High-resolution deconvolution methods for analysis of noisy γ-ray spectra

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ACAT 2014, Prague Sept. 1 – 5, 2014

Introduction

- The quality of the analysis of nuclear spectrometric data consists in general in correct identification of the existence of peaks and subsequently in good estimation of their positions and intensities (areas).
- The peaks as the main carrier of spectrometric information are very frequently positioned close to each other.
- The extraction of correct information out of spectra sections, where due to the limited resolution of the equipment, presence of noise, overlapped signals from various sources, is a very complicated problem.
- The deconvolution methods represent an efficient tool to improve the resolution in the data. It is of great importance mainly in the tasks connected with decomposition of overlapped peaks (multiplets) and subsequently for the determination of positions and intensities of peaks in gamma-ray spectra.

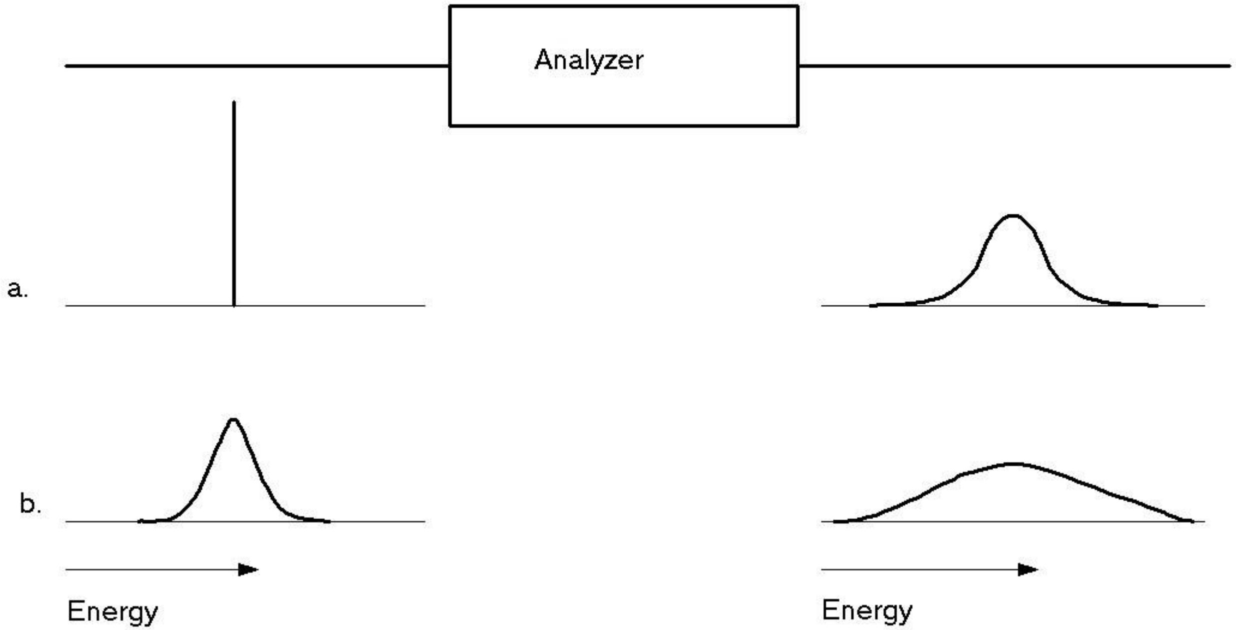
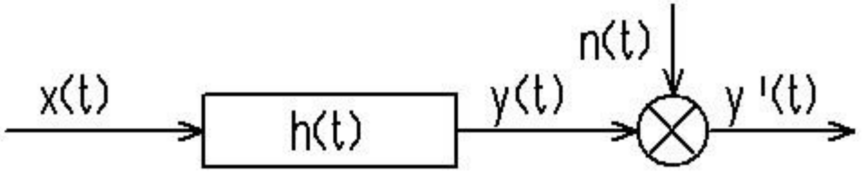


Illustration of smearing effects of an imperfect instrument - analyzer



Linear system with additive noise

The system can be identified
- according to theoretical knowledge,
- by measurement e.g. calibration source (only one peak) etc.

- Stationary discrete system that satisfies the superposition principle can be described by convolution sum

$$y(i) = \sum_{k=0}^{i} x(k)h(i-k) + n(i) = x(i) * h(i) + n(i) \quad i = 0,1,\dots,N-1$$

where $x(i)$ is the input into the system, $h(i)$ is its impulse function (response), $y(i)$ is the output from the system, $n(i)$ is additive noise and “ * “ denotes the operation of the convolution.

In matrix form it can be written

$$\boldsymbol{y} = H\boldsymbol{x} + \boldsymbol{n}$$

where the matrix ***H*** has dimensions N × M, the vectors ***y***, ***n*** have length N and vector ***x*** has length M, while N ≥ M (overdetermined system).

- To find least square solution of the above given system of linear equations the functional

$$\| H\boldsymbol{x} - \boldsymbol{y} \|^2$$

should be minimized.

- Unconstrained least squares estimate of the solution is

$$\hat{\boldsymbol{x}} = (H^T H)^{-1} H^{\boldsymbol{T}} \boldsymbol{y}$$

- For invariant convolution system the columns of the matrix H are represented by the response mutually shifted by one position

$$H = \begin{bmatrix} h(0) & 0 & \cdots & 0 \\ h(1) & h(0) & \cdots & 0 \\ \vdots & \vdots & \cdots & \vdots \\ h(L-1) & h(L-2) & \cdots & 0 \\ 0 & h(L-1) & \cdots & h(0) \\ 0 & 0 & \cdots & h(1) \\ \vdots & \vdots & \cdots & \vdots \\ 0 & 0 & \cdots & h(L-1) \end{bmatrix}$$

where $N = M + L - 1$.

Three types of regularization methods are very often used:
- smoothing,
- constraints imposition (for example only non-negative data are accepted),
- choice of a prior information probability function - Bayesian statistical approach.

