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The digitized energy spectrum, registered by multichannel analyzer, is the sum of 3 components:

$$s(x) = \sum_{i=1}^{n} A_i p_i(x) + B(x) + d(x), \qquad (1)$$

where x - channel, $A_i p_i(x)$ - i-th peak, B(x) - background, d(x)-statistical error. There it is assumed, that d(x) in each channel x has Gaussian distribution with expectation equal to zero and variance D(x); $d(x_1)$ and $d(x_2)$ are statistically independent in each $x_1 \neq x_2$; the background is formed by slowly changing details of the spectrum, which do not contain the useful information. The main problem of spectra processing is to obtain the estimates of such quantities as peak areas $S_i$, peak positions $N_i$ and the width W (fwhm). The commonly used method to solve this problem consists in following: /1 - 5/ the spectrum is divided into sections, which contain the isolated peaks or groups of unresolved peaks; as model is taken the function

$$f(x,A_1,\ldots,A_n,N_1,\ldots,N_n,W) = \sum_{i=1}^{n} A_i \varphi_i(x,N_i,W) + B(x), \qquad (2)$$

where $\varphi_i$ and B(x) are functions modelling peak and background, respectively; $\varphi_i$ and B(x) are differentiable with respect to parameters; after that the parameters $A_i, N_i, W$ are estimated by the least squares method (LSM); the area value is obtained from

$$S_i = A_i \int_{-\infty}^{+\infty} \varphi_i(x,N_i,W)\,dx \qquad (3)$$

One can note the following difficulties in using this method.

1) If the peak and background models are exactly corresponding to real peak and background, the parameter estimates are unbiased and their errors depend only on estimate variances. However, usually Gauss or Lorentz functions, which represent the real peaks, as a rule, only approximately are taken as models; the background models ignore usually local fluctuations of the real background. The result is that the estimates have a bias, the value of which is not determined by the method. Meanwhile , the uncontrolled systematic error is to be avoided while processing spectra with large statistic, because it can overbalance the statistic error manytimes.

The bias can decrease if some complementary varying parameters are introduced; however, this leads to the increase of estimate variances; this means that the problem of reduction of estimate uncertainties (variance plus bias) can not be solved merely by increasing amount of varying parameters.

One can, of course, determine some parameters previously and fix them varying only a small set of parameters. However, such a complication of parametric scheme requires a great caution, for if the quantities of interest: area, position and width are composite functions of nonphysical parameters and are not estimated immediately, their estimates can be inefficient (in statistical sense /6/).

2) Another difficulty is connected with stability of the estimates. First of all, one must take into account that the absolutely exact peak and background shapes are unknown. Moreover, some disagreement may occur between the suggested and real conditions of the problem. Hence, the estimates should be stable with respect to small changes of the problem conditions: a small variation of the conditions (for example, of the model) should lead to the small estimate variation.



The method, described below, enables to decrease the total error of the estimates (variance plus bias) and to control their stability. It is based on some ideas of pattern recognition theory /7/ and assumes that there exists the pattern of a peak, which represents the shape of this peak whatever sophistioated it may be. An experimentally measured isolated peak with large statistic (previously smoothed and with the extracted background), or a combination of analytical functions, which fit this experimental peak, or an analytical function, whioh desoribes the peak shape according to theoretical consiederations can be taken as such a pattern. Therefore, the real peaks are obtained from this pattern by some transformations.

The problem of recognition and description of these peaks can be very succesfully solved when these transformations are relatively simple and do not distort the shape very strongly /7/. One can admit such transformations as a shift, broadening and amplification (group of linear transformations in terms of ref. /7/). In this case, if the real peak has the amplitude A, position N and width W, its function may be denoted as $f(x,A,N,W)$ and it is connected with the pattern $\varphi(x)$ very simply:

$$f(x,A,N,W) = A\varphi\left(\frac{x-N}{W}\right). \qquad (4)$$

We can normalyze $\varphi(x)$, so that it has a center equal to zero, width and amplitude (or area) equal to unity. Then, (4) shows that the real peak is obtained from $\varphi(x)$ by shifting by N channels, broadening by W and amplification with the similarity coefficient A.

