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New statistical methods for exotic nuclei

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Abstract

When fitting spectra with a low number of counts per channel, the standard χ^2 fits will give systematic errors. The maximum likelihood method will perform better. Its behaviour in goodness-of-fit testing is analyzed and some alternative methods employing empirical distribution functions are mentioned.

In experiments with exotic nuclei one often will end up with spectra containing a low number of counts per channel. The standard statistical methods, see, e.g., [1,2], typically use "the law of large numbers" and assume a reasonable number of counts per bin (often values around 10 are quoted as being needed). To obtain this one might have to add so many channels that the resolution in the spectrum is lost. If binning is not done, one has to proceed carefully since the behaviour of the standard methods at a low number of counts can be quite different from the asymptotic limit. A general solution of this problem is to perform Monte Carlo simulations of the experiment. However, specific results could be useful and the aim of this contribution is to present some. In the general analysis we shall often look at "background spectra", i.e. spectra where all channels have the same number of expected counts μ (obeying the Poisson distribution), but we shall also for definiteness give examples of the use of the techniques for half-life spectra. Some earlier work in this direction was presented in [3].

Two versions of χ^2 tests are often met. The first using "theoretical errors" and the second using "experimental errors". To avoid confusion we shall follow Ref. [4] and refer to them as "Pearson's χ^2" and "Neyman's χ^2", respectively. They are given by $\chi^2_{\mathrm{P}} = \sum_i (n_i - y_i)^2/y_i$ and $\chi^2_{\mathrm{N}} = \sum_i (n_i - y_i)^2/n_i$. An independent way of proceeding

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is to use maximum likelihood. We shall use it in the form of the "likelihood χ^2" that is based on the likelihood ratio technique and for Poisson distributed data it is [4]

$$\chi^2_\lambda = 2\sum_i \bigl(y_i - n_i + n_i \ln(n_i/y_i)\bigr). \tag{1}$$

In the above formulae n_i and y_i are the count numbers and theoretical values in channel i. In order to handle the case $n_i = 0$, the last term in Eq. (1) should be changed to $n_i \ln(\max(n_i, 1)/y_i)$. This does not affect the numerical value.

For gaussian distributed data, χ^2_{P} will give correct fit values, but for low μ the difference between the Poisson and the gaussian distribution will be felt. For estimation of a constant background spectrum, χ^2_{P} will give a fit value 0.5 larger than the correct μ; this bias is felt stronger the smaller μ is. The alternative χ^2_{N} is even worse behaved and will give a fit value 1.0 smaller than μ (the detailed derivation of these results can be found in [5]). In contrast, χ^2_λ will give the correct value no matter how low μ gets. This bias in the standard χ^2 methods will of course also be felt for nonconstant spectra. As an example we shall look at the time distribution of the beta-delayed protons from ^{17}Ne based on the data in [6]. This spectrum had no background and extended for almost ten half-lives. Results from the three different fit methods are given in Table 1, the errors are determined as the parameter changes that increase χ^2 by one [1,2]. If the data are fit without a background term, the resulting half-life values differ. Introducing a background, the half-life values become more consistent, since the background term gets a value approximately equal to the bias given above. Note that binning improves the reliability of the χ^2 fits, but that the background remains at the bias value. (The half-life for ^{17}Ne quoted in [6] of 109.3 ± 0.6 ms was based on a χ^2_{N}-analysis with binned spectrum but no background. It should be replaced by 109.6 ± 0.7 ms.)

Maximum likelihood gives correct parameter values and error bars. We now turn to its use in goodness-of-fit tests. Although χ^2_λ asymptotically will be χ^2-distributed [1,4] and therefore have an expectation value equal to the number of degrees of freedom N, the behaviour for small count numbers will be different. For the case considered above (constant spectrum with expectation value μ per channel), one can derive explicit expressions for the behaviour and show that $\chi^2_\lambda \to N$ for large μ. The behaviour at lower values is given in Fig. 1. This figure also gives the variance of $\sqrt{2\chi^2_\lambda}$ (for a true χ^2

Table 1
The half-life of ^{17}Ne evaluated with different methods

Background in fit?	Bin width (ms/ch)	Half-life (ms) χ^2_{N}	χ^2_{P}	Max. likelihood
No	5.46	108.40 ± 0.54	110.10 ± 0.56	109.54 ± 0.56
Yes	5.46	109.69 ± 0.70	109.58 ± 0.74	109.61 ± 0.73
No	27.29	109.29 ± 0.55	109.67 ± 0.56	109.54 ± 0.56
Yes	27.29	109.65 ± 0.71	109.55 ± 0.74	109.59 ± 0.73
		Background (counts/ch)		
Yes	5.46	-1.1 ± 0.4	0.5 ± 0.5	-0.1 ± 0.4
Yes	27.29	-1.7 ± 2.1	0.6 ± 2.2	-0.2 ± 2.2

