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Determination of the detection limit and decision threshold for ionizing radiation measurements —

Part 8: Fundamentals and application to unfolding of spectrometric measurements without the influence of sample treatment

Détermination de la limite de détection et du seuil de décision des mesurages de rayonnements ionisants —

Partie 8: Principes fondamentaux et leur application à la déconvolution des spectres des mesurages de rayonnements ionisants négligeant l'influence de la préparation d'un échantillon

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ISO copyright office
Case postale 56 • CH-1211 Geneva 20
Tel. + 41 22 749 01 11
Fax + 41 22 749 09 47
E-mail copyright@iso.org
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Foreword

ISO (the International Organization for Standardization) is a worldwide federation of national standards bodies (ISO member bodies). The work of preparing International Standards is normally carried out through ISO technical committees. Each member body interested in a subject for which a technical committee has been established has the right to be represented on that committee. International organizations, governmental and non-governmental, in liaison with ISO, also take part in the work. ISO collaborates closely with the International Electrotechnical Commission (IEC) on all matters of electrotechnical standardization.

International Standards are drafted in accordance with the rules given in the ISO/IEC Directives, Part 2.

The main task of technical committees is to prepare International Standards. Draft International Standards adopted by the technical committees are circulated to the member bodies for voting. Publication as an International Standard requires approval by at least 75 % of the member bodies casting a vote.

Attention is drawn to the possibility that some of the elements of this document may be the subject of patent rights. ISO shall not be held responsible for identifying any or all such patent rights.

ISO 11929-8 was prepared by Technical Committee ISO/TC 85, *Nuclear energy*, Subcommittee SC 2, *Radiation protection*.

ISO 11929 consists of the following parts, under the general title *Determination of the detection limit and decision threshold for ionizing radiation measurements*:

— *Part 1: Fundamentals and application to counting measurements without the influence of sample treatment*

— *Part 2: Fundamentals and application to counting measurements with the influence of sample treatment*

— *Part 3: Fundamentals and application to counting measurements with high resolution gamma spectrometry, without the influence of sample treatment*

— *Part 4: Fundamentals and applications to measurements by use of linear-scale analogue ratemeters, without the influence of sample treatment*

— *Part 5: Fundamentals and applications to counting measurements on filters during accumulation of radioactive material*

— *Part 6: Fundamentals and applications to measurements by use of transient mode*

— *Part 7: Fundamentals and general applications*

— *Part 8: Fundamentals and applications to unfolding of spectrometric measurements without the influence of sample treatment*

Introduction

This part of ISO 11929 gives basic information on the statistical principles for the determination of the detection limit, of the decision threshold and of the limits of the confidence interval for general applications of nuclear radiation measurements.

ISO 11929-1 and ISO 11929-2 deal with integral counting measurements with or without consideration of the sample treatment. High-resolution spectrometric measurements, which can be evaluated without unfolding techniques, are covered in ISO 11929-3 while evaluations of spectra via unfolding have to be treated according to this part of ISO 11929. ISO 11929-4 deals with measurements using linear scale analogue ratemeters, ISO 11929-5 with monitoring of the concentration of aerosols in exhaust gas, air or waste water, and ISO 11929-6 with measurements by use of a transient measuring mode.

Parts 1 to 4 were elaborated for special measuring tasks in nuclear radiation measurements based on the principles defined by Altschuler and Pasternack [1], Nicholson [2], Currie [3]. ISO 11929-7 gives a general Bayesian-statistical approach for the determination of decision thresholds, detection limit and confidence intervals by separating the determination of these characteristic quantities from the evaluation of the measurement. Consequently ISO 11929-7 is generally applicable and can be applied to any suitable procedure for the evaluation of a measurement. Parts 5, 6 and 7 and this part of ISO 11929 are based on methods of Bayesian statistics (see [5] in the Bibliography) for the determination of the characteristic limits (see [6] and [7] in the Bibliography) as well as for the unfolding (see [8] in the Bibliography).

This part of ISO 11929 makes consequent use of the general approach of ISO 11929-7 and describes explicitly the necessary procedures to determine decision thresholds, detection limits and confidence limits for physical quantities which are derived from the evaluation of nuclear spectrometric measurements by unfolding techniques, without taking into account the influence of sample treatment (see [4] in the Bibliography). There are many types of such quantities, for example, the net area of a spectral line in gamma- or alpha-spectrometry.