In fact, the other characteristics of the peak shape such as asymmetry, for example, can change along the spectrum. However, it is not to be regarded as a serious obstacle , because one can always

divide the spectrum into sections, in which all characteristics, except for 3 above mentioned, are approximately constant, and process these sections correcting the shape model before transition from one section to another.

Furthermore, we can estimate unknown quantities A,N,W by LSM -fitting. The relation (4) enables a simple caloulation of the partial derivatives with respect to the parameters A,N,W, which are required by LSM. In fact:

$$\frac{\partial f}{\partial A} = \varphi(z); \quad \frac{\partial f}{\partial N} = -\frac{A}{W}\varphi'(z); \quad \frac{\partial f}{\partial W} = -\frac{Az}{W}\varphi'_z(z); \qquad (5)$$

$$\frac{\partial^2 f}{\partial A^2} = 0; \quad \frac{\partial^2 f}{\partial A \partial N} = -\frac{\varphi'_z}{W}; \quad \frac{\partial^2 f}{\partial A \partial W} = -\frac{z\varphi'_z}{W}; \quad \frac{\partial^2 f}{\partial N^2} = \frac{A}{W^2}\varphi''_{zz}; \qquad (6)$$

$$\frac{\partial^2 f}{\partial N \partial W} = \frac{A}{W^2}(\varphi'_z + z\varphi''_{zz}); \quad \frac{\partial^2 f}{\partial W^2} = \frac{Az}{W^2}(2\varphi'_z + z\varphi''_{zz}), \qquad (7)$$

where $z = \frac{x-N}{W}$.

If $\varphi(x)$ is given analytically, it is sufficient to know only $\frac{\partial \varphi}{\partial x}$ and $\frac{\partial^2 \varphi}{\partial x^2}$. If $\varphi(x)$ is given by a table, then the values $\varphi(x)$ in x, situated between the points of the table can be calculated by an interpolating formula and the derivatives by the difference formulas.

We can note the following advantages of this method:

1) $\varphi(x)$ can describe the peak shape with any exactitude and at the same time the amount of parameters is minimal; furthermore, they are of interest; thus, they are statistically efficient;

2) the method is universal and allows one to process the spectra of different kinds,without program transformation,merely by the substitution of the corresponding model table;

3) it is easy to prove whether the estimates are stable with respect to small model variations,because the appropriate model variations can be performed using, if necessary, visual control means.



Now let us consider some statistical aspects of the method. On the basis of the relation (4) a set of models can be considered:

$$CW^n\varphi\left(\frac{x-N}{W}\right), \text{ where } -\infty < n < +\infty. \qquad (8)$$

Practically, there are often used such Gaussian models as

$$\frac{S}{\sqrt{2\pi}\sigma}\cdot\exp\left(-\frac{(x-N)^2}{2\sigma^2}\right) \quad \text{and} \quad A\cdot\exp\left(-\frac{(x-N)^2}{2\sigma^2}\right).$$

They are the particular cases of (8) with n = -1 and n=0, respectively. We wish to consider each of models (8) in order to determine the most efficient way of parameter estimation. Let us construct for each model its Fisher matrix /6/. In our case we assume that the errors of the spectrum have the normal distribution so that the matrix desired will coincide with that of LSM-procedure. The minimized functional in LSM-procedure is

$$\sum_x \frac{1}{D(x)}(s(x)-f(x,\bar{p}))^2, \quad \text{where} \qquad (9)$$

$\bar{p}$ is the abbreviation for parameters to be estimated.

The element of its matrix is written

$$b_{ij} = \sum_x \frac{1}{D(x)}\frac{\partial f(x)}{\partial p_i}\frac{\partial f(x)}{\partial p_j} \qquad (10)$$

Thus, we have:

| | | |
|---|---|---|
| $W^{2n}a_{11}$ | - | $CW^{2n-1}(na_{11} - a_{13})$ |
| - | $C^2W^{2n-2}a_{22}$ | - |
| $CW^{2n-1}(na_{11}-a_{13})$ | - | $C^2W^{2n-2}(n^2a_{11}-2na_{13}+a_{33})$ |

where $a_{11} = \sum_x \frac{1}{D(x)} \varphi^2(z)$; $a_{13} = \sum_x \frac{1}{D(x)} \varphi(z)\varphi'_z(z)z$ ;

$a_{22} = \sum_x \frac{1}{D(x)} (\varphi'_z)^2$; $a_{33} = \sum_x \frac{1}{D(x)} (z\varphi'_z)^2$. (11)

We neglect the elements $b_{12}$, $b_{21}$, $b_{23}$, $b_{32}$, because they are comparatively small (if the asymmetry of $\varphi(x)$ is at a reasonable level).