- ***Tikhonov-Miller regularization.*** The functional

$\|H\mathbf{x}-\mathbf{y}\|^2+\alpha\|Q\mathbf{x}\|^2$ Q, α are the regularization matrix and parameter, respectively,

is minimized. The solution can be obtained by solving the equation

$$\mathbf{x}=\left(H^TH+\alpha Q^TQ\right)^{-1}H^T\mathbf{y}$$

Zero-th order or Tikhonov regularization for $Q=E$

$$\mathbf{x}=\left(H^TH+\alpha\right)^{-1}H^T\mathbf{y}$$

- ***Riley Algorithm (commonly called iterated Tikhonov regularization).*** To obtain smoother solution one may use algorithm of Tikhonov-Miller regularization with iterative refinement

$$\mathbf{x}^{(n+1)}=\mathbf{x}^{(n)}+\left(H^TH+\alpha Q^TQ\right)^{-1}\left(H^T\mathbf{y}-H^TH\mathbf{x}^{(n)}\right) \qquad \mathbf{x}^{(0)}=0$$

However, because of its iterative nature, the Riley algorithm lends itself to another type of regularization, so called Projections On Convex Sets – POCS. It means we set all negative elements to zero after each iteration.

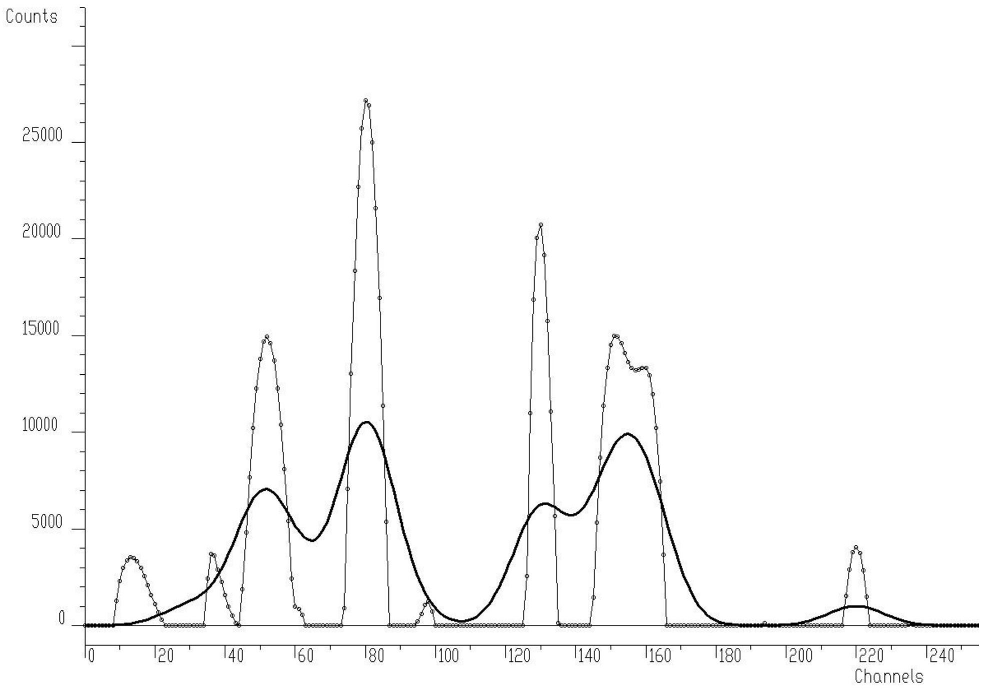


Fig. Riley deconvolution with POCS regularization - thick line is original spectrum, thin line represents spectrum after deconvolution.

Van Cittert Algorithm. The basic form of Van Cittert algorithm for discrete convolution system is

$$\boldsymbol{x}^{(n+1)} = \boldsymbol{x}^{(n)} + \mu\left(H^T H H^T \boldsymbol{y} - H^T H H^T H \boldsymbol{x}^{(n)}\right) = \boldsymbol{x}^{(n)} + \mu\left(\boldsymbol{y'} - A\boldsymbol{x}^{(n)}\right)$$

where:

A is system Toeplitz matrix,

n represents iteration number and

μ is the relaxation factor.

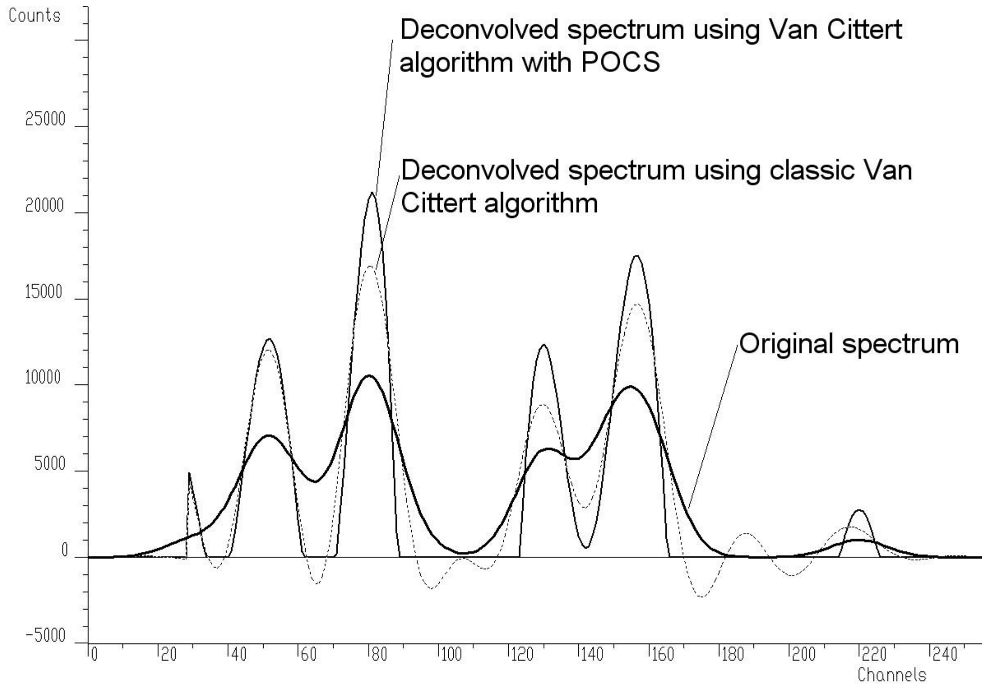


Fig. 65 Original spectrum (thick line), deconvolved spectrum using Van Cittert algorithm (without regularization) and deconvolved spectrum using Van Cittert algorithm regularized via POCS method.

