9) a *folding* when, in particular, the random variables X_i are independent and $Y = G(X_1, X_2, \ldots) = \sum_i a_i X_i$ with constant coefficients a_i. Then,

$$\mathrm{E}Y = \sum_i a_i\, \mathrm{E}X_i; \qquad \mathrm{Var}\,Y = \sum_i a_i^2\, \mathrm{Var}\,X_i;$$

$$\ln \varphi_Y(\omega) = \sum_i \ln \varphi_{X_i}(a_i \omega). \tag{10}$$

The *principle of maximum entropy* [22] can be used to establish the distribution $f(x \mid a)$ of a random variable X. It consists in maximizing the *(information) entropy*

$$S = -\int_G f(x \mid a) \ln(f(x \mid a) / f(x))\, dx = \max \tag{11}$$

observing the normalization condition and the constraints $\mathrm{E}G_i(X) = a_i$ with given functions $G_i(X)$ and data a_i summarily denoted by a. The entropy S is a measure of the probability of the distribution $f(x \mid a)$ which is itself taken as a random function. The principle of maximum entropy is ultimately based on the principle of assigning uniform probabilities to equally possible states of the same kind because of symmetry considerations. The integral must be replaced by a sum if X is discrete. G is the region of integration where the *prior* $f(x)$ of X is positive. The prior is the distribution of X before the data a_i are available. It may either be given, or set constant in G if it is not given, expressing that every value $x \in G$ is equally likely. It can sometimes be derived from invariance considerations, for instance, a prior const/ν for the parameter $\nu > 0$ of a Poisson distribution. taken as a random variable [23] (Sect. 4.1). The prior may be unnormalizable.

This property only indicates insufficient prior information to determine the expectation value of any function of X. With the well-known Lagrange method, the solution of the maximization problem is

$$f(x \mid a) = C f(x) \exp\left(-\sum_i \beta_i G_i(x) \right) \tag{12}$$

with the normalization constant C and Lagrange multipliers β_i which must be calculated from the data a and the constraints. $f(x \mid a)$ vanishes outside G.

In statistical tests of *hypotheses*, statements to be proved true or false, an *error of the first kind* results if a true hypothesis is rejected. Similarly, an *error of the second kind* results if a false hypothesis is accepted. The given probabilities of the errors of the first and second kind are denoted by α and β. The given *confidence level* of a *confidence interval* is denoted by $1 - \gamma$. The different meanings of the confidence level in Bayesian and conventional statistics are described in Sect. 3.

3 Definitions of the characteristic limits

An experiment, which may consist of a single measurement or a series of measurements independently repeated under the same nominal conditions, is carried out to determine the unknown *(true) value* of a *measurand*, a physical quantity involved (or, similarly, the values of several measurands). To estimate the (true) measurand value from the data obtained by the experiment or from elsewhere, a random variable $\hat{\xi}$ is assigned to the measurand and called an *estimator*. A particular value ξ of the estimator $\hat{\xi}$ is an *estimate* of the measurand. The *measurement result* of the measurand is such an estimate evaluated from the data and other given relevant information on the measurand.

In Bayesian statistics, the distribution $f(\xi \mid x; y)$ of the estimator $\hat{\xi}$ expresses the actual state of incomplete knowledge of the measurand, the degree of belief that a particular value ξ of the estimator $\hat{\xi}$ is the measurand value to be determined. This distribution is uniquely established using the principle of maximum entropy and only the data actually available and the other given information summarily denoted by x; y (example in Sect. 5). Known, more basic frequency distributions such as Poisson distributions of radiation events registered may also be part of the information and may already be sufficient for establishing the distribution of the estimator $\hat{\xi}$ using the Bayes theorem so that the principle of maximum entropy need not be applied [10, 15] (example in Sect. 4). The expectation value $E\,\hat{\xi}$ is taken and calculated as the best estimate of the measurand value, as far as the present data and information are considered, because the non-central second-order moment $E(\hat{\xi}-\xi_0)^2$ with respect to an estimate ξ_0 assumes its minimum value for $\xi_0 = E\,\hat{\xi}$. The square root of this moment serves as the measurement uncertainty $u(\xi_0)$ (of the measurand) associated with the estimate ξ_0. The best estimate $E\,\hat{\xi}$ is then taken as the measurement result of the measurand, and the standard deviation $\sigma(\hat{\xi})$ as the *standard uncertainty* associated with the measurement result [9, 10, 13, 14]. Moreover, the interval $E\,\hat{\xi} - \sigma(\hat{\xi}) \leq \xi \leq E\,\hat{\xi} + \sigma(\hat{\xi})$ contains the estimates of the measurand which are reasonable considering the measurement uncertainty [9, 13, 14]. This interval should not be confused with the confidence interval.

Let $\hat{\xi}$ be the estimator of a non-negative measurand of interest such as the activity of a sample. The measurand value zero means that the physical effect represented by the measurand is absent. This event, denoted by $H_0 = \{\hat{\xi} = 0\}$, will be our hypothesis when we establish the decision threshold.

For the definition of the decision threshold and the detection limit, we also introduce the probability distribution $f(x \mid \xi; y)$ of a random variable X. We call X the *decision variable*. It should preferably be defined such that $E\,X = \xi$, at least for H_0. Its distribution expresses the degree of belief that a particular value x of X will be obtained in the experiment to be carried out if ξ is the measurand value. y is a given datum obtained from a reference experiment already performed. It is also taken as a value of a random variable Y related to the decision variable X if H_0 holds true, for instance, $Y = X$. The Bayes theorem $f(x \mid \xi; y)\ f(\xi; y) = f(\xi \mid x; y)\ f(x; y) = f(\xi; x; y)$ similar to Eq. (6) establishes a relationship between the two distributions $f(\xi \mid x; y)$ and $f(x \mid \xi; y)$ mentioned. In this equation, y serves as a parameter only, and $f(x; y)$ and $f(\xi; y)$ are the distributions of the decision variable X and the estimator $\hat{\xi}$ after the reference experiment has been carried out. These distributions are priors with respect to the experiment in question. When $f(\xi; x; y)$ follows from general information and considerations on the experiments and the measurand, the distributions $f(x \mid \xi; y)$ and $f(\xi \mid x; y)$ can be obtained from the above stated Bayes theorem by normalization with respect to X or $\hat{\xi}$, respectively. The priors then act as normalization constants. When nothing is known except that the measurand is non-negative, priors may be set constant. A prior for $\hat{\xi}$ vanishes for $\xi < 0$. Priors may be unnormalizable and then indicate that the information is not sufficient for obtaining a reasonable estimate of the measurand before the measurements are performed.