The determinant of the matrix is

$$Det = C^4 W^{6n-4} a_{22}(a_{11}a_{33} - a_{13}^2) .$$

The area of model (8) will be

$$S = \int_{-\infty}^{+\infty} CW^n \varphi(\frac{x-N}{W})dx = CW^{n+1} \quad (12)$$

provided that the area of $\varphi(x)$ is equal to unity. Then we find:

$$Det = S^4 W^{2n-6} a_{22}(a_{11}a_{33} - a_{13}^2) , \quad (13)$$

i.e. if the area is fixed, the determinant is greater for the greater n. On the other hand, if we put $n = a_{13}/a_{11}$ , we make matrix almost diagonal, i.e. the estimates C,W,N will be uncorrelated.

The reciprocal of the matrix is:

| | | |
|---|---|---|
| $\frac{n^2 a_{11} - 2na_{13} + a_{33}}{W^{2n} d}$ | - | $-\frac{na_{11} - a_{13}}{W^{2n-1} Cd}$ |
| - | $\frac{1}{C^2 W^{2n-2} a_{22}}$ | - |
| $-\frac{na_{11} - a_{13}}{W^{2n-1} Cd}$ | - | $\frac{a_{11}}{C^2 W^{2n-2} d}$ |

where $d = a_{11}a_{33} - a_{13}^2$ .



Let us evaluate the variance of the area estimate. We can use the formula for variance of the function of random quantities $f(\eta_1, \ldots, \eta_k)$:

$$Df = \sum_{i,j=1}^{k} \frac{\partial f}{\partial \eta_i} \frac{\partial f}{\partial \eta_j} \operatorname{cov}(\eta_i, \eta_j) .$$

We obtain

$$DS = \frac{W^2}{d}(a_{11} + 2a_{13} + a_{33}) , \quad (14)$$

i.e. the area variance does not depend on n. One should notice that if the width W is varied, then (in the case of usually suggested Poisson distribution) the area variance differs from its expectation (otherwise, if W known and, therefore, fixed then the variance and the expeotation should be equal).

Further, the position and width variances are, respectively:

$$DN = \frac{1}{C^2 W^{2n-2} a_{22}} ; \quad DW = \frac{a_{11}}{C^2 W^{2n-2} d} . \quad (15),(16)$$

For a peak with the area $S_f$, taking into account (12), we have:

$$DN = \frac{W^4}{S_f^2 a_{22}} ; \quad DW = \frac{a_{11} W^4}{S_f^2 d} . \quad (17)$$

The relations (14),(15),(16) are available if the background has been previously subtracted. In the general case, we should estimate the peak and background parameters simultaneously. Then the accuracy of peak parameters estimates will depend on the amount of information about background. Commonly is assumed that the shape is known (polynomial, for instance) and only the amplitude is to be estimated. Then we can take the spectrum model in the form:

$$f(x) = A_1 b_1(x) + A_2 b_2(x) + \ldots + A_p b_p(x) + CW^n \varphi(\frac{x-N}{W})$$

where $b_i(x)$ - the background functions, $A_i$ - their amplitudes.

Further, we can construct Fisher matrix and see, that none of $A_i$ influences the variances of peak parameter estimates. Thus, we can conclude in this case, that the accuracy of peak parameters depends on the shape of background and does not depend on its level (the indirect dependence may be if, for example, the variance of the spectrum depends on its level: the case of Poisson distribution of the counts).