Gold Algorithm. If we choose the local variable relaxation factor $\mu_i = \dfrac{x^{(n)}(i)}{\sum_{m=0}^{M-1} A_{im} x^{(n)}(m)}$ and we substitute it into Van Cittert formula we get the Gold deconvolution algorithm:

$$x^{(n+1)}(i) = \frac{y'(i)}{\sum_{m=0}^{M-1} A_{im} x^{(n)}(m)} x^{(n)}(i) \qquad x^{(0)} = [1,1,\ldots,1]^T$$

Its solution is always positive when the input data are positive, which makes the algorithm suitable for the use for naturally positive definite data, i.e., spectroscopic data.

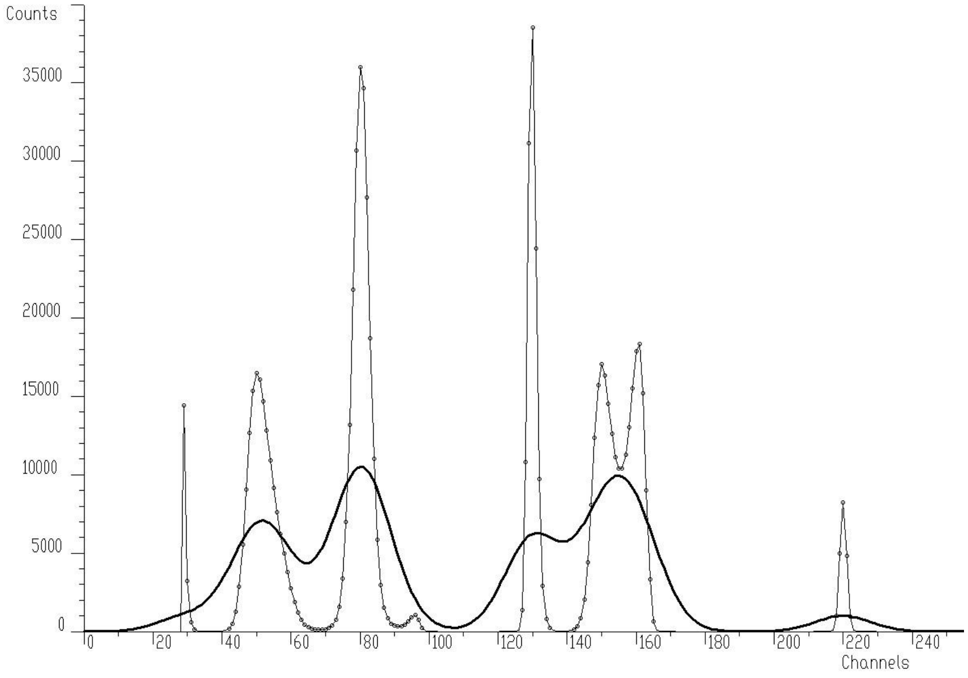


Fig.: Original spectrum (thick line) and deconvolved spectrum using Gold algorithm (thin line) after 10000 iterations. Channels are shown as small circles.

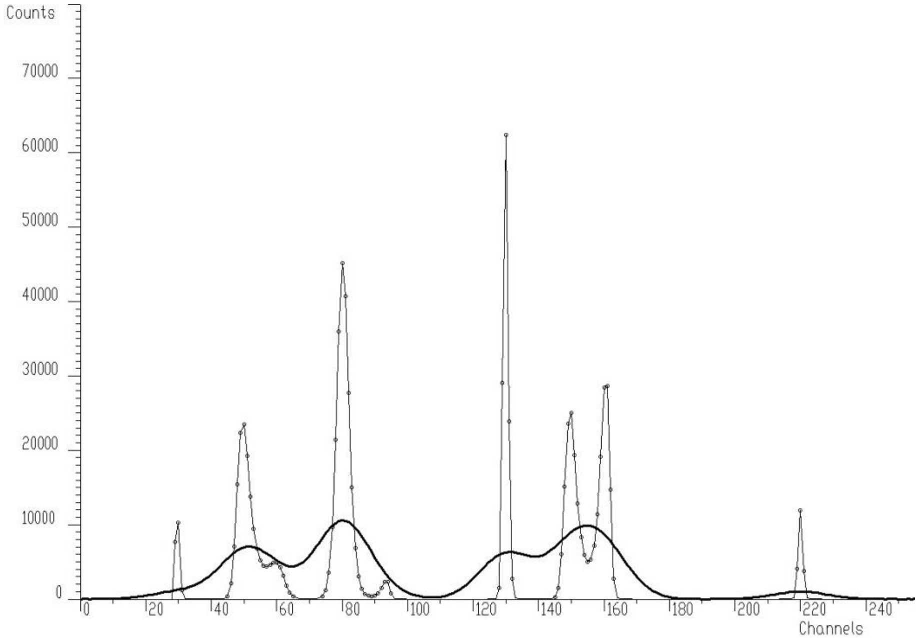


Fig.: Original spectrum (thick line) and deconvolved spectrum using Gold algorithm (thin line) after 50000 iterations.

- ***Richardson-Lucy Algorithm.*** Richardson-Lucy like algorithms use a statistical model for data formation and are based on the Bayes formula. The Bayesian approach consists of constructing the conditional probability density relationship

$$p(x|y)=\frac{p(y|x)p(x)}{p(y)}$$

The Bayes solution is found by maximizing the right part of the equation. The maximum likelihood (ML) solution maximizes the density p(y|x) over x. For discrete data the algorithm has the form

$$x^{(n+1)}(i)=x^{(n)}(i)\sum_{j=0}^{N-1}h(j,i)\frac{y(j)}{\sum_{k=0}^{M-1}h(j,k)x^{(n)}(k)} \qquad i\in\langle 0,M-1\rangle$$

This iterative method forces the deconvolved spectra to be non-negative. The Richardson-Lucy iteration converges to the maximum likelihood solution for Poisson statistics in the data. It is also sometimes called the expectation maximization (EM) method.