We are able now to define the decision threshold, the detection limit, and the confidence limits (Fig. 1):
- The decision threshold x^* is the quantile $x_{1-\alpha}$ of the distribution $f(x \mid \xi; y)$ with the hypothesis H_0. – Then, $\Pr(X > x^* \mid \hat{\xi} = 0; y) \leq \alpha$. If a value x of the decision variable X, obtained in the present or a later experiment, exceeds the decision threshold x^*, i.e. if $x > x^*$, we will decide that the physical effect in question is present, and we will reject our hypothesis H_0.
- The detection limit ξ^* is the minimum value ξ if the decision threshold x^* equals the quantile $\tilde{x}_\beta$ of the distribution $f(x \mid \xi; y)$. – Then $\Pr(X \leq x^* \mid \hat{\xi} = \xi^*; y) \geq \beta$ and $\Pr(X < x^* \mid \hat{\xi} = \xi^*; y) \leq \beta$. The measurement procedure will be unsuitable for the assigned purpose of the experiment if the detection limit ξ^* exceeds the given standard value ξ_r expressing the requirements to be met by the measurement procedure on scientific, legal, or other grounds, i.e. if $\xi^* > \xi_r$.
- If a value x of the decision variable X, obtained in the present or a later experiment, exceeds the decision threshold x^*, i.e. if $x > x^*$, then the lower limit ξ_l and the upper limit ξ_u of a confidence interval are the quantiles $\tilde{\xi}_{\gamma/2}$ and $\xi_{1-\gamma/2}$ of the distribution $f(\xi \mid x; y)$. – Then, $\Pr(\xi_l < \hat{\xi} < \xi_u \mid x; y) \leq 1-\gamma$ and $\Pr(\xi_l \leq \hat{\xi} \leq \xi_u \mid x; y) \geq 1-\gamma$. The quantile $\tilde{\xi}_{\gamma/2}$ is used to obtain the smallest interval in any case. The confidence interval defined in this way is generally not symmetrical with respect to the measurement result $E\,\hat{\xi}$. An alternative symmetrical confidence interval could be defined by the limits $\xi_{u,l} = E\,\hat{\xi} \pm \Delta\xi$, where $\Delta\xi$ is the maximum value so that $\Pr(\xi_l < \hat{\xi} < \xi_u \mid x; y) \leq 1-\gamma$. But a symmetrical confidence interval will no longer be reasonable if $\xi_l < 0$ is obtained. In this case, we should set $\xi_l = 0$.

The definitions of the decision threshold and the detection limit in conventional statistics are formally similar to the Bayesian-statistical definitions, but the probability distribution $f(x \mid \xi; y)$ of the decision variable X has a different meaning. It is the distribution of the relative frequencies with which values x will occur or are assumed to occur if the experiment is or
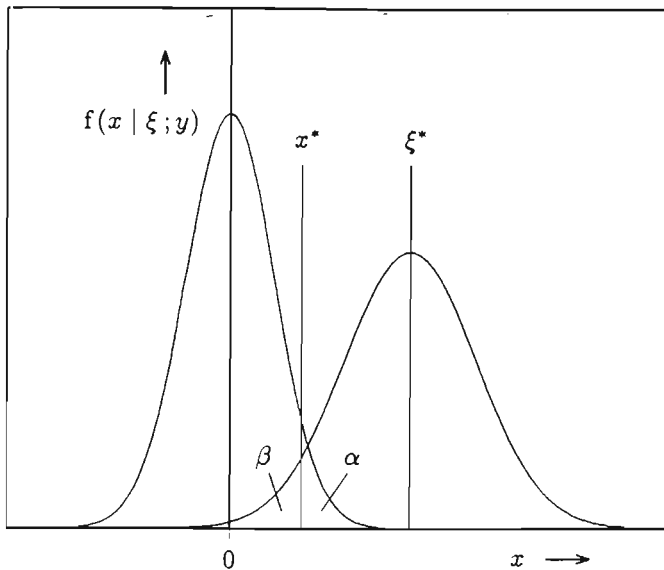
Fig. 1. Illustration of the decision threshold x^* and the detection limit ξ^* of a non-negative measurand (net effect) with a potential value ξ. The figure shows the distributions $f(x \mid \xi; y)$ of the decision variable X with values x and expectation value $E\ X = \xi$ for $\xi = 0$ and $\xi = \xi^*$. Given data are summarily denoted by y. The areas α and β below the distributions on the right-hand or left-hand side of the abscissa x^* are the probabilities of the errors of the first and second kind

was many times repeated independently under the same nominal conditions. The distribution is also assumed or derived from assumed or known, more basic frequency distributions such as Poisson distributions of radiation events registered. Parameters of these are calculated from the values x and y. These data also yield an estimate ξ of the measurand as a value of a suitable estimator $\hat{\xi}$ related to X and Y. The confidence limits are defined similarly but as the quantiles $\bar{x}_{\gamma/2}$ and $x_{1-\gamma/2}$ of the distribution $f(x \mid \xi; y)$ with the estimate ξ inserted and X so defined that $E\ X = \xi$. Numerically, all the characteristic limits turn out to be slightly different according to what statistics has been used (Sect. 4).

There is another difference which must be pointed out: In Bayesian statistics, the confidence level $1-\gamma$ is the probability, the degree of belief, of the confidence interval, obtained from the present data and other information, to contain the true measurand value. In contrast, the conventional-statistical confidence level is not a probability but must be interpreted as the fraction $1-\gamma$ of the different confidence intervals calculated in the same way from the data obtained each time if the whole experiment was repeated many times, and containing the true measurand value.

Miller et al. [15] (Sect. 1) define the decision threshold x^* essentially differently as the quantile $\xi_{1-\alpha}$ of a distribution $f(\xi \mid x)$. They derive this distribution from the Bayes theorem according to Eq. (6) with known or assumed distributions $f(x \mid \xi)$ and $f(\xi)$ and a constant $f(x)$. Their decision threshold is formally identical with our upper confidence limit if $\alpha = \frac{1}{2}\gamma$. That is the reason why it numerically differs quite significantly from the conventional-statistical and our decision thresholds. Furthermore, the distributions are interpreted as those of relative frequencies. For example, $f(\xi)$ is the reasonably assumed distribution of the measurand values in a population of samples, based also on information or assumptions on samples with measurand values zero, whereas we interpret the prior $f(\xi)$ as expressing our degree of belief assigned to the measurand value of the particular sample in question.

4 A basic case of radiation measurement

As a first example of deriving the characteristic limits generally defined in Sect. 3, we consider the important basic problem of nuclear radiation measurement in which the results of two measurements of counting radiation events are compared to detect a potential radiation contribution of a sample. This case is also the subject of the basic standard DIN 25482-1 [1] where it is dealt with in the usual way of conventional statistics. We also deal with this case in detail using and comparing the approaches both of Bayesian and conventional statistics to show their different philosophies and consequences.

4.1 Poisson and gamma distributions in a counting measurement

Let n be the number of nuclear radiation events registered during a counting measurement of 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 $v \geq 0$, the measurand value. A Poisson distribution can in many cases be assumed for physical reasons because nuclear events are physically independent and life time and dead time effects 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). Then we have

$$f(n \mid v) = e^{-v} v^n / n!: \quad (n = 0, 1, ...) \tag{13}$$

with $E\ N = \text{Var}\ N = v$.

In order to establish the distribution $f(v \mid n)$ for the parameter v now taken as a random variable $\hat{v}$ assigned to the measurand of interest in Bayesian statistics, we use the Bayes theorem $f(v \mid n)\ f(n) = f(n \mid v)\ f(v)$ according to Eq. (6). $f(n)$ is a constant for a given n, and a prior $f(v)$ is needed. This prior is the distribution of $\hat{v}$ before the measurement is performed. Jaynes [23] obtained $f(v) = \text{const}/v$ ($v > 0$) by a scaling consideration as follows: Assuming a steady physical Poisson process measured, the distribution of the count rate estimator $\hat{\varrho} = \hat{v}/t$ does not depend on the arbitrary duration t of measurement, that is, $f(\varrho \mid t) = f(\varrho) = t\ g(\varrho t)$, where the function $g(v)$ expresses the shape of the prior $f(v)$. Differentiation with respect to t yields the differential equation $\partial(t g(\varrho t))/\partial t = g(v) + v g'(v) = 0$ with the solution $g(v) = f(v) = C/v$ ($v > 0$; C is the integration constant). The fact that this distribution is not normalizable is due to the neglect of short-term and long-term influences on the measurement. Accordingly, $g(v)$ must be interpreted as an approximation of a more realistic, normalizable shape of the prior $f(v)$. Inserting $f(v) = C/v$ into the above stated Bayes theorem, and normalizing yields the *gamma distribution* $f(v \mid n) = e^{-v} v^{n-1}/(n-1)!$ ($v \geq 0$) which is set zero for $v < 0$. With $E\hat{v} = \text{Var}\ \hat{v} = n$, the number n of counted events is the measurement result, and $\sqrt{n}$ is the standard uncertainty (of the measurand) associated with this best estimate (Sect. 3).

