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Sophisticated algorithms of analysis of spectroscopic data

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Abstract:

The paper presents an overview of existing and new algorithms for the processing of spectroscopic data. These include algorithms for background elimination, for separation of peak containing regions from peak-free regions, deconvolution and identification of information carrier objects.

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1. Introduction

One of the basic problems in the analysis of the spectra is the separation of useful information contained in peaks from the useless information (background, noise). In order to process data from numerous analyses accurately and reproducibly, the background approximation must be, as much as possible, free of user-adjustable parameters. Baseline removal, as the first preprocessing step of spectrometric data, critically influences subsequent analysis steps. The more accurately the background is estimated the more precisely we can estimate the existence of peaks. In the contribution we present an algorithm to determine peak regions and separate them from peak-free regions. Subsequently it allows to propose a baseline estimation method based on sensitive non-linear iterative peak clipping with automatic local adjusting of width of clipping window. One of the most delicate problems of any spectrometric method is that related to the extraction of the correct information out of the spectra sections, where due to the limited resolution of the equipment, the peaks as the main carrier of spectrometric information are overlapping. Conventional methods of peak searching based usually on spectrum convolution are inefficient and fail to separate overlapping peaks. The deconvolution methods can be successfully applied for the determination of positions and intensities of peaks and for the decomposition of multiplets.

2. Background estimation

An accurate and fast method of background estimation, based on Statistics-sensitive Non-linear Iterative Peak-clipping algorithm (SNIP), has been developed in [1]. In [2] we extended the SNIP method for multidimensional spectra. In multidimensional spectra, the algorithm must be able to recognize not only continuous background but also to include all the combinations of coincidences of the background in some dimensions and the peaks in the other ones. In [3] we proposed several improvements of the SNIP algorithm. Further we have derived a set of modifications of the algorithm that allow estimation of specific shapes of background and ridges as well. Examples of one-, two-, and three-dimensional spectra before and after background elimination are given in Figs. 1-3.

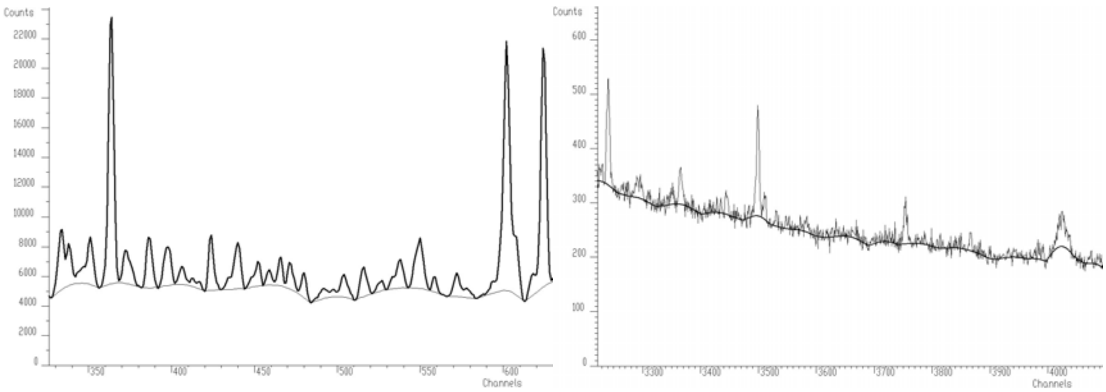

Fig. 1 An example of γ- ray spectrum with estimated background using decreasing clipping window and simultaneous smoothing.

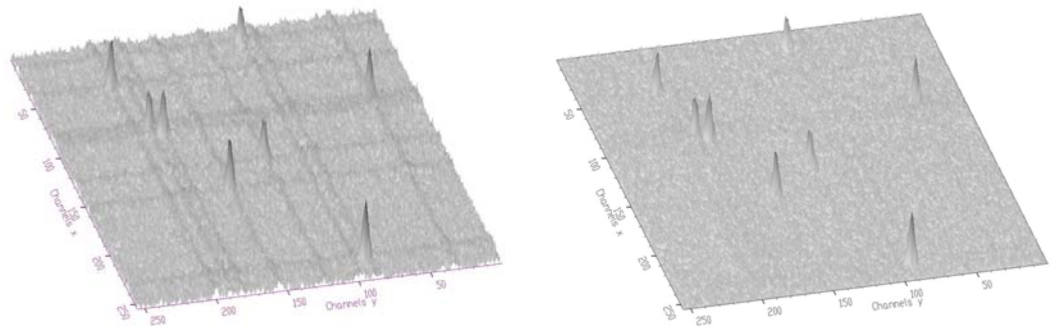

Fig. 2 An example of two-dimensional γγ - ray spectrum before and after background elimination using the algorithm with simultaneous smoothing.