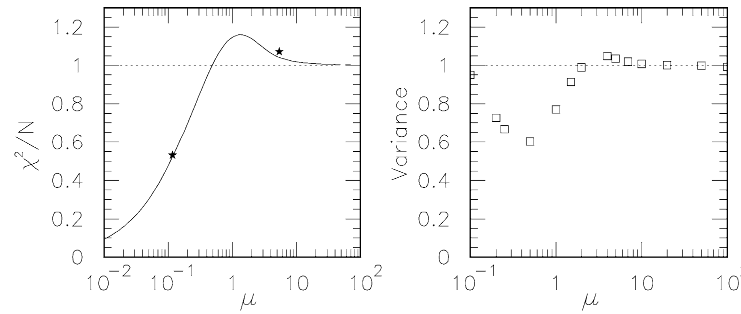

Fig. 1. Left: the value of the Poisson likelihood χ^2_λ per degree of freedom for a flat spectrum with a Poisson parameter μ. The line gives the result of an analysis done for a large number of channels N. The stars are experimental points for ^{12}Be decay spectra. Right: the variance of $\sqrt{2\chi^2_\lambda}$ calculated via Monte Carlo simulations of spectra with $N = 1000$ channels.

distribution this variance becomes 1 in the limit of large N) determined via Monte Carlo simulations. In both cases clear deviations from a χ^2 behaviour are seen for $\mu < 10$. The consequence is that χ^2_λ will take on unreasonably values if a large part of the spectrum has less than 10 counts per channel, an example is the half-life spectra from ^{12}Be shown in Fig. 1 in [7]. An analysis of the original data (binsize 0.1 ms, it is 3.2 ms in the figure) at times larger than 520 and 350 ms, respectively, i.e. when only background remains, gives the χ^2_λ-values shown in the left panel in Fig. 1. They agree with the theoretical values within the spread seen in the Monte Carlo simulations (cf. the variance in the right panel).

Even worse than this is that χ^2_λ in the limit of low count numbers effectively records only the total number of counts in the spectrum and therefore looses statistical power. In this limit, it is therefore logical to turn to other statistical methods in order to have a reliable estimate of goodness-of-fit. Several methods from robust analysis and exploratory data analysis should be considered, see, e.g., [8]. One class of methods that we shall look into here rely on the empirical distribution function (*EDF*), the equivalent of the theoretical cumulative distribution function. Formally, it can be defined for binned data as $EDF_k = \sum_{i=1}^{k} n_i/n_{\text{tot}}$ and therefore increases monotonically from 0 to 1. Given a theoretical distribution with probabilities p_i for lying in bin i and the corresponding cumulative distribution $F_k = \sum_{i=1}^{k} p_i$, several *EDF*-tests can be defined. The best known test is probably the Kolmogorov–Smirnov statistics that uses the maximum deviation between EDF_k and F_k. We shall employ here two tests that make use of the summed square deviation [9], namely the Cramér–von Mises statistics W^2 and the Anderson–Darling statistics A^2 that puts more weight on points at the ends of the distribution.

We are presently investigating the use of *EDF* tests for goodness-of-fit estimates for spectra with low count rates, since they have been shown in many cases to be superior to χ^2 tests [9,10]. The main problem in employing *EDF* tests is that the confidence levels must be estimated (e.g. with Monte Carlo methods) once the theoretical curves contain fit parameters. For the case of the (continuous) gaussian and exponential distributions, this is demonstrated in detail in [10]. However, most flat spectra turn out to give very similar confidence levels for W^2 and A^2 for a large range of count rates. As an example, the 95% confidence levels in the two cases are about 0.465 and 2.51. An ad hoc procedure for cases as the ^{12}Be half-life mentioned above would then be to employ χ^2_λ for the lowest part of the spectrum where the count rate varies with channel number and use, e.g., W^2 for the remaining "flat" part. The two resulting confidence levels can, if this is wanted, be combined as shown in [1]. For our example, the Cramér–von Mises test shows that there is less than 1% probability that the backgrounds in the two ^{12}Be spectra mentioned above are constant. This is due to small systematic deviations that can be seen in the binned spectrum in [7], but one should note that the χ^2_λ analysis (Fig. 1) was not sensitive to these deviations. The *EDF* tests are more powerful.

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