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Statistical analysis of low-level material screening measurements via gamma-spectroscopy

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ABSTRACT

Background estimations in neutrinoless double beta decay experiments ($0\nu\beta\beta$) require reliable statistical limits on gamma-spectrometric low-level material screening measurements. For this purpose a custom method based on Bayesian statistics with reference to the international standard ISO 11929-7 is presented. The analysis combines the data from sample- and background spectra and comprises the physical knowledge of non-negative counting rates. It allows to incorporate multiple gamma lines of radionuclides. The confidence intervals pass continuously from two-sided intervals into single-sided upper limits.

1. Introduction

At present a new generation of experiments is dedicated to the search of neutrinoless double beta decay ($0\nu\beta\beta$) at extremely low background rates. In case of the GERDA experiment (Abt et al., 2004) a background index of 10^{-3} counts/(kg a keV) or better at the $Q_{\beta\beta}$-value of 2039 keV in ^{76}Ge is aspired. In order to reach this background level strict material screening and selection of the construction and shielding materials for high radiopurity is essential. For this purpose a number of low-level gamma-spectrometers are employed which are designed to reach the required sensitivities ranging from mBq/kg (Budjáš et al., 2008) down to some 10 μBq/kg (Heusser et al., 2004; Neder et al., 2000).

Throughout the design phase of the experiment the background contribution is estimated for each component using the data from material screening in combination with Monte Carlo simulations. Vice versa the design may be adapted in consideration of new results from the screening measurements. This leads to the necessity to utilise a statistical, which is designed to provide characteristic limits at the edge of the sensitivity. This article proposes such a procedure for the case of low-level gamma-spectroscopy.

2. Ancillary conditions for the analysis

2.1. Desirable properties of the final result

Under the assumption that the result of a material screening measurement is used for the background estimation of a low-background experiment, it is necessary to provide an estimate and characteristic limits on the specific activity of radionuclides in the sample, regardless whether a peak is detected or not. In case of a positive result (peak detection), an estimate of the unknown true value of the specific activity should be quoted together with a two-sided confidence interval. In case of a null result, an *upper limit* (single-sided confidence interval) on the specific activity must be provided. The latter should be constructed such that it makes best use of the available data and reflects our knowledge about the smallness of the sample's activity.

At this point it must be stressed that the corresponding international standard ISO 11929-7 (2005) does not provide confidence limits for the case that the result of a measurement does not exceed the *decision threshold*. For this case it is recommended to add the comment "below the decision threshold" to the documentation, whereas no upper limit is specified. For this reason the standard does not provide us the necessary tool for the evaluation of our data.

Note that the standard advises to compare a guideline value to the *detection limit* of the measuring procedure prior to the measurement to check whether the procedure is suitable for the given purpose. In our case such a guideline value does not exist since it is generally the task to measure the specific activity to the lowest possible sensitivity.

2.2. Demands from the measurement process

In the following we presuppose that each measurement of the sample's specific activity is composed out of a sample spectrum and a separate background spectrum, recorded under comparable conditions. The net counting rates R_n and R_b of the peaks are determined independently for each spectrum, with the objective

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of substracting the background peak contribution from the corresponding peak in the sample spectrum. The classical formula to assess the specific activity A_{spec} with regards to one spectral line of a certain isotope reads

$$A_{spec} = w(R_n - R_b). \quad (1)$$

The sample's mass and the full energy peak efficiency are summarised in the factor w. As we premise low counting rates of only a few counts per day and peak or less, it is assumed that the counting statistics is the dominant source of uncertainty in the measurement.

The classical formula bears the problem of unphysical negative results due to statistical fluctuations of R_n and R_b. This is likely for the common case of having a non-detectable activity in the sample, whereas the background spectrum yields a non-zero net counting rate. On the other hand it is not desirable to subtract a negative R_b from R_n, in particular, if one background spectrum is used for several sample measurements. The introduced bias is of the order of the uncertainty of R_b and thus is relevant for low-level measurements. Therefore, we demand from the analysis to take into account the physical constraint of allowing only non-negative estimations for the true values underlying R_n, R_b and R_n–R_b.

Moreover, we request an optimal use of the available data, since the low counting rates allow a significant improvement only at the cost of several days or months of additional life time. Therefore, the analysis must allow to combine the information of multiple spectral lines, which can be assigned to one isotope or decay chain.

Both, the treatment of separate sample and background spectra in gamma-spectroscopy and the combination of multiple spectral lines are not covered explicitly in ISO 11929-7 or other parts of the ISO 11929 series. We focus on these aspects in this analysis, because we consider them essential for low-level measurements.

3. Deriving the probability distribution

As the foundation of the analysis, we derive the probability distribution $h(\kappa)$ for the unknown true values of the specific activity κ. We start by specifying the respective probability distributions for the sample and the background spectra separately.