The particular case $n = 0$ must be treated separately: $E\hat{v}$ and $\text{Var}\ \hat{v}$ vanish, and $f(v \mid n) = \delta(v)$ and a zero uncertainty follow. This is not reasonable in practice since we can never be sure that exactly $v = 0$ if no event happens to be registered in a measurement of finite duration. Thus, no reasonable statement can be made on v if $n = 0$. With any more realistic shape of the prior $f(v)$, we should always obtain $E\hat{v} > 0$ and $\text{Var}\ \hat{v} > 0$. In conventional statistics, N itself is usually used as an *unbiased* estimator of v, that is, $E\ N = v$. Thus, the number

n of events counted is an estimate of v. With Var $N = v$ also estimated by n, the standard uncertainty $\sqrt{n}$ of the measurand follows and also turns out to be unreasonable for $n = 0$.

To avoid this shortcoming which would lead into severe troubles in Sect. 4.2, we assume that the counting measurement will be carried out with a duration t chosen suitably large according to the experience of former, similar measurements, so that for any reasonable $v > 0$ at least a few counts can be expected. t is therefore no longer arbitrary. This will reduce the probability density for small v significantly. Moreover, $\hat{v}$ $(= \hat{\varrho}t)$ will be bounded for physical or experimental reasons, although a sufficiently large upper bound need not be specified explicitly. We represent this knowledge by equally likely v between zero and the upper bound, thus, by a constant prior $f(v)$. The Bayes theorem and normalization then yield the gamma distribution

$$f(v\,|\,n) = e^{-v}v^n/n!: \quad (v \geq 0) \tag{14}$$

with E $\hat{v}$ = Var $\hat{v}$ = $\sigma^2(\hat{v})$ = $n + 1$. This result is more reasonable for $n = 0$ since the standard uncertainty $\sqrt{n+1}$ does not vanish, and the interval E $\hat{v} - \sigma(\hat{v}) \leq v \leq$ E $\hat{v} + \sigma(\hat{v})$ of reasonable estimates of the measurand turns out to also contain the estimate $v = 0$. Asymptotically for large n, both approaches discussed lead to the same results. The main differences only occur for small n.

4.2 The Bayesian approach

Let a reference or *zero effect measurement* of a dummy sample or, if appropriate, the background be carried out as an experiment such as that considered in Sect. 4.1. In the following, all symbols for quantities referring to this zero effect measurement are primed. Thus, for instance, n' is the number of events registered during the zero effect measurement. It corresponds to y in Sect. 3. We now ask for the number n of events which will be counted in a second measurement of fixed duration t to be performed with a sample involved but otherwise with all nominal conditions identical. We assume the count rate of this *gross effect measurement* to be the sum of the count rate due to the zero effect and the count rate contribution of the sample, i.e. $\hat{v}/t = \hat{v}'/t' + \hat{\varrho}$. Here, $\hat{\varrho}$ is the estimator assigned to the sample count rate to be measured and corresponds to $\hat{\xi}$ in Sect. 3. The sample count rate is the measurand in question.

We need the distribution $f(n\,|\varrho;\,n')$ to establish the decision threshold with $\varrho = 0$ and the detection limit with a general $\varrho > 0$. We have

$$f(n|\varrho;n') = \int_0^\infty f(n\,|\,v';\varrho;n')\,f(v'\,|\,\varrho;n')\mathrm{d}v' \tag{15}$$

according to the expansion theorem in Eq. (7). If the parameter variables $\hat{v}'$ and $\hat{\varrho}$ are fixed, then N and N' are independent, and N has a Poisson distribution with the parameter $v = \varrho t + v't/t'$. This distribution is the first factor of the integrand in Eq. (15). The second factor is a gamma distribution according to Eq. (14) since the zero effect measurement does not depend on the sample, that is, on $\hat{\varrho}$. We obtain

$$f(n|\varrho;n')$$
$$= \int_0^\infty \Big(\exp\big(-(\varrho t + v't/t')\big)(\varrho t + v't/t')^n/n!\big) \cdot \big(e^{-v'}(v')^{n'}/n'!\big)\,\mathrm{d}v'$$
$$= \frac{e^{-\varrho t}}{n!\,n'!}\sum_{k=0}^n \binom{n}{k}(\varrho t)^k (t/t')^{n-k}\int_0^\infty (v')^{n+n'-k}\,e^{-v'/q}\mathrm{d}v'$$
$$= \frac{p^n q^{n'+1} e^{-\varrho t}}{n'!}\sum_{k=0}^n \frac{(n+n'-k)!}{k!\,(n-k)!}(\varrho t/p)^k \tag{16}$$

with $p = t/(t+t')$ and $q = t'/(t+t')$ and with the expectation value EN = ϱt + $(n'+1)p/q$ and the variance Var $N = \varrho t$ + $(n'+1)p/q^2$. We introduce R = N/t - $(n'+1)/t'$ as the decision variable corresponding to X in Sect. 3. Then we obtain E $R = \varrho$ as is suitable, and Var $R = \varrho/t$ + $((n'+1)/t')(1/t+1/t')$.

It must again be pointed out that the distribution according to Eq. (16) expresses the degree of belief assigned to the outcome n of the gross effect measurement before this is performed, and by no means a distribution of counts n occurring in measurements repeated many times with the same sample involved. For $\varrho = 0$, it is a *negative binomial distribution*

$$f(n\,|\,\hat{\varrho} = 0; n') = \frac{(n+n')!}{n!\,n'!}\,p^n\,q^{n'+1} \tag{17}$$

with E N = $(n'+1)p/q$ and Var $N = (n'+1)p/q^2$ and E $R = 0$. According to Sect. 2 and the negative binomial distribution of Eq. (17), the quantile $n_{1-\alpha}$ of N for the probability $1-\alpha$ is the smallest natural number n which meets the condition

$$\Pr(N \leq n\,|\,\hat{\varrho} = 0; n') = \frac{q^{n'+1}}{n'!}\sum_{k=0}^n \frac{(k+n')!\,p^k}{k!} \geq 1 - \alpha. \tag{18}$$

The decision threshold r^* of the decision variable R = N/t - $(n'+1)/t'$ then follows immediately:

$$r^* = n_{1-\alpha}/t - (n'+1)/t'. \tag{19}$$

The measured value $r = n/t - (n'+1)/t'$ of the decision variable R must be compared with r^* to decide whether or not the sample has contributed to the events registered. r corresponds to x in Sect. 3. If $r > r^*$, the hypothesis $H_0 = \{\hat{\varrho} = 0\}$ is rejected. Results for r^* are shown in Fig. 2. r^* is fluctuating due to the discreteness of $n_{1-\alpha}$.