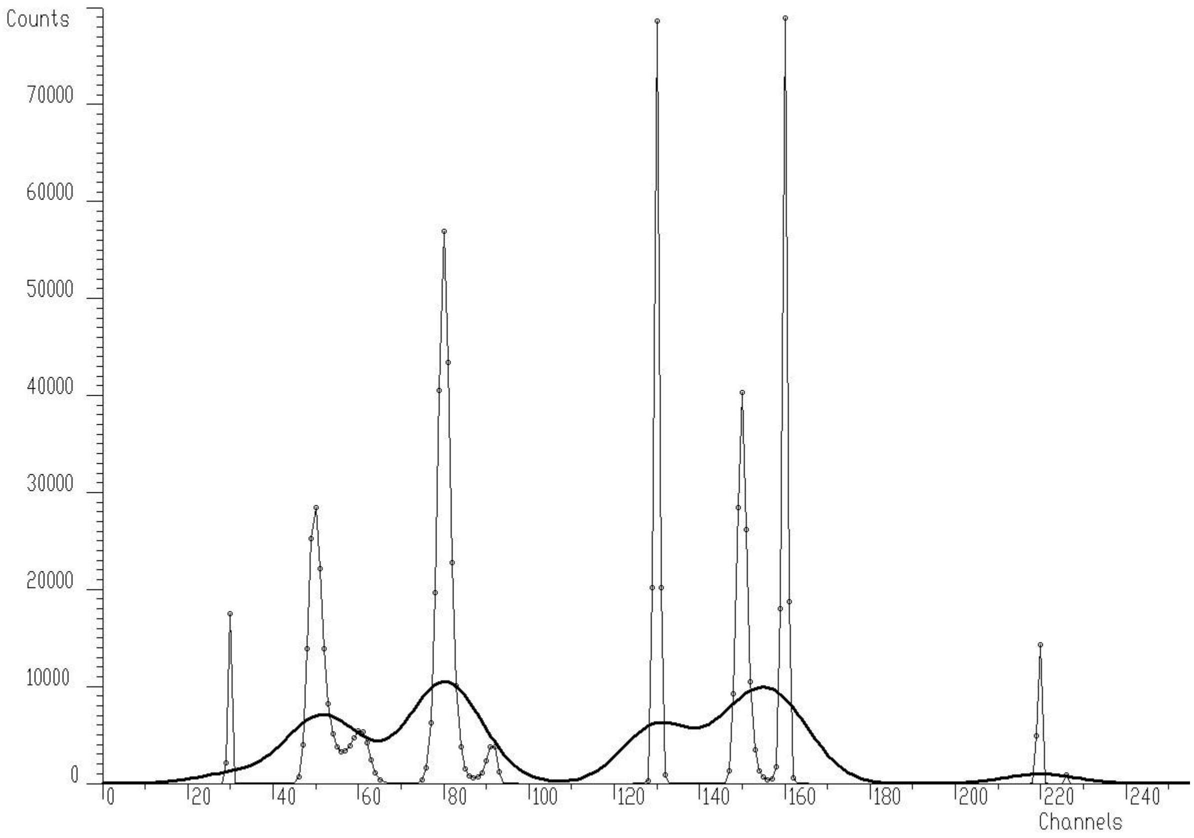


Fig.: Original spectrum (thick line) and deconvolved spectrum using Richardson-Lucy algorithm (thin line) after 50 000 iterations.

- ***Maximum A Posteriori Deconvolution Algorithm.*** The maximum a posteriori (MAP) solution maximizes over x the product $p(y\,|\,x)p(x)$. For discrete data the algorithm has the form

$$x^{(n+1)}(i) = x^{(n)}(i)\exp\left\{\sum_{j=0}^{N-1} h(j,i)\left[\frac{y(j)}{\sum_{k=0}^{M-1} h(j,k)\,x^{(n)}(k)} - 1\right]\right\}$$

Positivity of the solution is assured by the exponential function. Moreover the non-linearity permits superresolution.

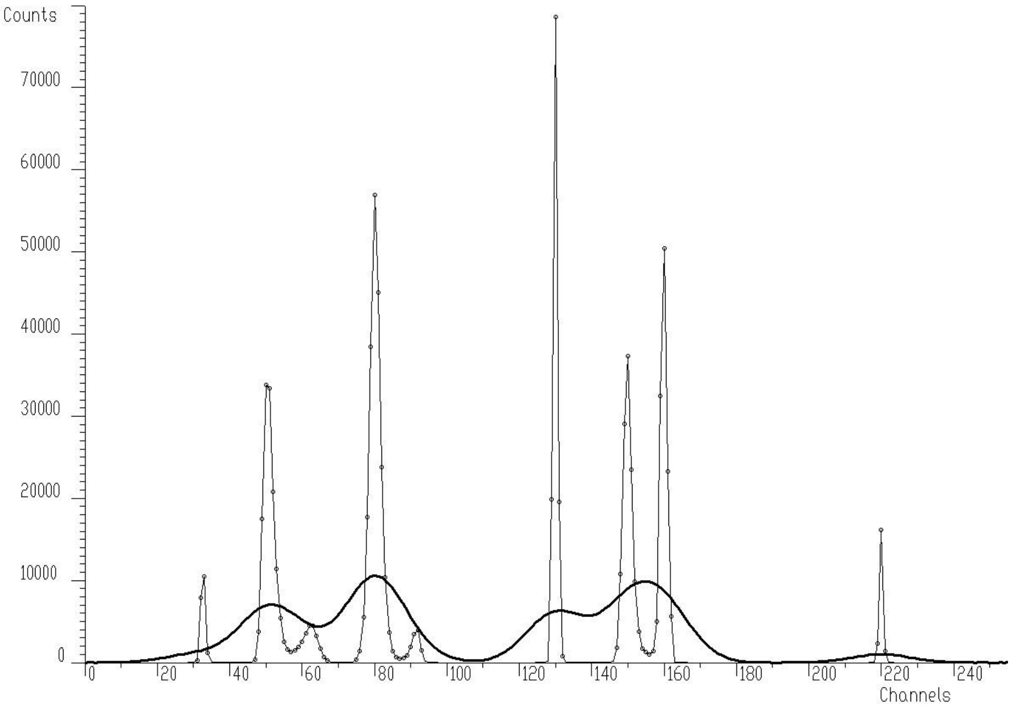


Fig.: Original spectrum (thick line) and deconvolved spectrum using MAP algorithm (thin line) after 50000 iterations.

Robustness of the deconvolution methods in respect to increasing level of noise

- In the following figure we present a matrix, which is composed of the original spectrum (Fig.(a)) and noise vector with increasing amplitude ranging from 0% up to 120% of the amplitude of small peaks (#1, #5 and #9), Fig.(c).
- Matrix composed of deconvolved spectra using classic Gold deconvolution algorithm and 10 000 iteration steps is presented in Fig. (d).
- One can observe that classic Gold deconvolution algorithm is robust to noise. Peaks do not change their positions and deconvolved spectra are smooth even for high level of noise. On the other hand, the method is not able to resolve peaks #3, #5 and to decompose peaks #7 and #8 even for noiseless data.