While processing the section with many peaks the parameters of one peak do not influence those of another if the peaks are not overlapped. Otherwise, the correlations between the parameters of the overlapped peaks arise. In this case the quality of estimates will depend on the parametrisation way. Let us consider the doublet, which can be described by two different models:

$$\psi_1 = C_1\varphi_1 + C_2\varphi_2; \qquad \psi_2 = (A - B)\varphi_1 + (A + B)\varphi_2$$

We have fixed here the position and the width.

The determinants of LSM - matrices are

$$det_1 = a^2 - b^2 ; \quad det_2 = 4(a^2 - b^2) ,$$

where $$a = \sum_x \frac{1}{D(x)} \varphi_1^2(x) \approx \sum_x \frac{1}{D(x)} \varphi_2^2(x); \quad b = \sum_x \frac{1}{D(x)} \varphi_1(x)\varphi_2(x) .$$

The second matrix will be approximately diagonal.

The variances are

$$DC_1 = DC_2 = \frac{a}{a^2-b^2} ; \quad DA = \frac{1}{2(a+b)} ; \quad DB = \frac{1}{2(a-b)} . \qquad (18)$$

The second model gives the more efficient estimates. By analogy to that let us consider the optimal parametrisation of the position (the amplitudes and the width are fixed). Let us take two models:

$$\psi_1 = A_1\varphi(x-N_1) + A_2\varphi(x-N_2); \quad \psi_2 = A_1\varphi(x-N+S) + A_2\varphi(x-N-S). \qquad (19)$$



The determinants are

$$det_1 = A_1^2A_2^2(a^2-b^2) ; \qquad det_2 = 4A_1^2A_2^2(a^2-b^2) .$$

The variances are

$$DN_1 = \frac{a}{A_1^2(a^2-b^2)}; \qquad DN_2 = \frac{a}{A_2^2(a^2-b^2)}$$

$$DN = \frac{(A_1^2 + A_2^2)a - 2A_1A_2b}{4A_1^2A_2^2(a^2-b^2)} ; \quad DS = \frac{(A_1^2 + A_2^2)a + 2A_1A_2b}{4A_1^2A_2^2(a^2-b^2)} . \qquad (20)$$

The second model gives here more efficient estimates too. Thus, it is more appropriate to describe the doublet by such characteristics:

1) the center of gravity N ;
2) the deviation from center of gravity S ;
3) the mean amplitude A ;
4) the deviation from the mean amplitude B .

This parametrisation is more suitable when the decomposition of the doublet is not necessary.

The full matrix for simultaneously estimated parameters of several peaks and background has, of course, the more complicated structure and its consideration in the general case does not give the possibility to obtain the analytical formulas for estimate variances, but if we neglect some unessential details and small quantities, we reduce the consideration of full matrix to above given considerations of separate blocks of this matrix.

We must point out one more source of estimate errors, namely, the computational one. Usually, if the LSM - matrix is well conditioned (its determinant is great) and minimisation process is correctly performed, the computational error, compared with statistical

one and error due to uncertainty of models, is neglectibly small. However, when the determinant is close to zero, the computational error becomes great. It is difficult to evaluate it, thus one can only recommend to use the models with well conditioned matrix.

The premature interruption of the iterational process can increase the computational error too: the estimates are not in this case least squares estimates and have a bias and non-minimal variance. It occurs usually while using the minimisation methods with slow and non-monotonous convergency: gradient, stochastic and so on. In order to avoid this error, the following minimisation procedure is the most desirable:

1) at first, the method with great radius of convergency should be employed (gradient, Gauss-Newton or some others);
2) at last, the method with great rate of convergency, e.g. Newton; the Newton's method has also the advantage: its matrix is the 2-nd derivative of the functional and if it is positively defined, then we are at minimum point.

Taking into account (11),(14),(15),(16),(18),(20), we can conclude: if the models are in agreement with the real objects and the computation is correctly performed, the errors of estimates depend only on following factors:

1) the variance of the spectrum D(x) (an unfavourable factor);
2) the statistic $S_i$ (a favourable one);
3) the width W (an unfavourable one);
4) the shape of background (an unfavourable one).

Thus, the accuracy of the estimates is defined by these factors and in order to improve it, the improvement of the factors is required.