The detection limit follows from Eq. (16) as the solution $\varrho = \varrho^*$ of the equation (Fig. 1)

$$\Pr(N \leq n_{1-\alpha}\,|\,\varrho; n')$$
$$= \frac{q^{n'+1}e^{-\varrho t}}{n'!}\sum_{n=0}^{n_{1-\alpha}}p^n\sum_{k=0}^n \frac{(n+n'-k)!}{k!\,(n-k)!}(\varrho t/p)^k = \beta. \tag{20}$$

Solving this equation for the ϱ of the exponential factor $e^{-\varrho t}$ yields an equation of the form $\varrho = h(\varrho)$ which should be solved numerically by iteration, beginning, for instance, with $\varrho = (1 + k_{1-\beta}/k_{1-\alpha})\,r^*$. This iteration converges. Results are shown in Fig. 3.

The distribution $f(\varrho\,|\,n; n')$ is needed to calculate the confidence limits. It follows from the Bayes theorem $f(\varrho\,|\,n; n')\,f(n; n')$ = $f(n\,|\,\varrho; n')\,f(\varrho\,|\,n')\,f(n')$. In this equation, $f(n\,|\,\varrho; n')$ is given according to Eq. (16) and $f(n; n')$ and $f(n')$ are constants for n and n' fixed. $\hat{\varrho}$ characterizes the sample, $\hat{\varrho}t$ is assigned to the parameter of the Poisson distribution of the sample events registered. $\hat{\varrho}$ is therefore independent of N' which belongs to the zero effect measurement. Thus, $f(\varrho\,|\,n')$ = $f(\varrho)$ = const according to Sect. 4.1. We obtain

$$f(\varrho|n;n') = C\,H(\varrho)t e^{-\varrho t}\sum_{k=0}^n \frac{(n+n'-k)!}{k!\,(n-k)!}(\varrho t/p)^k. \tag{21}$$

$H(\varrho)$ is the Heaviside unit step function with $H(\varrho) = 0$ for $\varrho < 0$ and $H(\varrho) = 1$ for $\varrho \geq 0$. It is used to make the distribution vanish for $\varrho < 0$. The moments are

$$\mathrm{E}\,\hat{\varrho}^m = \frac{C}{t^m}\sum_{k=0}^n \frac{(n+n'-k)!\,(k+m)!}{k!\,(n-k)!\,p^k}. \tag{22}$$

The normalization constant C follows from the relationship E $\hat{\varrho}^m = 1$ for $m = 0$. E $\hat{\varrho}$ is the best estimate of the measurand,
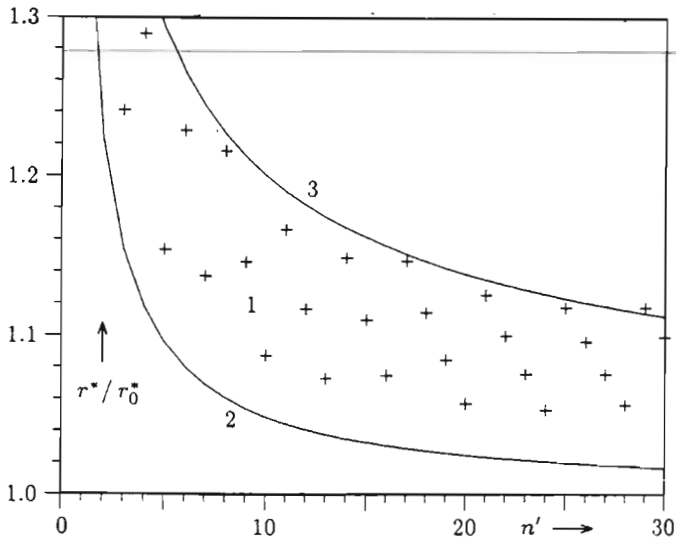
Fig. 2. *(1, crosses) Exact and (2) approximate Bayesian-statistical and (3) approximate conventional-statistical decision thresholds r* for the detection of the radiation event rate of a sample, versus the registered number n' of zero effect events according to Eqs. (19), (25) and (31), respectively. Identical durations t = t' of the gross and zero effect measurements and an error probability α = 0.05 are assumed. $r_0^* = (k_{1-\alpha}/t)\sqrt{2\,n'}$ is the asymptotic decision threshold for large n' and both statistics*
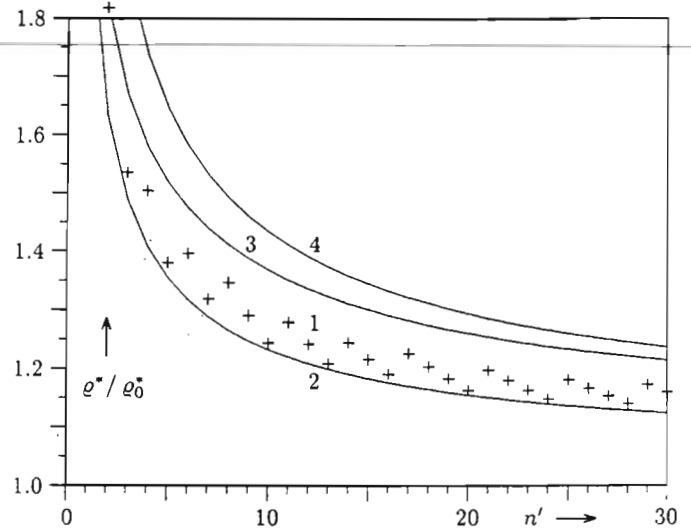

Fig. 3. *(1, crosses) Exact and (2) approximate Bayesian-statistical and (3) approximate conventional-statistical detection limits ϱ* for the detection of the radiation event rate of a sample, versus the registered number n' of zero effect events according to Eqs. (20), (26) and (32), respectively. Identical durations t = t' of the gross and zero effect measurements and error probabilities α = β = 0.05 are assumed. $\varrho_0^* = (2\,k_{1-\alpha}/t)\sqrt{2\,n'}$ is the asymptotic detection limit for large n' and both statistics. (4) approximation according to Ref. [1]*

the sample count rate, and $\sigma(\hat{\varrho})$ is the standard uncertainty associated with this estimate. The measured value $r = n/t - (n'+1)/t'$ of the decision variable R is also an estimate of the measurand, but it may be negative, whereas $\mathrm{E}\,\hat{\varrho}$ is always non-negative. Using the Jaynes prior $f(\varrho) = \mathrm{const}/\varrho$ (Sect. 4.1) instead of the constant prior would lead to an unnormalizable $f(\varrho\,|\,n;\,n')$ and, thus, to the unacceptable result that no reasonable statement can be made on the sample count rate.

The confidence limits ϱ_l and ϱ_u are obtained by equating the distribution integrals from $\varrho = 0$ up to these limits with $\eta = \frac{1}{2}\gamma$ and $\eta = 1 - \frac{1}{2}\gamma$:

$$\Pr(\hat{\varrho} \le \varrho\,|\,n;n') = \int_0^\varrho f(\varrho'\,|\,n;n')\,\mathrm{d}\varrho'$$

$$= 1 - C\mathrm{e}^{-\varrho t}\sum_{k=0}^n \frac{(n+n'-k)!}{(n-k)!\,p^k}\sum_{j=0}^k \frac{(\varrho t)^j}{j!} = \eta \qquad (23)$$

with $\varrho \ge 0$. This distribution function can be verified by comparing its derivative with the probability density according to Eq. (21) and by the fact that the second term vanishes for $\varrho \to \infty$. Eq. (23) can be solved numerically by iteration for the confidence limits in a similar way as Eq. (20), beginning, for instance, with $\varrho_{u.1} = r$. See Fig. 4 for results.