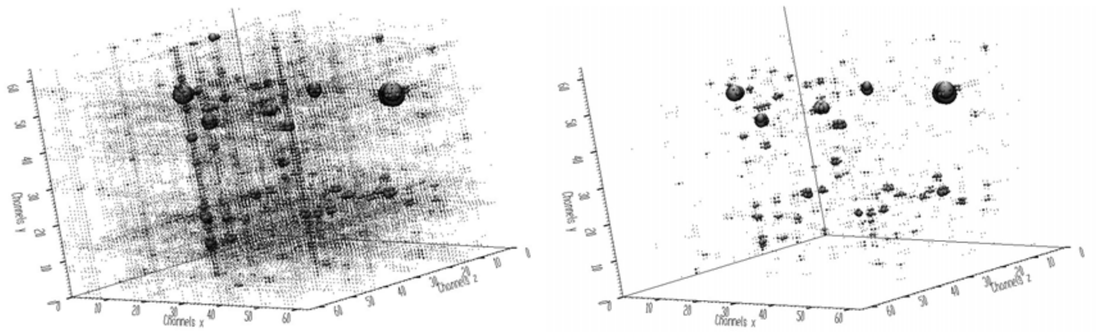

Fig. 3 An example of three-dimensional γγγ - ray spectrum before and after background elimination using the algorithm with simultaneous smoothing.

3. Estimation of peak regions

In [4-5] the authors propose a peak-search method based on two-pass convolution of the spectrum with the first derivative of the Gaussian. Besides of the identification of peaks the method can be utilized for the determination of peaks intervals [6]. Based on this approach we proposed an improved background estimation algorithm with clipping window adaptive to peak regions widths. The comparison of both methods is presented in Fig. 4.

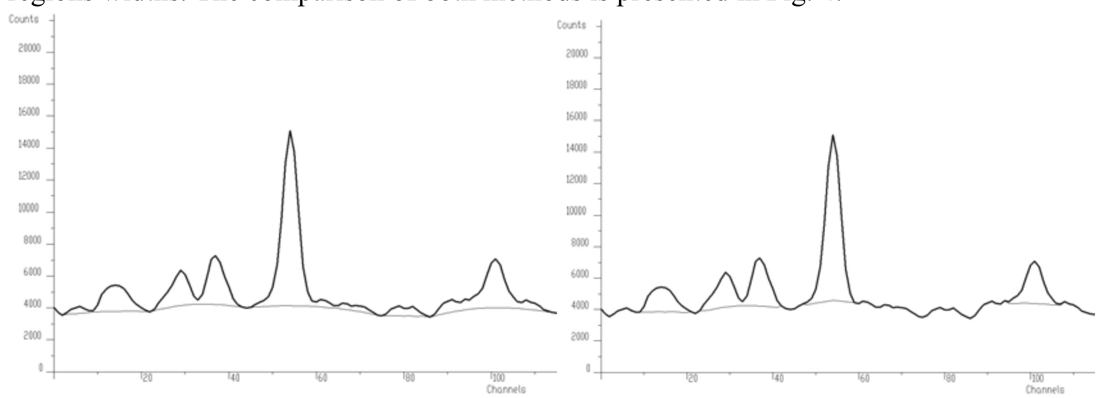

Fig. 4 Experimental γ-ray spectrum with estimated background using fixed width of clipping window and width automatically adjustable to the widths of peak regions.

