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A New Quantity to Determine the Best Model by Least-Squares Fit

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The usual χ^2 per degrees of freedom test is not reasonable to assess the quality of fit for determining the best model of spectrum shape, i.e.,

$$\chi^2/(n-q),$$

where n is the total channel number of the measured spectrum and q is the number of free parameters in a theoretical model used in the fit. A new quantity available for that purpose, i.e.,

$$(\chi^2+2q)/n,$$

is proposed in the present work.

KEYWORDS : /Non-linear Least-Squares Fit/χ^2/AIA/

1. INTRODUCTION

In the non-linear least-squares fit for analyzing spectrum data obtained by counting nuclear radiations, the χ^2 function defined by

$$\chi^2=\sum_{j=1}^{n} w_j(M_j-F_j)^2, \tag{1}$$

is minimized to estimate the most probable values of free parameters in theoretical model for spectrum shape, where M_j,($j=1,2,\cdots,n$) is the spectrum data which is usually given by a set of radiation counts in each channel j, n is the total number of channels of the spectrum and w_j is the weight for M_j. Generally, w_j is given by $1/\sigma_j{}^2$, where σ_j is the standard deviation of M_j, i.e.,

$$\sigma_j=M_j{}^{1/2}. \tag{2}$$

The theoretical model for spectrum shape is expressed by $F_j(a_1,a_2,\cdots,a_q)$ ($j=1,2,\cdots,n$) in Eq. (1), where a_j($j=1,2,\cdots,q$) is the free parameter in the model and q is the number of the parameters.

A purpose of the non-linear least-squares fit is usually to extract information about energies or intensities of nuclear radiations from measured spectra, i.e., peak counts, position or width.

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Since these quantities are related to free parameters in the theoretical model, they are estimated from the most probable values of free parameters determined by the fit. Any results from the fit suffers from two kinds of uncertainties. One is the random uncertainty in spectra obtained by counting nuclear radiations, which can be treated by the theory of statistics. The other is the systematical deviation between theoretically assumed and real spectrum shapes.

Since a computer program for analyzing the gamma-ray spectra was developed by Helmer et al. more than twenty years ago[1], χ^2 per degrees of freedom given by

$$\chi^2/(n-q)$$

has been used in the test of theoretical models. It is often required to select the best in several possible models for spectrum shape. Then, a model which results in the smallest $\chi^2/(n-q)$ is employed as the best one. The same quantity has been also used in the error estimation of free parameters. The following matrix is usually used as error matrix for the most probable values of free parameters:

$$(E)=(L^{-1})_{ij}\chi^2/(n-q), \tag{3}$$

where $(L)_{ij}$ is the normal matrix deduced from the theory of statistics[2], i.e.,

$$\begin{aligned}(L)_{ij}&=\sum_{k=1}^{n}\frac{1}{M_k}\left(\frac{\partial F_k}{\partial a_i}\cdot\frac{\partial F_k}{\partial a_j}-\frac{M_k-F_k}{M_k}\cdot\frac{\partial^2 F_k}{\partial a_i\partial a_j}\right),\\ &\simeq\sum_{k=1}^{n}\frac{1}{M_k}\cdot\frac{\partial F_k}{\partial a_i}\cdot\frac{\partial F_k}{\partial a_j},\quad (i,j=1,2,\cdots,q).\end{aligned} \tag{4}$$

The $\chi^2/(n-q)$ in Eq. (3) may be regarded as a correction for the systematic deviation between true and assumed (model) spectra, i.e., the impreciseness of the model used in the fit.

The above method to test models by means of $\chi^2/(n-q)$ and also to estimate errors from Eq. (3) which includes the same quantity are now quite popular. However, there has not so far been performed any verification for their theoretical consistencies. A more reasonable quantity for determining the best model is deduced in the present paper. An improved method for estimating uncertainties in the most probable values of free parameters is also suggested.

2. A NEW QUANTITY FOR ASSESSING QUALITY OF FIT

The most probable values of free parameters determined by the minimization of Eq. (1) actually fluctuate depending on statistics of the measured spectrum and impreciseness of the model function employed in the fit. $\chi^2/(n-q)$ has the same form as the unbiased estimate or for the variance of errors, which appears in the theory of statistics[2]. Therefore, if the systematical deviations between a model function and true spectrum shape would behave like the statistical fluctuation, $\chi^2/(n-q)$ would equal to the variance of errors. However, the systematic deviation at each channel are not independent, that is, the deviation is quit different from the statistical fluctuation. It is clearly wrong to use Eq. (3) for estimating errors of data including systematic uncertainties. Thus, we have not any theoretical basis to use $\chi^2/(n-q)$ in the non-linear least-squares fit.