In the Appendix, the distributions according to Eqs. (13), (14), (16) and (17) are proved to converge (in distribution), when standardized, to the standardized normal distribution if a suitable parameter τ, actually the respective parameters ν, n, n', n' of the distributions mentioned, approaches infinity. The normal distribution with the same expectation value μ and standard deviation σ as those of any of these distributions can then serve as an approximation of this distribution in question for large parameter values, and, as it is also shown in the Appendix, a quantile x_η of this distribution can be approximated by

$$x_\eta = \mu + k_\eta\,\sigma. \qquad (24)$$

We are able now to establish approximations of the decision threshold and the detection limit. Because $\mu = \mathrm{E}\,R = \varrho$ and

$\sigma^2 = \mathrm{Var}\,R = \varrho/t + ((n'+1)/t')(1/t+1/t')$ (see passage below Eq. (16)) and using Eq. (24), $\varrho = 0$, and $\eta = 1 - \alpha$, the approximate decision threshold reads (Fig. 2)

$$r^* = k_{1-\alpha}\sqrt{((n'+1)/t')(1/t+1/t')}. \qquad (25)$$

Except of $n'+1$ instead of n', this decision threshold is identical to the approximation for large n' given in Ref. [1] of the conventional-statistical decision threshold. The detection limit is easily obtained with $\varrho = \varrho^* > 0$ and $\eta = \beta$ (Figs. 1 and 3):

$$\varrho^* = r^* + k_{1-\beta}\sqrt{\varrho^*/t + ((n'+1)/t')(1/t+1/t')}. \qquad (26)$$

This implicit equation can be solved analytically for ϱ^* or again by iteration. In particular for $\alpha = \beta$, we obtain $\varrho^* = 2\,r^* + k_{1-\beta}^2/t$.

Similarly, the distribution according to Eq. (21) can be approximated by a normal distribution with $\mu = (n+1)/t - (n'+1)/t'$ and $\sigma^2 = (n+1)/t^2 + (n'+1)/t'^2$, but truncated at $\varrho = 0$. if both parameters $n \to \infty$ and $n' \to \infty$ (Appendix). Nonetheless, a quantile ϱ_η of the truncated normal distribution which approximates that of the distribution considered, can be expressed by those of the standardized normal distribution which has the distribution function $\Phi(z)$. With the probability $\eta_0 = \Phi(\mu/\sigma)$, we obtain

$$\varrho_\eta = \mu + k_{\bar{\eta}}\,\sigma; \quad \bar{\eta} = \eta_0\,\eta + 1 - \eta_0. \qquad (27)$$

This can be seen as follows: It is $\Pr(\hat{\varrho} \ge 0) = \eta_0$ for the untruncated normal distribution with the parameters μ and σ. Thus, for abscissae $\varrho \ge 0$, the truncated normal distribution is larger than the untruncated one by a factor $1/\eta_0$, and $\Pr(0 \le \hat{\varrho} \le \varrho_\eta) = \eta$ of the truncated normal distribution corresponds to $\Pr(0 \le \hat{\varrho} \le \varrho_\eta) = \eta_0\eta$ of the untruncated normal distribution. Here, $\Pr(\hat{\varrho} < 0) = 1 - \eta_0$ must be added to obtain $\Pr(\hat{\varrho} < \varrho_\eta) = \bar{\eta}$ of the untruncated normal distribution. It is stressed that the parameters μ and σ^2 are not the expectation
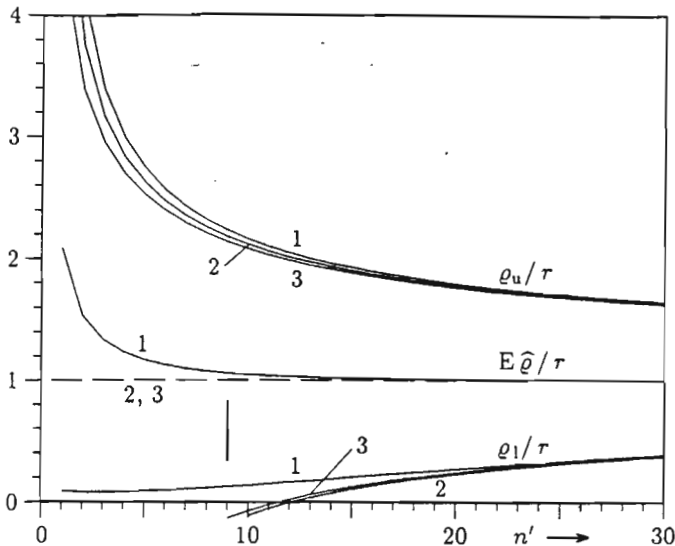
Fig. 4. (1, crosses) Exact and (2) approximate Bayesian-statistical and (3) approximate conventional-statistical lower and upper confidence limits ϱ_l and ϱ_u for the detection of the radiation event rate of a sample, versus the registered number n' of zero effect events according to Eqs. (23) and (29) and the end of Sect. 4.3, respectively. Identical durations $t = t'$ of the gross and zero effect measurements, $n = 2n'$ registered events of the gross effect measurement, and a confidence level $1 - \gamma = 0.95$ are assumed. $E \hat\varrho$ and r are the Bayesian-statistical and conventional-statistical measurement results, respectively, $r = n'/t$ in this case, $E \hat\varrho$ according to Eq. (28). Both the Bayesian-statistical and the approximate conventional-statistical decision thresholds correspond to $n' = 9$ (vertical bar). For $n' < 9$ corresponding to $n < 18$, the hypothesis of a zero radiation event rate of the sample cannot be rejected

value and variance of the truncated normal distribution. Instead, the latter are

$$E \hat\varrho = \mu + \frac{\sigma \exp(-\mu^2/(2\sigma^2))}{\eta_0 \sqrt{2\pi}}; \quad Var \hat\varrho = \sigma^2 - E \hat\varrho \cdot (E \hat\varrho - \mu). \quad (28)$$

The confidence limits ϱ_l and ϱ_u follow from Eq. (27) for $\eta = \frac{1}{2}\gamma$ and $\eta = 1 - \frac{1}{2}\gamma$. For $\mu \gg \sigma$, the truncation of the distribution can be neglected. In this case, the confidence limits are identical to those obtained from the normal distribution (Fig. 4):

$$\varrho_{u,l} = \frac{n+1}{t} - \frac{n'+1}{t'} \pm k_{1-\gamma/2} \cdot \sqrt{\frac{n+1}{t^2} + \frac{n'+1}{t'^2}}. \quad (29)$$

4.3 The conventional approach

With the Bayesian approach, the parameter v' of the Poisson distribution is left unknown and taken into account as a random variable with a constant prior distribution. In contrast, v' is an unknown constant in conventional statistics and estimated as follows:

The random variables N and N' are again assumed to be Poisson-distributed with the expectation values $E N = v$ (= $v't/t'$ for the hypothesis $\varrho = 0$, where ϱ is also a constant now) and $E N' = v'$ and variances $Var N = v$ and $Var N' = v'$. The usual conventional-statistical estimate n' could be used for v' (similarly, n for v). If n is available and as long as $r = n/t - r'$ with $r' = n'/t'$ does not exceed the decision threshold r^*, i.e. as long as the hypothesis $\varrho = 0$ cannot be rejected, n can also be used as information for estimating v'. We then introduce coefficients a and b and the estimator $\hat\vartheta = aN + bN'$ for v'. $\hat\vartheta$ should be unbiased, i.e. $E\hat\vartheta = v'$, and of minimum variance. This implies $E\hat\vartheta = v' = av't/t' + bv'$ or $at + bt' = t'$ and $Var\hat\vartheta = a^2v't/t' + b^2v' = min$ or $a^2t + b^2t' = min$ resulting in $a = b = $

$t'/(t+t')$ and the value $\vartheta = (n + n')t'/(t + t')$ of $\hat\vartheta$ as the estimate for v'. This is a quite natural result which we would also obtain when putting both experiments together and estimating the common count rate v'/t' by $(n + n')/(t + t')$ since $N + N'$ also follows a Poisson distribution.