Since the uncertainty of measurement plays a fundamental role in this part of ISO 11929, evaluations of measurements and the determination of the uncertainties of measurement have to be performed according to the Guide for the Expression of Uncertainty in Measurement.

For this purpose, Bayesian statistical methods are used to specify statistical values characterized by the following given probabilities:

— The *decision threshold*, which allows a decision to be made for each measurement with a given probability of error as to whether the result of a measurement indicates the presence of the physical effect quantified by the measurand.

— The *detection limit*, which specifies the minimum true value of the measurand which can be detected with a given probability of error using the measuring procedure in question. This consequently allows a decision to be made as to whether a measuring method checked using this part of ISO 11929 satisfies certain requirements and is consequently suitable for the given purpose of measurement.

— The *limits of the confidence interval*, which define an interval which contains the true value of the measurand with a given probability, in the case that the result of the measurement exceeds the decision threshold.

Determination of the detection limit and decision threshold for ionizing radiation measurements —

Part 8: Fundamentals and application to unfolding of spectrometric measurements without the influence of sample treatment

1 Scope

This part of ISO 11929 specifies a method for determination of suitable statistical values which allow an assessment of the detection capabilities in spectrometric nuclear radiation measurements, and of the physical effect quantified by a measurand (for example, a net area of a spectrometric line in an alpha- or gamma-spectrum) which is determined by evaluation of a multi-channel spectrum by unfolding methods, without the influence of sample treatment. For this purpose, Bayesian statistical methods are used to specify characteristic limits.

2 Normative references

The following referenced documents are indispensable for the application of this document. For dated references, only the edition cited applies. For undated references, the latest edition of the referenced document (including any amendments) applies.

BIPM/IEC/IFCC/ISO/IUPAC/IUPAP/OIML, *Guide to the expression of uncertainty in measurement*, Geneva, 1993

BIPM/IEC/IFCC/ISO/IUPAC/IUPAP/OIML, *International vocabulary of basic and general terms in metrology.* 2nd edition, Geneva, 1993.

ISO 11929-3:2005, *Determination of the detection limit and decision threshold for ionizing radiation measurements — Part 3: Fundamentals and application to counting measurements with high resolution gamma spectrometry, without the influence of sample treatment*

ISO 11929-7:2005, *Determination of the detection limit and decision threshold for ionizing radiation measurements — Part 7: Fundamentals and general applications*

3 Terms and definitions

For the purposes of this document, the following terms and definitions apply.

3.1
measuring method
any logical sequence of operations, described generically, used in the performance of measurements

NOTE Adapted from the International Vocabulary of Basic and General Terms in Metrology:1993.

3.2
measurand
particular quantity subject to measurement

[International Vocabulary of Basic and General Terms in Metrology:1993]

NOTE In this part of ISO 11929, a measurand is non-negative and quantifies a nuclear radiation effect. The effect is not present if the value of the measurand is zero. It is characteristic of this part of ISO 11929 that the measurand is derived from a multi-channel spectrum by unfolding methods. An example of a measurand is the intensity of a line in a spectrum above the background in a spectrometric measurement.

3.3
uncertainty (of measurement)
parameter, associated with the result of a measurement, that characterizes the dispersion of the values that could reasonably be attributed to the measurand

[Guide for the expression of uncertainty in measurement:1993]

NOTE The uncertainty of a measurement derived according to the Guide for the expression of uncertainty in measurement comprises, in general, many components. Some of these components may be evaluated from the statistical distribution of the results of series of measurements and can be characterized by experimental standard deviations. The other components, which also can be characterized by standard deviations, are evaluated from assumed or known probability distributions based on experience and other information.

3.4
mathematical model of the evaluation
a set of mathematical relationships between all measured and other quantities involved in the evaluation of measurements

3.5
decision quantity
random variable for the decision whether the physical effect to be measured is present or not

3.6
decision threshold
fixed value of the decision quantity by which, when exceeded by the result of an actual measurement of a measurand quantifying a physical effect, one decides that the physical effect is present

NOTE The decision threshold is the critical value of a statistical test to decide between the hypothesis that the physical effect is not present and the alternative hypothesis that it is present. When the critical value is exceeded by the result of an actual measurement, this is taken to indicate that the hypothesis should be rejected. The statistical test will be designed such that the probability of wrongly rejecting the hypothesis (error of the first kind) is at most equal to a given value α.