4. Deconvolution

The peaks as the main carrier of spectrometric information are very frequently positioned close to each other. The extraction of the correct information out of the spectra sections, where due to the limited resolution of the equipment, signals coming from various sources are overlapping, is a very complicated problem. Deconvolution and restoration are the names given to the endeavor to improve the resolution of an experimental measurement by mathematically removing the smearing effects of an imperfect instrument, using its resolution function. As a rule deconvolution problems are very ill-conditioned, i.e., very small errors or noise in the deconvolved spectrum cause enormous oscillations in the resulting data. In the contribution we have studied only positive definite deconvolution algorithms (Gold [7], Richardson-Lucy [8], [9] and Maximum a posteriori [10]). In [11] we proposed boosted positive definite deconvolution algorithm. In [12] we developed deconvolution algorithm based on Tikhonov regularization of squares of negative values. Both allow to improve the resolution up to delta functions. Examples of one-, and two-dimensional spectra before and after deconvolution are given in Figs. 5 and 6, respectively.

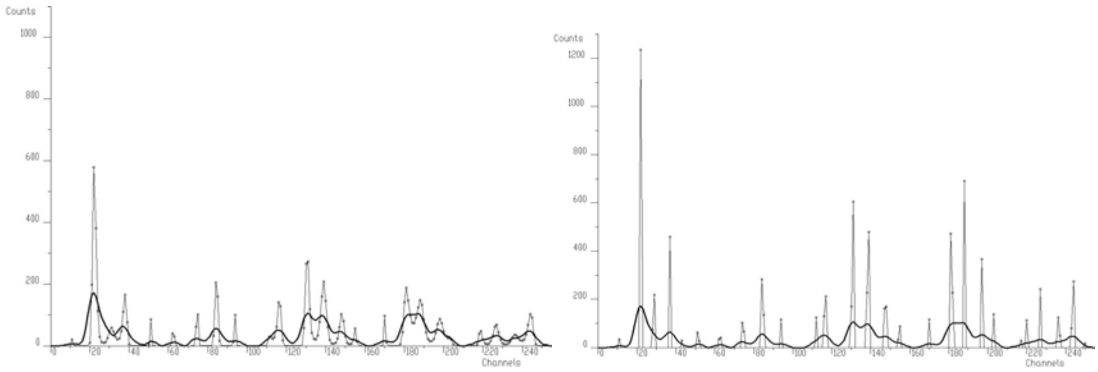

Fig. 5 Original and deconvolved γ-ray spectrum using classic and boosted Gold algorithm.

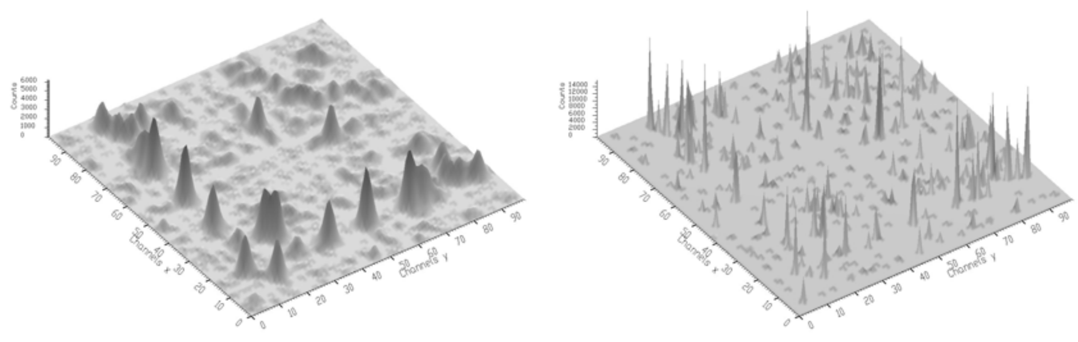

Fig. 6 Original and deconvolved $\gamma\,\gamma$-ray spectrum using boosted Gold algorithm.

5. Identification of spectroscopic information carrier objects

In [13] we proposed a peak searching algorithm based on convolution with the second derivative of Gaussian for multidimensional spectra. The algorithm is able to recognize crossing points of ridges of lower-fold coincidences from n-fold coincidence peaks (Fig. 7).