To obtain the decision threshold, we need an estimate s^2 of the variance of $R = N/t - N'/t'$ which reads $Var R = v'/t^2 + v'/t'^2 = (v'/t')(1/t+1/t')$. Inserting the above-stated estimate ϑ of v', we obtain $s^2 = (n + n')/tt'$. We again approximate the distribution of R by a normal distribution the quantile of which serves as the decision threshold $r^* = k_{1-\alpha} s$. We reject our hypothesis $\varrho = 0$ if $r > r^*$. The largest value of $r = n/t - r'$ which can be accepted as conforming to our hypothesis, is r^* implying the largest value $n = r^*t + n't/t' = (r^* + r')t$ which we insert now into the expression for s^2. This finally yields

$$r^* = k_{1-\alpha} \sqrt{r^*/t' + r' \cdot (1/t + 1/t')}. \quad (30)$$

This implicit equation can be analytically solved for r^*, resulting in

$$r^* = \frac{k_{1-\alpha}^2}{2t'} \left(1 + \sqrt{1 + (2t'/k_{1-\alpha})^2 \cdot r' \cdot (1/t + 1/t')} \right). \quad (31)$$

This is the equation presented in Ref. [1] to specify the decision threshold. The results for r^* according to Eq. (31) are a bit larger than those from Eq. (25) (Fig. 2). Eq. (31) is an approximation, based on a normal distribution used for R, but it is sufficient for practice. To obtain a more accurate result would require a complex calculation including a folding of the two Poisson distributions involved with the unknown parameter r^*, yielding the distribution of R. r^* then must be implicitly determined by comparing it with the quantile of the distribution also depending on r^*. We dispense with this calculation.

The detection limit is established according to Fig. 1 and similar to Eq. (26) with $r^* = k_{1-\alpha} s$ but with n/t in the expression of s^2 estimated by $\varrho^* + r'$ since n is not available now. This yields the implicit formula

$$\varrho^* = k_{1-\alpha} \sqrt{\varrho^*/t' + r' \cdot (1/t + 1/t')} + k_{1-\beta} \sqrt{\varrho^*/t + r' \cdot (1/t + 1/t')} \quad (32)$$

which should be iteratively solved for ϱ^* beginning with $\varrho^* = 0$. In contrast to Ref. [1], r' is here not replaced by the unknown v'/t' (= ϱ_0 in Ref. [1]) since a numerical estimate of the detection limit is required in practice but cannot otherwise be calculated (Fig. 3).

If $r > r^*$, the hypothesis $\varrho = 0$ is rejected, and v' cannot be estimated as described above. In this case, R is used as an estimator of the measurand, and r as an estimate of ϱ. The distribution of R is again approximated by a normal distribution with the expectation value ϱ estimated by r, and a variance estimated by $n/t^2 + n'/t'^2$. The quantiles $r \pm k_{1-\gamma/2} \sqrt{n/t^2 + n'/t'^2}$ of this normal distribution for $\eta = \frac{1}{2}\gamma$ and $\eta = 1 - \frac{1}{2}\gamma$ are then taken as the confidence limits turning out to be asymptotically identical for large n and n' to the Bayesian-statistical approximations according to Eq. (29). A negative ϱ_l cannot always be avoided with the conventional approach, whereas the Bayesian-statistical ϱ_l is always non-negative (Fig. 4).

5 Example of general application

We now investigate a simple, but basic and typical example which generally cannot be dealt with in the framework of conventional statistics since underlying frequency distribu-

tions either do not exist or are unknown and cannot be assumed. Likewise, we again deal with the problem investigated in Sect. 4, but forgetting the shape of the Poisson frequency distribution involved and only taking into account that its expectation value and its variance are identical.

Let a primary estimate x and the associated standard uncertainty $u(x)$ of a non-negative measurand be given or obtained from a measurement data evaluation procedure according to the Guide [9] or DIN 1319-3 [13] or -4 [14], for instance, a spectrum unfolding [12], and let no further information on the measurand be available at all. The primary estimate x may be negative even if the measurand is known to be non-negative. The symbol $u(x)$ in general should not and cannot be interpreted as a function of x, although x and $u(x)$ are in most cases obtained from the same data set which also includes the zero effect measurement data y. Nevertheless, we need $u(x)$ also for a general x not actually available and different measurand values ξ. Therefore, we cautiously use $u(x)$ also as a given function of ξ and then denote it by $\tilde{u}(\xi)$. This function will also depend on y. According to Ref. [10], x is the expectation value and $u^2(x)$ the variance of a random variable $\hat{\xi}$ called the *estimator* of the measurand. Similar to Sect. 3, the measurand is assumed to be suitably defined so that $\xi = 0$ indicates the absence of the physical effect represented by the measurand. The primary distribution $f_0(\xi \mid x; y)$ of the estimator, the *data prior* [10], is established using the principle of maximum entropy yielding the normal probability density

$$f_0(\xi \mid x; y) = C \exp\left(-\frac{1}{2}(\xi - x)^2/u^2(x) \right). \tag{33}$$

The principle of maximum entropy (Sect. 2) here consists in maximizing the entropy

$$S = -\int f_0(\xi \mid x; y) \ln\left(f_0(\xi \mid x; y)/f_0(\xi) \right) d\xi \tag{34}$$

using a constant prior $f_0(\xi)$ and observing the constraints $E\,\hat{\xi} = x$ and $Var\,\hat{\xi} = u^2(x)$ [10].

It is known that the measurand is non-negative. This independent information not yet used is taken into account by a factor $H(\xi)$, the *model prior* [10], in this particular case the Heaviside unit step function (Sect. 4.2), yielding the final distribution $f(\xi \mid x; y)$ as a truncated normal distribution:

$$f(\xi \mid x; y) = C\,H(\xi)\,\exp\left(-\frac{1}{2}(\xi - x)^2/u^2(x) \right). \tag{35}$$

First the normalization constant C and then the confidence limits are calculated similar to Eq. (27) as quantiles of this distribution. The expectation value $E\,\hat{\xi}$ and the variance $Var\,\hat{\xi}$ are calculated similar to Eq. (28). The factor $H(\xi)$ can be neglected if $x \gg u(x)$. We then obtain the confidence limits

$$\xi_{u,l} = x \pm k_{1-\gamma/2}\,u(x). \tag{36}$$

In general, $E\,\hat{\xi}$ and $Var\,\hat{\xi}$ of $f(\xi \mid x; y)$ differ from x and $u^2(x)$. This reflects the fact that the knowledge of the measurand to be non-negative is included in $f(\xi \mid x; y)$ but not in $f_0(\xi \mid x; y)$. $E\,\hat{\xi}$ and the confidence limits are always non-negative.