- In the following figures we show the results after non-boosted deconvolutions (10 000 iterations) and boosted ones (200 iterations repeated 50 times with boosting coefficient $p = 1.2$).

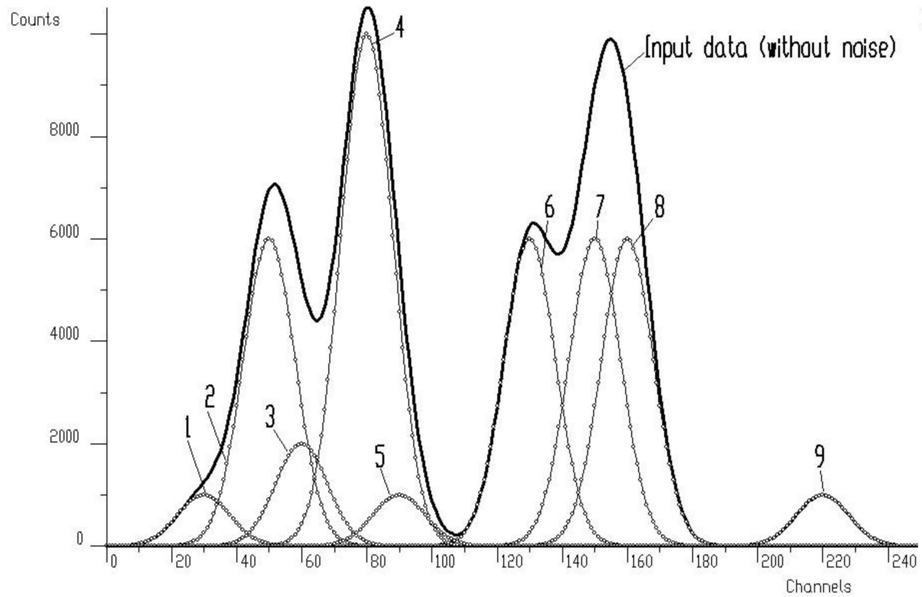


Fig. (a): Original spectrum composed of 9 Gaussians.

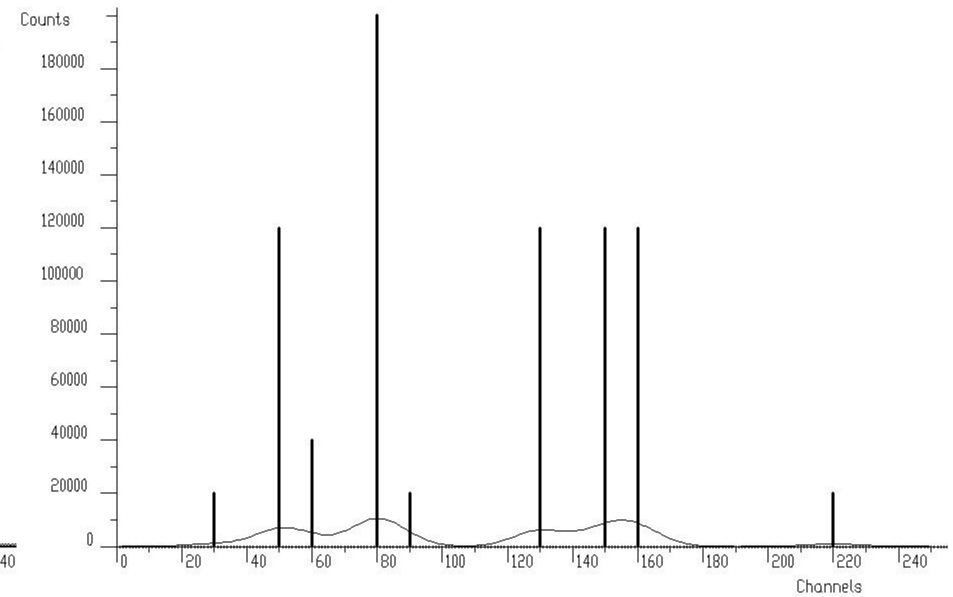


Fig.(b): Original synthetic spectrum (thin lines) and the ideal solution (thick bars).

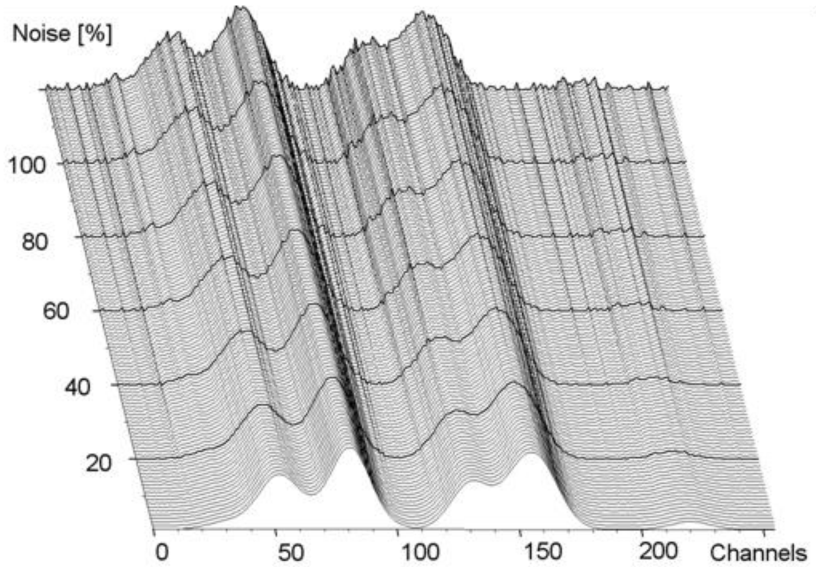


Fig.(c): Original spectrum with added increasing noise (in % of the amplitude of small peaks #1, #5, #9).