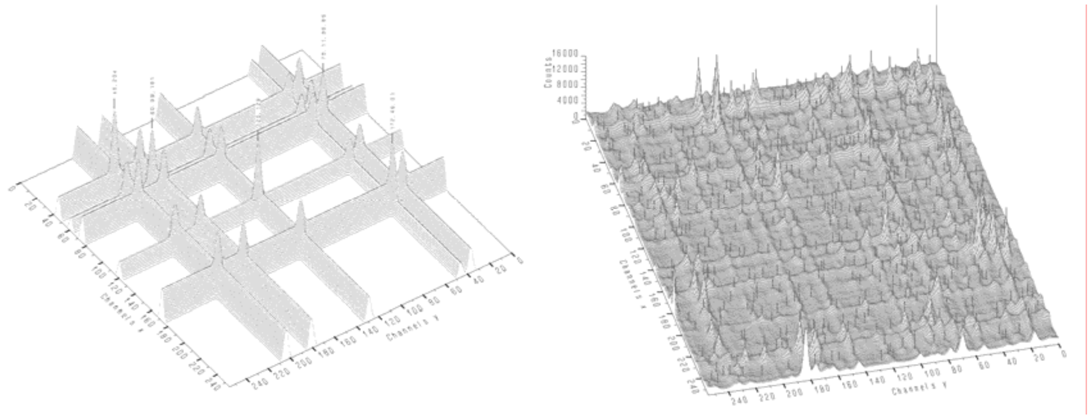

Fig. 7 Synthetic and experimental two-dimensional spectra with found peaks denoted by marks.

In many cases in low-statistics spectra we need to smooth data before application of peak searching algorithm. In [14] we proposed a smoothing and peak enhancement method based on Markov chains. Again we generalized the method for multidimensional data. In Figs. 8 and 9 we illustrate the smoothing and peak enhancement properties of the method.

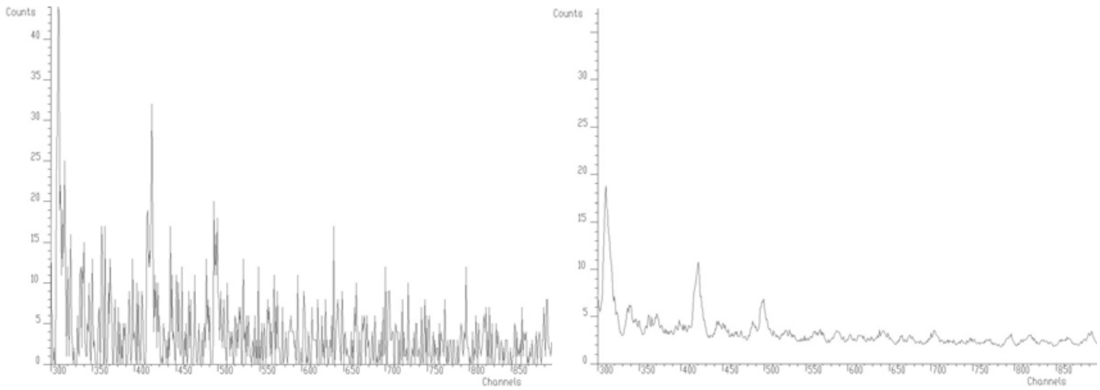

Fig. 8 Low-statistics γ -ray spectrum before and after application of Markov smoothing.

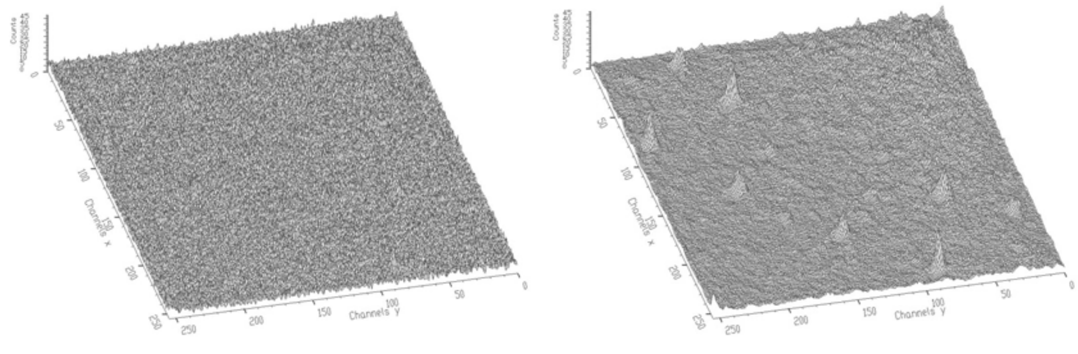

Fig. 9 Low-statistics $\gamma\,\gamma$ -ray spectrum before and after application of Markov smoothing.