3.7
detection limit
smallest true value of the measurand which is detectable by the measuring method

NOTE The detection limit is the smallest true value of the measurand which is associated with the statistical test and hypotheses according to 3.6 by the following characteristics: if in reality the true value is equal to or exceeds the detection limit, the probability of wrongly not rejecting the hypothesis (error of the second kind) will be at most equal to a given value β.

3.8
confidence limits
values which define confidence intervals to be specified for the measurand in question which, if the result exceeds the decision threshold, includes the true value of the measurand with the given probability $(1 - \gamma)$

3.9
guideline value
value which corresponds to scientific, legal or other requirements for which the measuring procedure is intended to assess

EXAMPLE Activity, specific activity or activity concentration, surface activity, or dose rate.

4 Quantities and symbols

$\hat{\xi}$ Random variable as estimator for a non-negative measurand quantifying a physical effect

ξ Value of the estimator; true value of the measurand

$\tilde{u}(\xi)$ Standard uncertainty of the decision quantity X as a function of the true value ξ of the measurand

X Random variable as decision quantity; estimator of the measurand

x Result of a determination of the decision quantity X

$u(x)$ Standard uncertainty of the measurand associated with the measurand result x of a measurement

z Best estimate of the measurand

$u(z)$ Standard uncertainty of the measurand associated with the best estimate z

x^* Decision threshold for the measurand

ξ^* Detection limit for the measurand

ξ_l, ξ_u Respectively, lower and upper limit of the confidence interval for the measurand

i Number of a channel in a multi-channel spectrum obtained by a spectrometric nuclear radiation measurement; ($i = 1, ..., m$)

ϑ Continuous parameter (for example, energy or time) related to the different channels in a multi-channel spectrum

ϑ_i Value of ϑ connected with channel i; ($i = 1, ..., m$)

t Measuring time

m Number of channels in the spectrum

N_i Independent Poisson-distributed random variables of events counted in a channel i during the measurement of duration t; ($i = 1, ..., m$)

n_i Number of events counted in a channel i during the measuring time t; ($i = 1, ..., m$)

X_i Independent random variable of the rate of events counted in a channel i during a measurement of duration t, input quantities of the evaluation; $X_i = N_i / t$; ($i = 1, ..., m$)

$\boldsymbol{X}$ Column matrix of the X_i

x_i Rate of events counted in a channel i during a measurement of duration t; $x_i = n_i / t$; ($i = 1, ..., m$)

$\boldsymbol{x}$ Column matrix of the x_i

$\boldsymbol{x}'$ Column matrix $\boldsymbol{x}' = \boldsymbol{A}\boldsymbol{y}'$

$u(x_i, x_j)$ Covariance associated with x_i and x_j

Y_k Output quantity Y_k derived from the multi-channel spectrum by unfolding methods; $k = 1, ..., n$

$\boldsymbol{Y}$ Column matrix of the Y_k

y_k Estimate of an output quantity (parameter), Y_k; ($k = 1, ..., n$)

$u(y_k)$ Standard uncertainty of y associated with y_k

$\boldsymbol{y}'$ Column matrix $\boldsymbol{y}$ after replacement of y_1 by ξ

$H(\vartheta_i)$ Functional relationship representing the spectral density at ϑ_i of a multi-channel spectrum; $H(\vartheta_i) = \sum_{k=1}^{n} \Psi_k(\vartheta_i) \cdot Y_k$

p Number of input quantities t_i which are not subject to fit

$\Psi_k(\vartheta)$ Function describing the shapes of the individual spectral lines and of the background contributions; ($k = 1, ..., n$)

n Number of output quantities

$\boldsymbol{v}$ Column matrix of input quantities; $\boldsymbol{v} = (x_1, ..., x_m, t_1, ..., t_p)$

t_i Input quantities which are not subject to fit

$\boldsymbol{M}(\boldsymbol{Y})$ Column matrix of the $H(\vartheta_i)$

$\boldsymbol{A}$ Response matrix of the spectrometer

A_{ik} Elements of the response matrix $\boldsymbol{A}$

$\boldsymbol{U_x}$ Uncertainty matrix of $\boldsymbol{X}$

$\boldsymbol{U_y}$ Uncertainty matrix of $\boldsymbol{Y}$

G_k Function of the input quantities X_i, ($i = 1, ..., m$)