With the Bayes theorem $f(x \mid \xi; y)\,f(\xi; y) = f(\xi \mid x; y)\,f(x; y)$ according to Eq. (6), using constant $f(x; y)$ and $f(\xi; y)$ for $\xi \geq 0$ and approximating $u(x)$ by the function $\tilde{u}(\xi)$ assumed to be varying slowly enough for $\xi \approx x$, we obtain

$$f(x \mid \xi; y) = C \exp\left(-\frac{1}{2}(x - \xi)^2/\tilde{u}^2(\xi) \right); \quad (\xi \geq 0). \tag{37}$$

Here, x is interpreted as a value of the decision variable X, thus, $E\,X = \xi$ and $Var\,X = \tilde{u}^2(\xi)$. It is pointed out that this normal distribution of X based on Bayesian statistics is derived using the principle of maximum entropy and the Bayes theorem. It is not an assumption as often in conventional statistics. But it must be properly interpreted as representing the degree of belief, based on present information, that a value x will occur in an experiment to be carried out later on. It is *not* the real, approximated, or assumed distribution of values x which will actually occur in experiments repeated many times.

The decision threshold is easily obtained using $f(x \mid \xi; y)$ according to Eq. (37) with $\xi = 0$:

$$x^* = k_{1-\alpha}\,\tilde{u}(0). \tag{38}$$

The detection limit also follows from $f(x \mid \xi; y)$ according to Eq. (37) (Fig. 1):

$$\xi^* = x^* + k_{1-\beta}\,\tilde{u}(\xi^*), \tag{39}$$

an equation which should then be solved iteratively for ξ^* beginning with $\xi^* = 0$. With an $\tilde{u}(\xi)$ varying slowly enough, the iteration can be expected to converge. Here, it becomes clear that the uncertainty must be given as a function of ξ. Otherwise, the given value $u(x)$ must be used as an approximation. Then, $x^* = k_{1-\alpha}\,u(x)$ and $\xi^* = (k_{1-\alpha} + k_{1-\beta})\,u(x)$. In many cases of H_0, $x = y_1 - y_0$ will be a small difference of two values y_1 and y_0 similar to y, obtained from two measurements to be compared. If the standard uncertainties $u(y_1)$ and $u(y_0)$ associated with y_1 and y_0 are available, $u^2(0) = u^2(y_1) + u^2(y_0)$ may be used. Moreover, the interpolation $\tilde{u}^2(\xi) = \tilde{u}^2(0)(1 - \xi/x) + u^2(x)\xi/x$ will be applicable if $\tilde{u}(0)$ is available and $x > 0$.

We now apply the example dealt with to the important basic problem of common practice in nuclear radiation measurements already investigated in Sect. 4. We deal with this problem here again in the case of limited information when data of the measurand involved are given as above only as estimates and associated uncertainties, whereas it is dealt with in Sect. 4 in more detail, extensively using the knowledge and the properties of underlying Poisson frequency distributions of radiation events registered.

We compare two independently obtained primary estimates r and r' and the associated standard uncertainties $u(r)$ and $u(r')$ of two measurands of the same kind in order to detect a measurand difference known to be non-negative for physical reasons. Let, for instance, $r = n/t$ be the rate of n radiation events counted during a gross effect measurement of a sample. t is the fixed duration of the measurement. Then, if a Poisson frequency distribution can be assumed for the random variable N the value of which is n, then $u^2(r) = n/t^2$ according to Refs. [13, 14]. Similarly, for a zero effect measurement, using primed symbols corresponding to the unprimed ones, $r' = n'/t' = y$, $u^2(r') = n'/t'^2$. Furthermore, introducing the decision variable $X = N/t - r'$ with its value $x = r - r'$, and the net count rate $\hat{\xi} = \hat{\varrho}$, our measurand as in Sect. 4, we have $u^2(x) = u^2(r) + u^2(r') = n/t^2 + n'/t'^2$ according to the uncertainty propagation law valid also in Bayesian statistics [10]. If only the zero effect measurement is actually carried out, we will assume $r \approx r'$ or $n/t \approx n'/t'$ with $\xi = 0$ and therefore $u^2(x) = \tilde{u}^2(0) = r'(1/t+1/t')$ in this case, and we will obtain the decision threshold asymptotically identical to that in Eq. (25) and Ref. [1] in the case of sufficiently large n and n' (Sect. 4). Furthermore, for a net rate $\xi > 0$, we approximate $r = n/t \approx \xi + n'/t'$ yielding $u^2(r) \approx (\xi + n'/t')/t$ and $\tilde{u}^2(\xi)$

$= (\xi + n'/t')/t + n'/t^2$ as a function of ξ. According to Eq. (39), this leads to

$$\xi^* = x^* + k_{1-\beta} \sqrt{\xi^*/t + r' \cdot (1/t + 1/t')} \,. \tag{40}$$

This equation can be solved analytically for ξ^*, or iteratively beginning with $\xi^* = 0$. The first approximation is $\xi^* = (k_{1-\alpha} + k_{1-\beta}) \, \bar{u}(0)$. For $\alpha = \beta$, we obtain $\xi^* = 2x^* + k_{1-\beta}^2/t$. These results are also asymptotically identical to those in Eq. (26) and Ref. [1] in the case of sufficiently large n and n' except for the expectation value ϱ_0 of the zero effect count rate occurring in Ref. [1] which here corresponds to the estimate r'. But for large n', ϱ_0 and r' will become approximately identical. The confidence limits must be calculated with $f(\xi \mid x; y)$ according to Eq. (35) using the above-stated x and $u(x)$. They are also asymptotically identical to those in Ref. [1].

Appendix:
Asymptotic behaviour of several distributions related to the Poisson distribution

We consider a random variable X with the expectation value μ and the variance σ^2, both depending on an increasing parameter τ, and with the characteristic function $\varphi(\omega) = E \exp(i\omega X)$. The standardized random variable $Y = (X-\mu)/\sigma$ has the characteristic function $\bar{\varphi}(\omega) = \exp(-i\omega\mu/\sigma) \, \varphi(\omega/\sigma)$, the Taylor-expanded logarithm of which reads

$$\ln\bar{\varphi}(\omega) = -\frac{1}{2}\omega^2 + \varepsilon; \quad \varepsilon = (\ln\varphi(\omega))'''|_{\theta\omega/\sigma} \cdot \omega^3/(3!\,\sigma^3); \quad (0 \le \theta \le 1) \,. \tag{41}$$

If the remainder $\varepsilon \to 0$ with $\tau \to \infty$ for any fixed ω, then $\bar{\varphi}(\omega) \to \exp(-\frac{1}{2}\omega^2)$ which is the continuous characteristic function of the standardized normal distribution. According to the following direct limit theorem, the distribution of Y then *converges in distribution* to the standardized normal distribution.

Convergence in distribution means pointwise convergence of a sequence of distribution functions $F_Y(y)$ of a random variable Y to a limiting distribution function at the abscissae where the limiting distribution function is continuous (at other abscissae, pointwise convergence is not required). It expresses in addition that the integral $I = \int_a^b G(y) \, dF_Y(y)$ (a Stieltjes integral similar to Eq. (3)) of any continuous function $G(Y)$ over the interval $a \le y \le b$ with constant a and b, converges to the corresponding integral with respect to the limiting distribution, here the standardized normal distribution. The limiting distribution function must be continuous at $y = a$ and $y = b$, and $G(Y)$ must be bounded if $a = -\infty$ or $b = +\infty$.