In the spectra of nuclear multifragmentation one needs to determine ridges of corresponding points from very sparsely distributed two-dimensional experimental data. In [15] we proposed an algorithm based on linearization and smoothing using inverted positive second derivative of

Gaussian. Application of Gold deconvolution allows decomposition of identified ridges to subridges. An illustrative example is presented in Figs. 10 and 11.

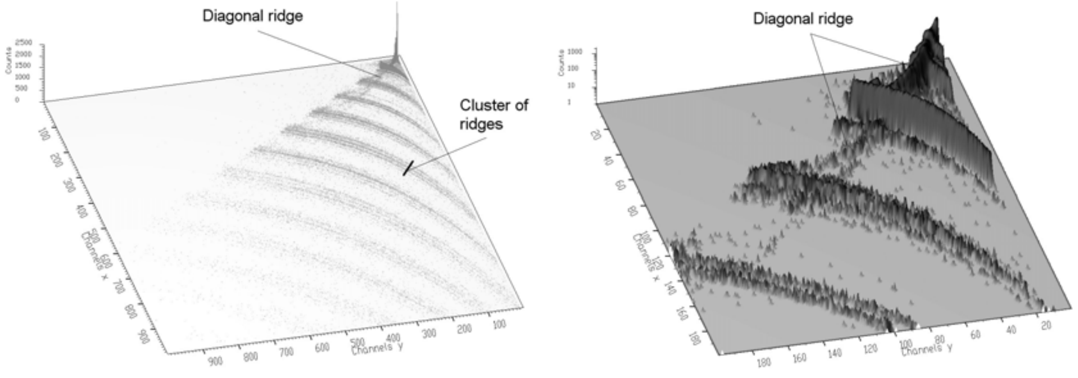

Fig. 10 Original Si-Si spectrum and its detail.

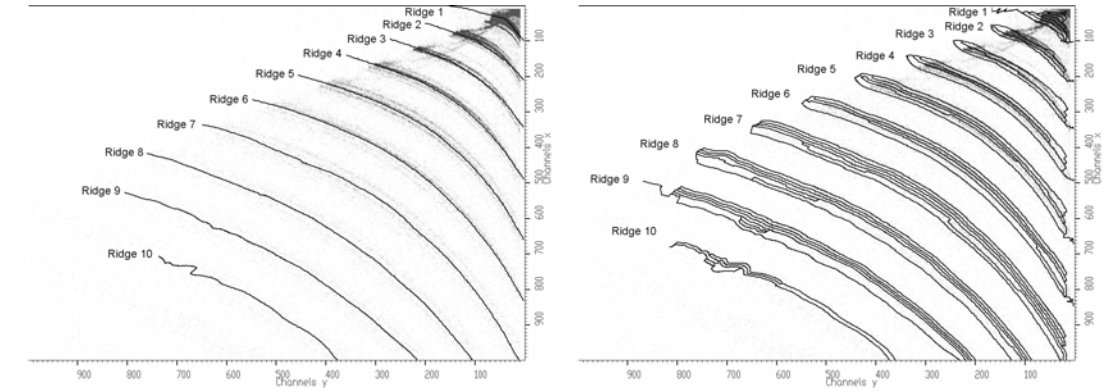

Fig. 11 Spectrum from Fig. 10 with determined ridges and decomposed to subridges.

6. Conclusions

We have generalized and extended the existing basic SNIP algorithm for additional parameters and possibilities that make it possible to improve substantially the quality of the background estimation. We have included these modifications and derived the algorithms for two-, three-, up to n-dimensional spectra.

We proposed an algorithm for the determination of the peak regions. In the contribution we suggested an algorithm of background estimation with the clipping window adaptable to the widths of peak regions as well. Moreover the algorithm for separation of peaks containing regions from peak-free regions can be utilized for fitting purposes to confine the fitting regions.

To improve resolution in spectra we analyzed a series of deconvolution methods. We proposed boosted deconvolution algorithms and the algorithm based on Tikhonov regularization of squares of negative values. Both algorithms are able to decompose the overlapped peaks practically to δ functions while concentrating the peak areas to one channel.

Further in the contribution we present peak searching algorithm based on the second derivatives of Gaussian and peak searching algorithm for low-statistic spectra based on Markov chain method. The presented algorithms were implemented in DaqProVis system [16] and partially in ROOT system in form of TSpectrum classes[17].

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