3.1. Probability density function for the separate spectra

The quantities to be measured are defined as the effective net counting rates of the sample and the background spectrum, in the dimension of the specific activity. These measurands are estimated by

$$x = w \cdot R_n \quad \text{and} \quad y = w \cdot R_b \quad (2)$$

and the corresponding unknown true values are μ and η. Note that $\kappa = \mu - \eta$.

The probability distribution $f(x|\mu)$ is the conditional probability density for obtaining a measured value x given the true value μ. It is shown in Weise et al. (2006) to have the form of a gaussian distribution

$$f(x|\mu) = C \cdot \exp\left[-\frac{1}{2}\left(\frac{x-\mu}{\tilde{u}(\mu)}\right)^2\right] \quad (\mu \geqslant 0), \quad (3)$$

where $\tilde{u}(\mu)$ is the standard uncertainty of μ, and C is the normalisation constant. It can also be interpreted as the likelihood function, which contains the full information with respect to the unknown parameter μ, according to the likelihood principle (Berger and Wolpert, 1984; Basu, 1988).

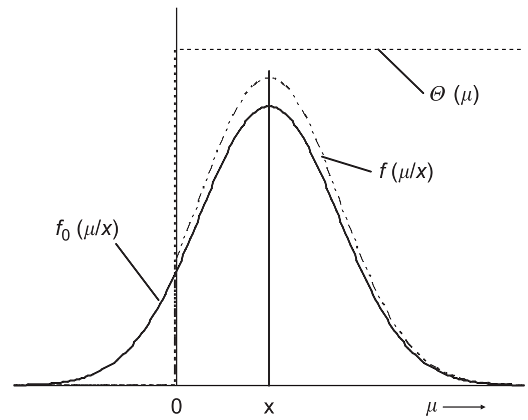

Fig. 1. Illustration of the probability distribution and constituents given in Eq. (5).

The application of the Bayes theorem allows to change from $f(x|\mu)$ to the probability distribution $f(\mu|x)$ for the true values μ in dependence on x,

$$f(\mu|x) \cdot f(x) = f(x|\mu) \cdot f(\mu). \quad (4)$$

The distribution $f(\mu)$ is called the *model prior* and represents all the information about the measurand before the experiment is performed. For our case of non-negative event rates we choose $f(\mu) = \Theta(\mu)$ to be the heaviside step function, which is constant for $\mu \geqslant 0$ and zero for $\mu < 0$. $f(x)$ is uniform for all x and may be utilised for normalisation.

For $f(\mu|x)$ we obtain the "truncated gaussian" distribution (see Fig. 1)

$$f(\mu|x) = C \cdot \Theta(\mu) \cdot f_0(\mu|x), \quad (5)$$

with $f_0(\mu|x)$ being the gaussian distribution originating from Eq. (3), however, the parameter μ becomes the variable and x becomes the parameter. For the standard uncertainty it holds $u(x) = \tilde{u}(\mu)$, whereas $u(x)$ can be determined from the input quantities of x. C now contains the normalisation factor of Eq. (3) as well as $f(x)$. In the following C can always be considered the proper normalisation constant, since $f(x)$ can be chosen accordingly.

So far, the origin and relation of $f(x|\mu)$ to $f(\mu|x)$ has been described according to Weise et al. (2006), which established the statistical basis for ISO 11929-7. In analogy, we obtain the distribution functions $g(y|\eta)$ and $g(\eta|y)$ for the background spectrum.

3.2. Combining the sample and background spectrum

In the next step, we combine the information of the two spectra by introducing the condition $\kappa = \mu - \eta \geqslant 0$ for a non-negative specific activity and convoluting the distribution functions. The product of the single distribution functions $f(x|\mu)$ and $g(y|\eta)$ yields the probability density of receiving a set of (x,y) with a given set of (μ,η),

$$h(x,y|\mu,\eta) = f(x|\mu) \cdot g(y|\eta). \quad (6)$$

Now, the Bayes theorem is applied to obtain the distribution function for the true values. In addition to the model priors $\Theta(\mu)$ and $\Theta(\eta)$ from above, we insert the condition $\mu - \eta \geqslant 0$,

$$h(\mu,\eta|x,y) = C \cdot \Theta(\mu) \cdot \Theta(\eta) \cdot \Theta(\mu - \eta) \cdot f_0(\mu|x) \cdot g_0(\eta|y). \quad (7)$$

The relation $\kappa = \mu - \eta$ allows to change from the variables (μ,η) to a new set of variables, including the variable of interest κ,

$$(\mu,\eta) \Leftrightarrow (\mu,\mu-\kappa) \Leftrightarrow (\kappa+\eta,\eta). \quad (8)$$