$\boldsymbol{G}$ Column matrix of the G_k

α Probability of the error of the first kind; the probability of rejecting the hypothesis if it holds true

β Probability of the error of the second kind; the probability of accepting the hypothesis if it is false

$1 - \gamma$ Probability attributed to the confidence interval of the measurand; probability that the true value of the measurand is included by the confidence interval

k_p Quantiles of the standardized normal distribution for the probability p (see Table 1); $p = 1 - \alpha$, $1 - \beta$, $1 - \gamma$

E Operator for the formation of the expectation of a random variable

Var Operator for the formation of the variance of a random variable

diag Indicator for a diagonal matrix

5 Statistical values and confidence interval

5.1 Principles

5.1.1 General aspects

For a particular task involving nuclear radiation measurements, first the particular physical effect which is the objective of the measurement has to be described. Then a non-negative measurand has to be defined which quantifies the physical effect and which assumes the value zero if the effect is not present in an actual case.

A random variable, called a decision quantity X, has to be attributed to the measurand. It is also an estimator of the measurand. It is required that the expectation value EX of the decision quantity X equals the true value ξ of the measurand. A value x of the estimator X derived from measurements is a primary estimate of the measurand. The primary estimate x of the measurand, and its associated standard uncertainty $u(x)$, have to be calculated as the primary complete result of the measurement according to the Guide for the expression of uncertainty in measurement, by evaluation of measured quantities and of other information using a mathematical model of the evaluation which takes into account all relevant quantities. Generally, the fact that the measurand is non-negative will not be explicitly made use of. Therefore, x may become negative, in particular, if the true value of the measurand is close to zero.

NOTE The model of the evaluation of the measurement need not necessarily be given in the form of explicit mathematical formulas. It can also be represented by an algorithm or a computer code.

For the determination of the decision threshold and the detection limit, the standard uncertainty of the decision quantity has to be calculated, if possible, as a function $\tilde{u}(\xi)$ of the true value ξ of the measurand. In the case that this is not possible, approximate solutions are described below.

ξ s the value of another, non-negative estimator $\hat{\xi}$ of the measurand. The estimator $\hat{\xi}$, in contrast to X, makes use of the knowledge that the measurand is non-negative. The limits of the confidence interval to be determined refer to this estimator $\hat{\xi}$ (compare 5.4). Besides the limits of the confidence interval, the expectation value E$\hat{\xi}$ of this estimator as a best estimate z of the measurand, and the standard deviation $[\mathrm{Var}(\hat{\xi})]^{1/2}$ as the standard uncertainty $u(z)$ associated with the best estimate z of the measurand, have to be calculated (see 6.3).

For the numerical calculation of the decision threshold and the detection limit, the function $\tilde{u}(\xi)$ is needed, which is the standard uncertainty of the decision quantity X as a function of the true value ξ of the measurand. The function $\tilde{u}(\xi)$ generally has to be determined by the user of this part of ISO 11929 in the course of the evaluation of the measurement according to the Guide for the expression of Uncertainty in Measurement. For examples see Annex A. This function is often only slowly increasing. Therefore, it is justified in many cases to use the approximation $\tilde{u}(\xi) = u(x)$. This applies, in particular, if the primary estimate x of the measurand is not much larger than its standard uncertainty $u(x)$ associated with x. If the value x is calculated as the difference (net effect) of two approximately equal values y_1 and y_0 obtained from independent measurements, that is $x = y_1 - y_0$, one gets $\tilde{u}^2(0) = u^2(y_1) + u^2(y_0)$ with the standard uncertainties $u(y_1)$ and $u(y_0)$ associated with y_1 and y_0, respectively.

If only $\tilde{u}^2(0)$ and $u(x)$ are known, an approximation by linear interpolation is often sufficient for $x > 0$ according to:

$$\tilde{u}^2(\xi) = \tilde{u}^2(0) \cdot (1 - \xi / x) + u^2(x) \cdot \xi / x \tag{1}$$

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

For setting up the mathematical model of the evaluation of the measurement, one has to distinguish two types of physical quantities, input and output quantities. The output quantities Y_k ($k = 1, ..., n$) are viewed as measurands (for example, the parameters of an unfolding or fitting procedure) which have to be determined by the evaluation of a measurement. The decision quantity X is one of them. They depend on the input