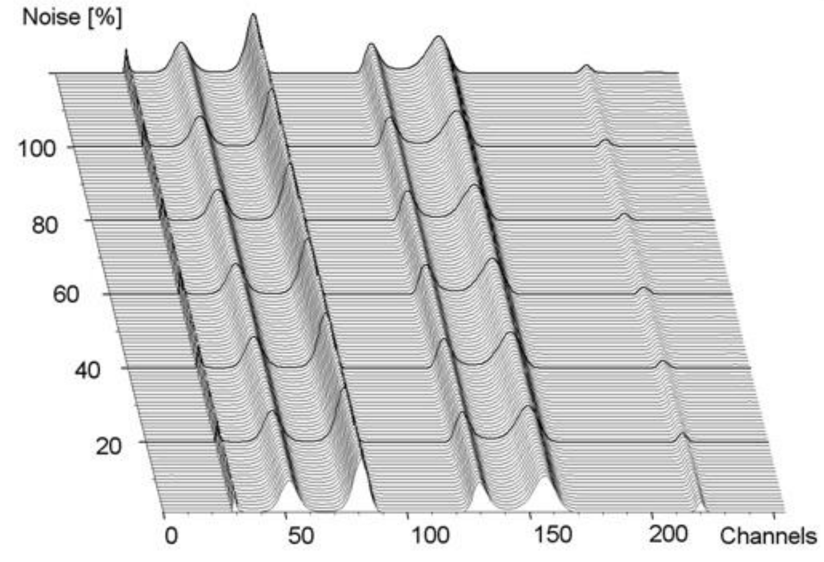


Fig.(d): Matrix composed of deconvolved spectra using classic Gold deconvolution algorithm.

Gold deconvolution algorithm

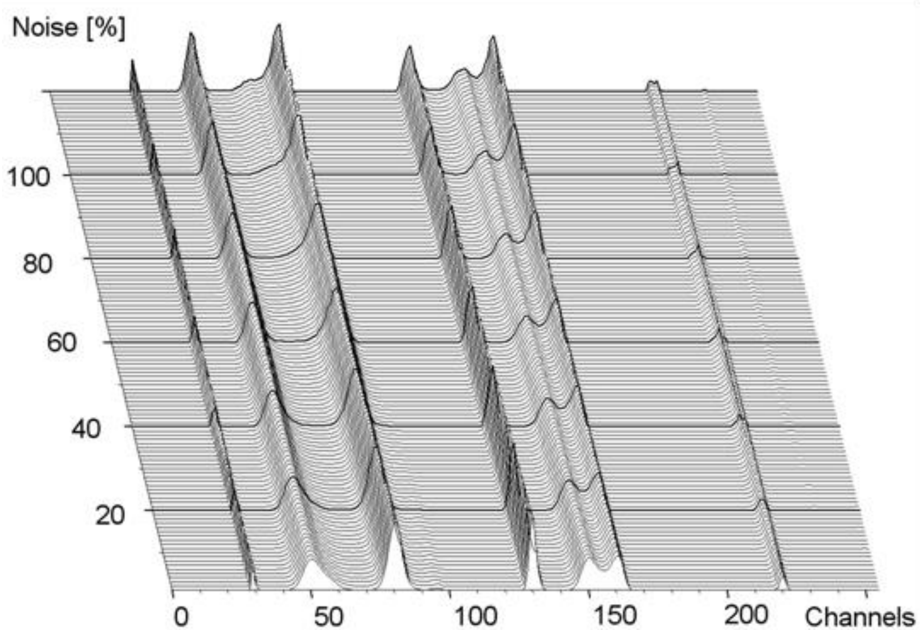


Fig. (a): Result of one-fold Gold deconvolution for increasing level of noise.

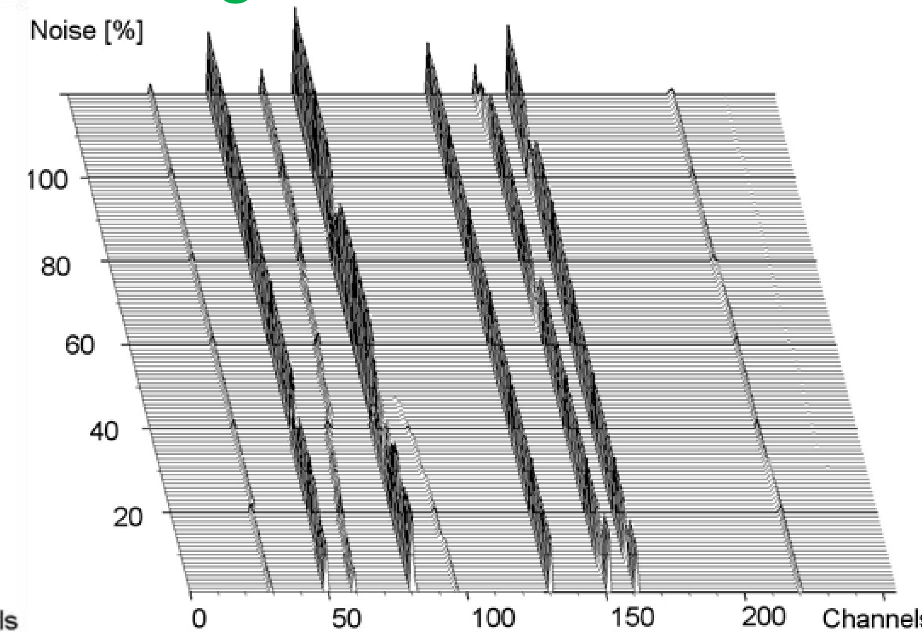


Fig. (b): Result of boosted one-fold Gold deconvolution for increasing level of noise.

- One-fold Gold deconvolution (Fig.(a)) is relatively robust to increasing level of noise. It resolves the doublet composed of peaks #7 and #8, respectively. Nevertheless the resolution capabilities are quite limited.
- The boosted one-fold deconvolution (Fig.(b)) decomposes all peaks practically to one channel. However for higher levels of noise the peak #3 changes its position. The peak #5 for more than 40% of noise disappears. Other peaks practically do not change their positions.