The *direct limit theorem* is a part of the important Lévy-Cramér limit theorem [18] and reads: If the characteristic functions of a sequence of distribution functions converge everywhere pointwise to a function $\varphi(\omega)$ which is continuous in an interval $|\omega| < \omega_0$ with some ω_0, then the distribution functions converge in distribution to a distribution function the characteristic function of which is $\varphi(\omega)$.

The following conclusion is important for the practice of applying the characteristic limits defined in Sect. 3: In particular with $G(Y) \equiv 1$ and $a = -\infty$, we have $I = \Pr(Y \le b) = F_Y(b)$, an increasing, continuous function of b in the case of the standardized normal distribution, that is, $I = \eta$ for a given probability η if and only if $b = k_\eta$. The same integral I with a fixed b and with respect to the distribution of Y then will converge to η if this distribution converges in distribution to the standardized normal distribution and if and only if $b =$

k_η. Thus, k_η is the unique limit of the quantile y_η. This is the reason why we can use the approximation $x_\eta = \mu + k_\eta \sigma$ for the quantile x_η if τ is large enough.

Introducing the constants a_i $(i = 1, ..., m)$ and the independent random variables X_i with their characteristic functions $\varphi_i(\omega)$, the characteristic function of $Y = \sum_{i=1}^m a_i X_i$ is $\varphi(\omega) = \prod_{i=1}^m \varphi_i(a_i\omega)$. If the X_i are standardized and $\sum_{i=1}^m a_i^2 = 1$, then Y is also standardized. If, in addition, the remainders ε_i of X_i according to Eq. (41) approach zero and the distributions of X_i thus converge in distribution to the standardized normal distribution, then the same holds true for Y. This can easily be seen when $\ln\varphi(\omega)$ is examined.

The Poisson distribution $f(n \mid v) = e^{-v} v^n/n!$ with $\mu = \sigma^2 = v$ has the characteristic function $\varphi(\omega) = \exp((e^{i\omega}-1)v)$ with $(\ln\varphi(\omega))''' = -ive^{i\omega}$. According to Eq. (41), we obtain $\varepsilon = -i \exp(i\theta\omega/\sqrt{v}) \cdot \omega^3/(3!\,\sqrt{v}) \to 0$ for $\tau = v \to \infty$. The standardized Poisson distribution thus converges in distribution to the standardized normal distribution.

The gamma distribution $f(v \mid n) = e^{-v} v^n/n!$ with $\mu = \sigma^2 = (n + 1)$ has the characteristic function $\varphi(\omega) = (1-i\omega)^{-n-1}$ with $(\ln\varphi(\omega))''' = -2i \, (n+1) \, (1-i\omega)^{-3}$. According to Eq. (41), we obtain $\varepsilon = -i \, (1 - i\theta\omega/\sqrt{n+1})^{-3} \cdot \omega^3/(3\sqrt{n+1}) \to 0$ for $\tau = n \to \infty$. The standardized gamma distribution thus also converges in distribution to the standardized normal distribution.

For the negative binomial distribution $f(n \mid n') = (n + n')!$ $p^n q^{n'+1}/(n! \, n'!)$ with $p > 0$, $q > 0$, and $p + q = 1$, we have $\mu = (n' + 1)p/q$ and $\sigma^2 = (n' + 1)p/q^2$. The sum of $f(n \mid n')$ over n must yield $1 = (1-p)^{-n'-1} q^{n'+1}$. We easily obtain the characteristic function by replacing p by $pz = p \, e^{i\omega}$ in this sum, which results in $\varphi(\omega) = (1-pz)^{-n'-1} q^{n'+1}$ and $(\ln\varphi(\omega))''' = -i \, (n' + 1) pz \, (1 + pz) \, (1-pz)^{-3}$. With Eq. (41), $|pz| \le p < 1$, and $\sigma^2 = (n' + 1)p/q^2$, we obtain $|\varepsilon| \le (1 + p) \, \omega^3/ (3! \, \sqrt{(n' + 1) \, p}) \to 0$ for $\tau = n' \to \infty$. The standardized negative binomial distribution thus also converges in distribution to the standardized normal distribution.

The probability function of Eq. (16) is identical with the distribution of the sum $N = N_1 + N_2$ of the independent random variables N_1 and N_2, where N_1 is Poisson-distributed with the parameter ϱt, and N_2 follows a negative binomial distribution according to Eq. (17) with the parameters n'. $p = t/(t+t')$, and $q = t'/(t + t')$. Applying the Markov formula according to Eq. (9) yields for N the folded distribution

$$f(n \mid \varrho; n') = \sum_{n_1, n_2=0}^{\infty} \delta_{n, n_1+n_2} \cdot \frac{e^{-\varrho t}(\varrho t)^{n_1}}{n_1!} \cdot \frac{(n_2 + n')!}{n_2! \, n'!} p^{n_2} \, q^{n'+1}. \tag{42}$$

Replacing n_1 by k and n_2 by $n - k$ and observing $0 \le k \le n$, we easily obtain the probability function of Eq. (16). Because of the additivity of expectation values, variances, and logarithms of the characteristic functions according to Eq. (10) when independent random variables are added, we obtain $E \, N = \varrho t + (n' + 1)p/q$ and $\text{Var} \, N = \varrho t + (n' + 1)p/q^2$, and the standardized distribution of N also converges in distribution to the standardized normal distribution if $\varrho t \to \infty$ and $n' \to \infty$.

The probability density according to Eq. (21) can also be derived by folding two gamma distributions of independent random variables $\hat{v}$ and $\hat{v}'$ whereby $\hat{\varrho} = \hat{v}/t - \hat{v}'/t' \ge 0$. If, for the moment, the Heaviside factor $H(\varrho)$ is omitted in Eq. (21), then, according to the first, general part of this Appendix, the distribution of $\hat{\varrho}$, standardized with its expectation value $\mu = (n + 1)/t - (n'+1)/t'$ and variance $\sigma^2 = (n + 1)/t^2 + (n' + 1)/t'^2$, converges in distribution to the standardized normal distribution if $n \to \infty$ and $n' \to \infty$. The factor $H(\varrho)$ then truncates that standardized distribution at the abscissa $-\mu/\sigma$ corresponding to $\varrho = 0$. The remaining distribution is not nor-

mal and not standardized except if $\mu/\sigma \rightarrow \infty$. But $\mu/\sigma \gg 1$ will not always be found.

Conclusion

The decision threshold, the detection limit, and the confidence limits have been defined on the basis of Bayesian statistics as close as possible to the corresponding conventional-statistical characteristic limits. They can also be used in cases often occurring in practice, in which not only repeated or counting measurements are involved and, thus, conventional statistics fails. At least in the important basic case of counting measurements where a potential contribution of a particular nuclear radiation in question is to be detected and both statistics are applicable, the numerical differences between the differently defined characteristic limits turn out to be small and to even vanish asymptotically. There is thus no need to change the usual practice of applying the characteristic limits specified in DIN 25482-1 [1] in the case of a fixed duration of measurement.

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The author of this contribution

Dr. *Klaus Weise*, Parkstr. 11, D-38179 Schwülper, Germany. E-mail: klaus.weise@t-online.de