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EFFICIENT ALGORITHMS OF MULTIPARAMETER γ-RAY SPECTRA PROCESSING*

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In the paper, the efficient algorithms to process multiparameter γ-ray spectra are presented. They allow to search for peaks, to separate useful information from background and to improve resolution in 1-, 2- and 3-parameter γ-ray spectra. The algorithms are generalized to n-parameter data.

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1 Introduction

Experimental progress in the understanding of nuclear structure depends critically on the ability to analyze coincidence data in multidimensional space. The requirements for using higher dimensions and higher resolutions are continuously increasing. The classical techniques developed to analyze one-parameter spectra cannot be directly extended to higher-fold data. Some operations are extremely time consuming. This problem is becoming relevant for big sizes and for multidimensional spectra, where the number of operations grows exponentially with the sizes. The implementations of some methods, mainly on PC computers, without optimization would be impossible. In the paper we present algorithm of multidimensional peak searching, multidimensional background elimination and deconvolution.

2 Peak searching

Without being interested in details we outline the algorithm of peak searching for 2-parameter spectra. We assume that the peak can be described by Gauss function and that the background

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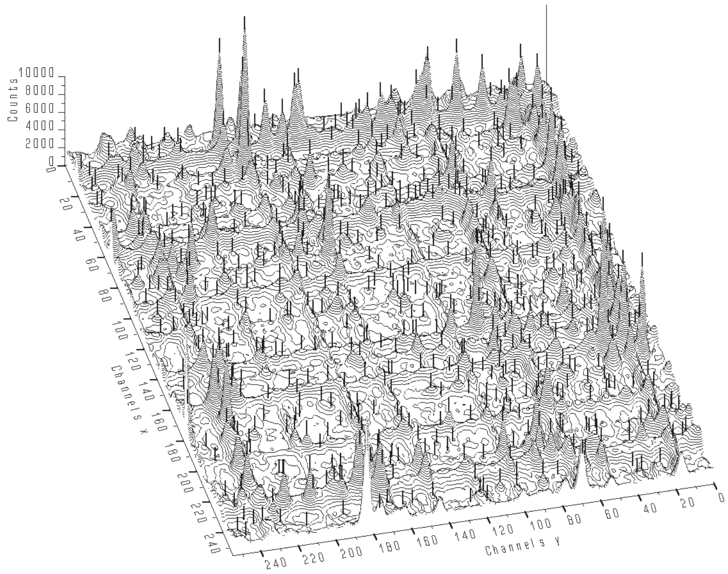

Fig. 1. Example of 2-parameter spectrum with peaks found.

can be approximated by a linear function within short interval. Then the number of counts as a function of the channel position x, y is

$$N(x,y) = G_1(x,y) + G_2(x) + G_3(y) + B + Cx + Dy \tag{1}$$

where $G_1(x,y)$ represents a 2-dimensional Gaussian, $G_2(x)$ and $G_3(y)$ represent 1-dimensional Gaussian ridges and $B + Cx + Dy$ is linear background. The second partial derivative of 1 in both variables is independent of $G_2(x), G_3(y)$ and background. It implies that the method is not sensitive to either of both ridges or their sum. Then maxima in the second derivative of a spectrum correspond to positions of a 2-dimensional peaks. The slices in the maxima in both directions are compared to their standard deviations. Applying conditions for the existence and the shape of peaks [1] the positions of 2-dimensional Gaussians can be determined. The method was extended also to 3-dimensional spectra. An example of Gaussians found in a 2-parameter spectrum is presented in Fig. 1. Positions of found peaks can be used as initial estimates to fit 2-parameter peaks in spectrum. An alternative way is to eliminate background from spectrum and then improve resolution sufficiently enough to obtain separated peaks.

3 Background estimation algorithm

The aim of algorithm is to separate useless information (background, combinations of coincidences of the background with peaks - ridges) from useful information contained in n-fold coincidence peaks of n-parameter spectrum.

Let us suppose that we estimate baseline spectrum of one-parameter spectrum stored in the vector $v(i)$. From $v(i)$ we shall calculate step by step the vectors $v_1(i), v_2(i)$ up to $v_m(i)$, where

m is a free parameter. The new value in the channel i in the pth iteration step is obtained by comparison of average of the values $v_{p-1}(i-p), v_{p-1}(i+p)$ with the value $v_{p-1}(i)$. We accept the minimum of these values, i.e.,

$$v_p(i) = \min\left\{ v_{p-1}(i),\ \frac{1}{2}\left[v_{p-1}(i+p) + v_{p-1}(i-p)\right] \right\}. \tag{2}$$

Analogously to one dimensional background estimation one can proceed in derivation of an algorithm to determine background of 2-parameter spectrum. From the 2-parameter spectrum $v(i,j)$ we shall successively create matrices $v_1(i,j), v_2(i,j)$ up to $v_m(i,j)$.