Richardson-Lucy deconvolution methods

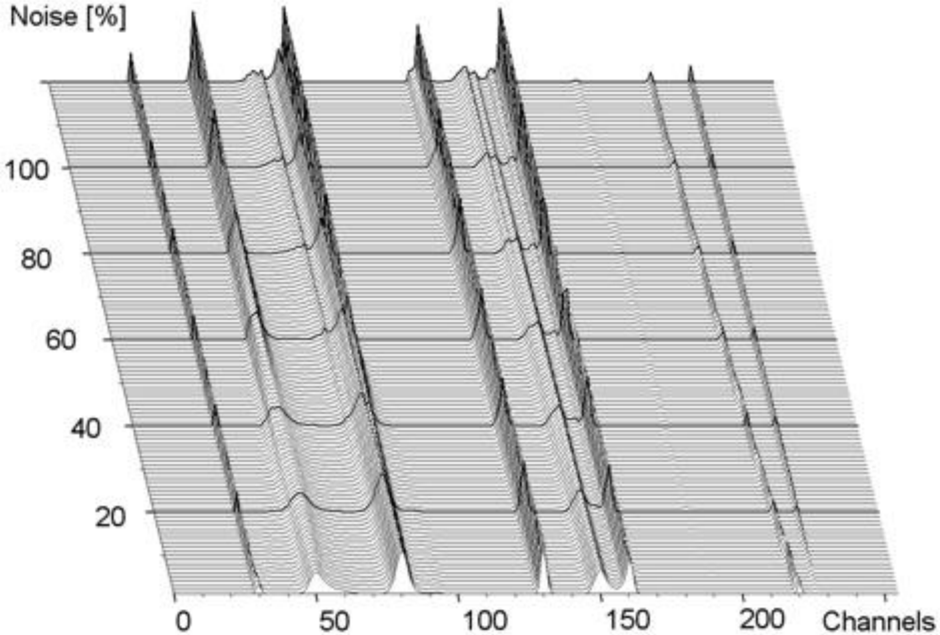


Fig.(c): Result after Richardson-Lucy deconvolution for increasing level of noise.

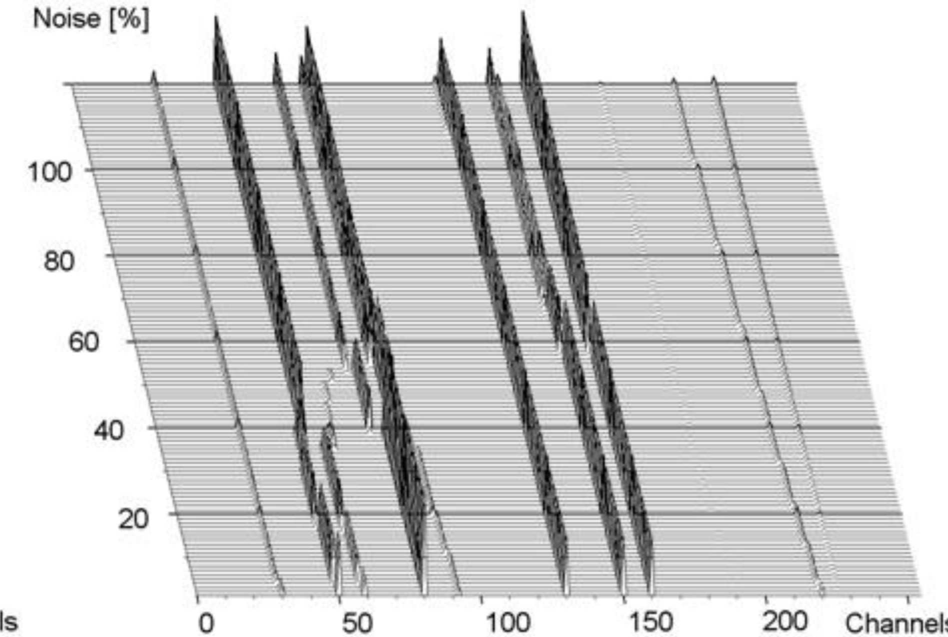


Fig.(d): Result of boosted Richardson-Lucy deconvolution for increasing level of noise.

- Richardson-Lucy deconvolution splits the peak #9 to two peaks, the second one being fake.
- The boosted Richardson-Lucy algorithm improves resolution, but it also generates false twin peak to the peak #9. The positions of other peaks change more dramatically than in one-fold Gold deconvolution.

MAP deconvolution algorithm

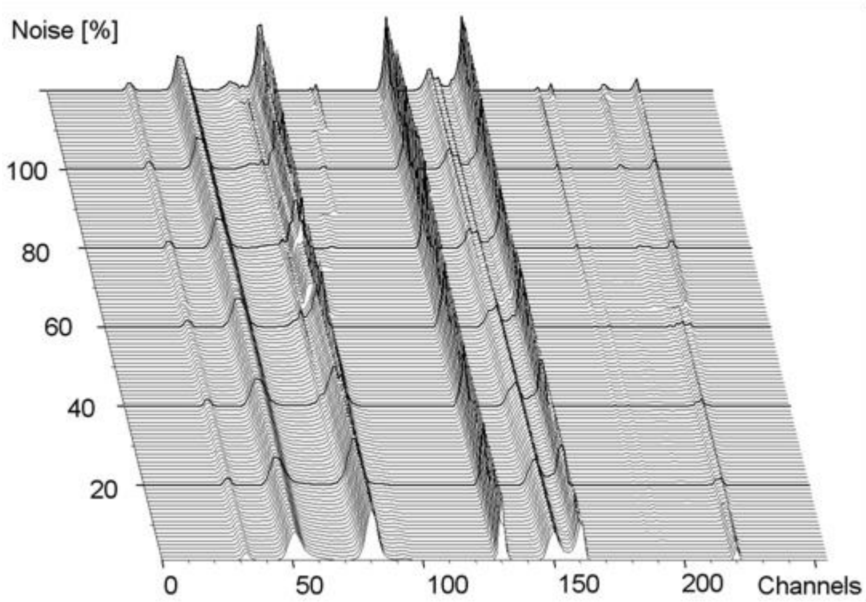


Fig. (a): Result of MAP deconvolution algorithm for increasing level of noise.

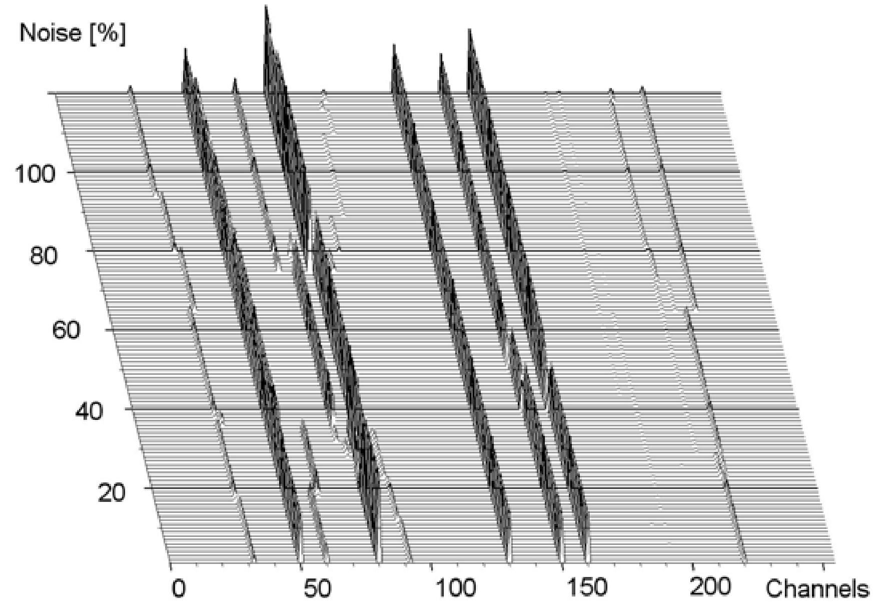


Fig. (b): Result of boosted MAP deconvolution algorithm for increasing level of noise.