In our previous work[3], a theoretical basis of the χ^2 fit was reviewed with attention to two error sources; one is the random uncertainty in spectra obtained by counting nuclear radiations while the other is the systematical deviation between theoretically assumed and real spectrum shape. According to our work[3] and others[4], the χ^2 function is approximately divided into two parts, i.e., random and systematic parts:

$$\chi^2 \simeq \chi^2(\text{random}) + \chi^2(\text{systematic}). \tag{5}$$

The random part, χ^2(random), comes from statistical fluctuations of measured data M_j. It is easily deduced from the statistical theory that the mean of this part is equal to the degree of freedom i.e., $(n-q)$. Therefore, the random part is approximately given by

$$\chi^2(\text{random}) \simeq n-q. \tag{6}$$

The systematical part comes from the deviation between theoretically assumed and real spectrum shapes, which is expressed by

$$\chi^2(\text{systematic}) = (\mu_j - F_j)^2/M_j, \tag{7}$$

where μ_j is the mean of M_j, i.e., the real spectrum shape. Note that we cannot estimate the systematic part independently because we cannot know the real spectrum shape in principle. Using the χ^2 function given by Eq. (1), the systematical part can be approximately given by

$$\chi^2(\text{systematic}) = \chi^2 - (n-q). \tag{8}$$

Now, we have to consider what is the best fit when we have many theoretical models for spectrum shape. If the statistics of measured data is very low, χ^2 for any model is near the degree of freedom, i.e., $n-q$ and χ^2(systematic) becomes near zero. This means that we cannot determine the best in the many models. If the statistics is high enough, χ^2 can be considerably larger than $n-q$ and χ^2(systematic) can be much larger than zero. In theoretical models with the same degree of freedom, the best fit is given by a model which make χ^2(systematic) smallest. However, it is not so simple to determine the best fit in models with different degrees of freedom. In an extreme case, we can aproach χ^2 to zero as we want by increasing the number of free parameters up to n. Then, we lose completely the degree of freedom of the least-squares fit.

Therefore, the best model will satisfies the following two conditions at the same time:

i) χ^2(random), i.e., the degree of freedom, is as large as possible,

ii) χ^2(systematic) is as small as possible.

A simple parameter to express the condition is

$$\chi^2(\text{systematic}) - \chi^2(\text{random}) = \chi^2 + 2q - 2n. \tag{9}$$

In the present treatment, we can say that the best fit is given by a model minimized in the difference between χ^2(random) and χ^2(systematic).

The parameter given by Eq. (9) is easily derived from the Akaike's Information Criteria (AIC)[5], which is one of most important results in the development of the theory of information. At 1974, Akaike introduced a new estimate minimum information theoretical criterion estimate (MAICE) which is designed for the purpose of statistical identification. When there are several competing models, the MAICE is defined by the model and the maximum likelihood estimates of the parameters which give the minimum of AIC:

$$AIC = -2 \log \text{(maximum likelihood)} + 2 \text{ (number of independently adjusted parameters within the model)}. \tag{10}$$

MAICE provides a versatile procedure for statistical model identification, which is free from the ambiguities inherent in the application of conventional hypothesis testing procedure. In the present case of non-linear least squares fit for spectrum data, the maximum likelihood in Eq. (10) is given by

$$\text{maximum likelihood} = \exp(-\chi^2/2). \tag{11}$$

The above equation is easily deduced from the conventional theory of statistics[2]. The number of independently adjusted parameters in Eq. (10) is q in the present case. Then we obtain

$$AIC = \chi^2 + 2q. \tag{12}$$

Using MAICE, the best fi is given by a model which makes AIC of Eq. (12) smallest. Note that Eq. (12) is equivalent to Eq. (9) when we can ignore the number of data n.

We now propose a new quantity for assessing the quality of fit and determining the best model of spectrum shape:

$$(\chi^2 + 2q)/n$$

$\chi^2/(n-q)$ conventionally used is to be substituted for $(\chi^2+2q)/n$. χ^2 becomes near $(n-q)$ when a model is good enough. Then, the new parameter is near $1+q/n$, which becomes near unity if $q \ll n$. Thus, the new quantity is defined to approach to unity for better fits as the conventional quantity $\chi^2/(n-q)$ is.

3. DISCUSSION

In our previous work[3], a method for examining results obtained by the fit and stating the uncertainties was developed with two parameters, i.e., the random misfit MR and the systematical misfit MS, which are quantitative representations of the random uncertainty and the systematical deviations, respectively:

$$MR=[(n-q)/S]^{1/2}, \tag{13}$$

$$MS=[(\chi^2+q-n)/S]^{1/2}, \tag{14}$$

where S is sum counts of spectrum data. MS can be used as an absolute measure for quality of fit, as shown in our previous work[3]. However, this quantity is not a measure for determining the best model of spectrum shape. To determine the best model, it is necessary not only to decrease systematic deviations but also to keep the degree of freedom as high as possible. One possible parameter for that purpose is $(\chi^2+2q)/n$, as described before.

Errors of free parameters optimized by the non-linear least-squares fit are usually estimated by a method based on the error matrix given by Eq. (3). Everyone, who carefully analyzes spectrum data by the fit, suspects that parameter errors such estimated are sometimes too small. This comes from the fact that the other uncertainty except the random uncertainty, i.e., the systematical deviation between theoretically assumed and real spectrum shapes, is not consistently taken into account. There has not so far been developed a theoretical method which can deduce reliable values for errors of free parameters optimized by the fit. A new consistent theory to treat uncertainties in free parameters is clearly required.

Following our previous theory[3], the present treatment may be developed to estimate the random and the systematical errors separately; random errors can be deduced from the ordinary theory of statistics while systematical errors are estimated from the new treatment for the systematical uncertainty. Estimations of random and systematical errors for various radiation spectra are now in progress. Detailed description of the new treatment will be given elsewhere.

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