The matrix elements that enter background estimation in the pth iteration step are denoted

$$\begin{aligned}
P_1 &= v_{p-1}(i+p, j+p); \quad & P_2 = v_{p-1}(i-p, j+p),\\
P_3 &= v_{p-1}(i+p, j-p); \quad & P_4 = v_{p-1}(i-p, j-p),\\
S_1 &= v_{p-1}(i+p, j); \quad & S_2 = v_{p-1}(i, j+p),\\
S_3 &= v_{p-1}(i, j-p); \quad & S_4 = v_{p-1}(i-p, j).
\end{aligned} \tag{3}$$

Our aim is that the peak ridges in both directions (coincidences of peaks with linear background) as well as their sum were incorporated into the background estimate. Therefore we compare the values in the elements S with the average value of neighbouring elements P. Then we replace the new values S by

$$\begin{aligned}
S_1 &= \max\{S_1,\ (P_1+P_3)/2\} - (P_1+P_3)/2;\\
S_2 &= \max\{S_2,\ (P_1+P_2)/2\} - (P_1+P_2)/2;\\
S_3 &= \max\{S_3,\ (P_3+P_4)/2\} - (P_3+P_4)/2;\\
S_4 &= \max\{S_4,\ (P_2+P_4)/2\} - (P_2+P_4)/2.
\end{aligned} \tag{4}$$

Then the new value in the matrix element i,j in the pth iteration step is

$$v_p(i,j) = \min\{v_{p-1}(i,j),\ (S_1+S_4)/2 + (S_2+S_3)/2 + (P_1+P_2+P_3+P_4)/4\}. \tag{5}$$

Background elimination algorithm can be generalized to three and multidimensional data [2]. An example of 2-parameter spectrum before and after background elimination is given in Fig. 2.

4 Deconvolution

The Gold method of deconvolution [3], [4] proved to be the most efficient for nuclear spectra deconvolution. In this section we outline the algorithm of Gold deconvolution. For a discrete system the relationship between a measured value $x(i)$ and the raw result of measurement $y(i)$ can be expressed as

$$y(i) = \sum_{k=o}^{N-1} h(i-k)x(k) \qquad i = 0, 1, \ldots, N-1 \tag{6}$$

where $h(i)$ is an impulse response and N is the number of samples of vectors h, x. The knowledge of the instrumental function $h(i)$ is required. Eq. 6 can be written in matrix form as

$$\bar{y} = H\bar{x} \tag{7}$$

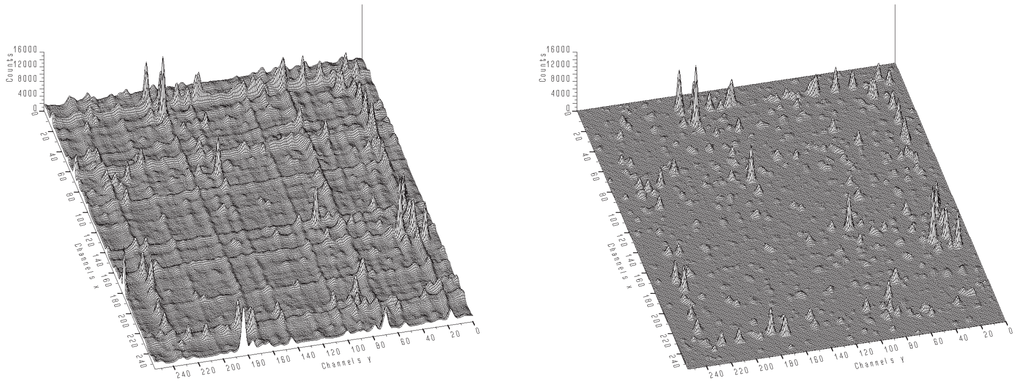

Fig. 2. Two-parameter spectrum before (a) and after (b) background suppression.

where columns of H are represented by the vectors h shifted by one position. Multiplying both sides of 7 by H^T yields

$$H^T \bar{y} = H^T H \bar{x} \tag{8}$$

wherefrom one gets

$$\bar{y_1} = H_1 \bar{x}. \tag{9}$$

The direct inversion of H_1 cannot lead to a stable solution. Therefore the method of regularization must be employed.