It was assumed above, that the amount of peaks in the spectrum



is known. However, the situation often occurs when it is unknown and the experimentator can only construct some hypotheses about it. Further, he tests these hypotheses in order to accept those of significance. Recently a set of methods was proposed to construct these hypotheses automatically[8,9]. Omitting the analysis of details of these methods we consider only the final stage of testing the hypotheses. There are difficulties in two following situations:

1) if the spectrum contains the overlapped peaks;
2) if the spectrum contains the weak peaks.

Let us consider both cases. Suppose that the real spectrum has m peaks and there are two hypotheses:

$H_m$ - the spectrum has m peaks;

$H_n$ - the spectrum has n peaks.

We can put for simplicity m=2, n=1. Let us use the most powerful criterion of likelyhood ratio[10]. If the spectrum s(x) has sufficiently large statistic in each channel (s(x)> 5-10), then it has approximately Gaussian distribution, so that the ratio of likelyhoods is:

$$\frac{L(H_1)}{L(H_2)} = \frac{\exp(-\sum_x \frac{1}{D(x)}(s(x) - A\varphi(\frac{x-N}{W_1}))^2)}{\exp(-\sum_x \frac{1}{D(x)}(s(x) - \sum_{j=1}^{2} B_j \varphi(\frac{x-N}{W_2}j))^2)} = C_1 , \qquad (21)$$

where A,N,$W_1$ and $B_1$, $B_2$, $N_1$, $N_2$, $W_2$ are LSM - estimates of parameters for the hypotheses $H_1$ and $H_2$, respectively. It may be written:

$$C_1 = \exp(-\sum_x \frac{1}{D(x)}(A^2\varphi^2 - (\sum_{j=1}^{2} B_j \varphi_j)^2 + 2s(x)(A\varphi - \sum_{j=1}^{2} B_j \varphi_j))) . \qquad (22)$$

Only one of hypotheses is acceptable, but we can surely reject the other hypothesis only when $C_1$ differs essentially from 1. Otherwise, they will be simultaneously significant and we can not draw safe in-

ference about amount of peaks. However, if $N_1$ is close to $N_2$, N is situated with great probability within the range $(N_1,N_2)$ and expanding $\sum B_j\varphi_j$ in the Taylor's power series in $(N_j-N)$ we can show that if $N_2-N_1$ tends to zero, then $B_1+B_2$ tends to A and $W_2$ to $W_1$, whence $C_1$ tends to unity. Thus, a minimally admissible limit for the difference $N_2-N_1$ should be put, in order to guarantee the unique significance. Denote it R (resolution). In the case m=1, n=2 we come to the same conclusion.

The analogous consideration of the 2-nd situation (weak peaks) enables to conclude: a minimally admissible limit for the amplitude of peak should be put, in order to have only one hypothesis from all significant. Denote it S (sensibility).

These limits remove not unique significance of the hypotheses as well as prevent the degeneration of the LSM-matrix. It follows from (22), that they depend on the same factors as the accuracy of estimates: the variance D(x), the statistic $S_f$ and the width W.
Certainly the shape of background influences the safety of the inference too. Moreover, the local background fluctuation, which looks as a peak, and the real peak can not be distinguished by statistical means, if the complementary physical information is not used. This emphasizes the necessity of development of such methods of automatic peak finding, which imply also the physical analysis of the spectrum (e.g. the prediction of the lines belonging to known isotopes in $\gamma$ or x ray spectra, using the available tables, or the calculation of the resonance energies in neutron diffraction spectra and so on).

The computer program UPEAK as the implementation of the method described is written in FORTRAN-IV and was used, most successfully when the decomposition of lines with non-Gaussian asymmetry



and excess was required. The peak models are given by tables and can vary along the spectrum; two different models are admissible for simultaneously analysed peaks (e.g. photo and escape peaks in $\gamma$-spectrum). The resolution R and sensibility S can be given or taken from statistical conditions. The initial values for the positions and width are required. Each parameter may be fixed or restricted by lower and upper limits.
The memory capacity needed for the program is less than 32K for the 4096 - channel spectra analysis. An average time is about 1-2s per analysed peak ( CDC-6200 ).

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