The basic form of iterative method of deconvolution for a general linear discrete system is

$$\bar{x}^{k+1} = \bar{x}^k + \mu(\bar{y} - A \cdot \bar{x}^k) \tag{10}$$

where A is system matrix, k represents the number of iterations and μ is the relaxation factor. In our case the matrix $H^T H$ in 8 is symmetric, so its eigenvalues are real. The eigenvalues of matrix $(H^T H) \cdot (H^T H)$ are the squares of eigenvalues of matrix $H^T H$ and therefore must be positive. The real positive eigenvalues of the system matrix is basic condition of stable solution of 9. Then 10 becomes

$$\bar{x}^{k+1} = \bar{x}^k + \mu[H^T H H^T \bar{y} - H^T H H^T H \bar{x}^k] \tag{11}$$

wherefrom one gets

$$\bar{x}^{k+1} = \bar{x}^k + \mu[\bar{y}' - H' \cdot \bar{x}^k] \tag{12}$$

By choosing relaxation factor μ according to [3] we obtain the Gold algorithm of deconvolution

$$x_i^{k+1} = \frac{y_i'}{\sum_{m=0}^{N-1} H'_{im} \cdot x_m^k} \cdot x_i^k \tag{13}$$

The advantage of Gold method in nuclear spectra deconvolution is the positivity of solution $\bar{x}$. The method can be generalized to 2-parameter spectra [4]. The example of 2-parameter spectrum before and after the deconvolution using the Gold method is given in Fig. 3.

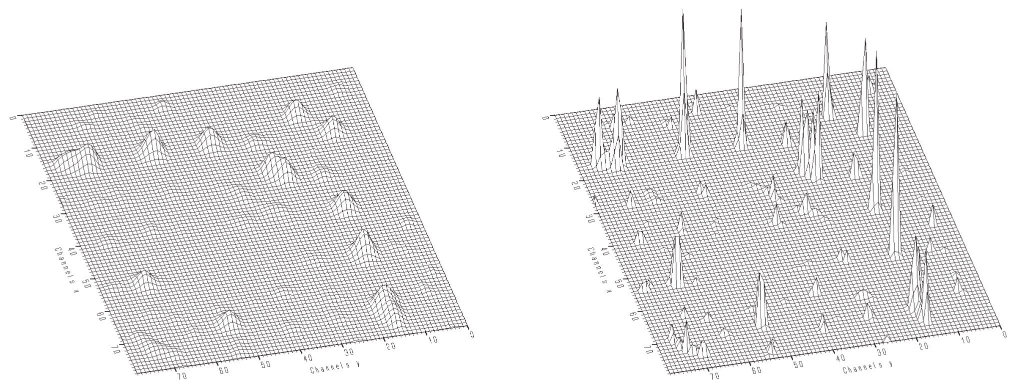

Fig. 3. Two-parameter spectrum before (a) and after (b) deconvolution.

The direct extension of the computational algorithm of one dimensional non-optimized Gold deconvolution to two-, three- and multidimensional system leads to exponential growth of numerical operations. Given a rather slow convergence speed of iterative Gold method one needs considerable number of iteration steps ($\approx$ 1000). Therefore in practical cases the method without optimization is not directly applicable in multidimensional deconvolution.Optimization can be achieved according to two facts. Fist, in γ-ray spectroscopy the number of channels of impulse response with non-zero counts is of the order of 10. Outside this interval the counts vanish to zeros. This can be exploited in matrix vector multiplication in the denominator of 13. It is useless to multiply with zeros. Second, in 13 one can observe that if for an i, y_i or x_i^k equals zero then for all following iteration steps $j > k\, x_i^j$ will remain zero. It means that for such a point one can stop corrections in the iteration step k. Both these facts allow to decrease dramatically computing time of 13.

5 Conclusions

All the algorithms described so far were implemented in "Integrated Multiparameter Nuclear Data Analysis Package" [5]. It includes standard conventional procedures and routines as well as new developed algorithms. The package is a tool that integrates multiparameter data taking, processing and display. It was used to process data from multidetector system Compact Pocket Ball (ORNL Oak Ridge) and Gammasphere (LBL) Berkeley with the aim to obtain information on high excited states of neutron-rich nuclei from spontaneous fission. It is also utilized in the field of relativistic nuclear physics in experiments on NUCLOTRON accelerator (JINR Dubna) in the frame of programme SPHERE.

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