- Non-boosted MAP deconvolution algorithm starts to generate false peaks for the noise level higher than 40%.
- Boosted MAP algorithm gives good results up to 20% of noise. After that one can observe changing positions of the peaks. There appear fake peaks in deconvolved data as well.

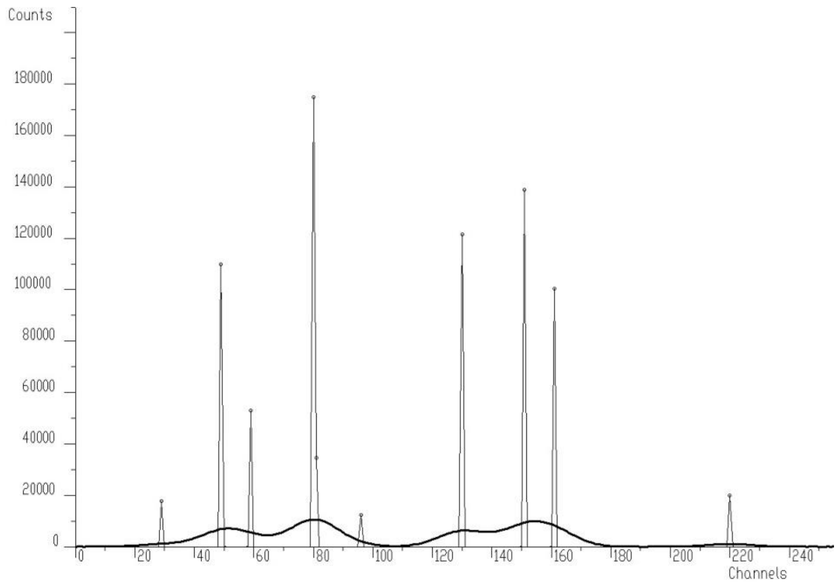


Fig.: Original spectrum (thick line) and deconvolved spectrum using boosted Gold algorithm (thin line) after 200 iterations and 50 repetitions (p=1.2).

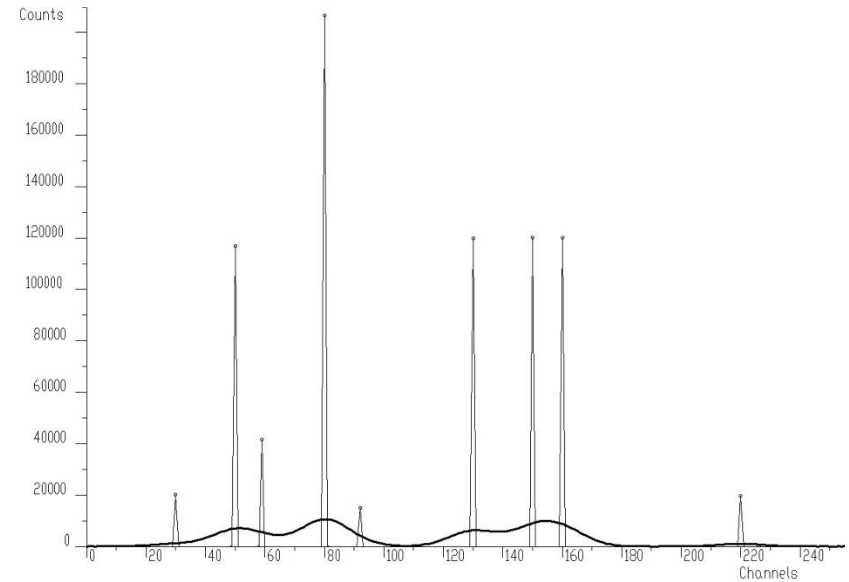


Fig.: Original spectrum (thick line) and deconvolved spectrum using boosted Richardson-Lucy algorithm (thin line) after 200 iterations and 50 repetitions.

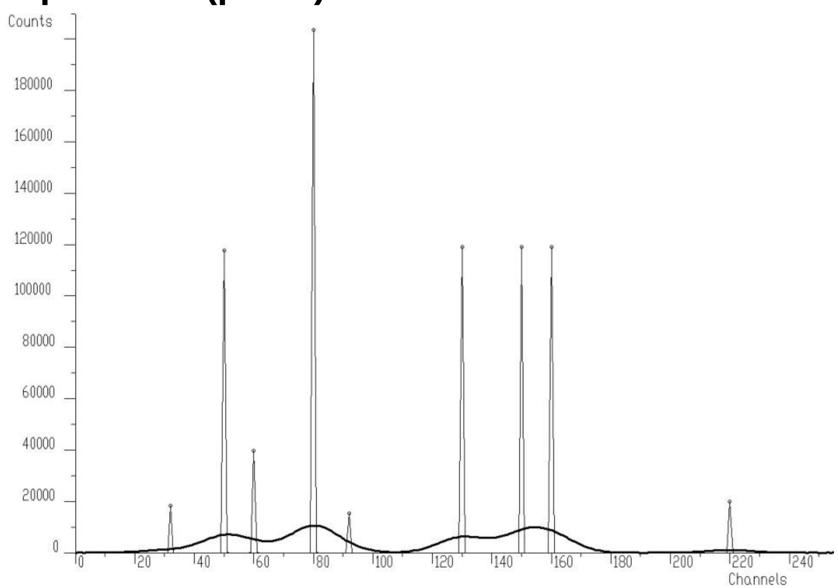


Fig.: Original spectrum (thick line) and deconvolved spectrum using boosted MAP algorithm (thin line) after 200 iterations and 50 repetitions.

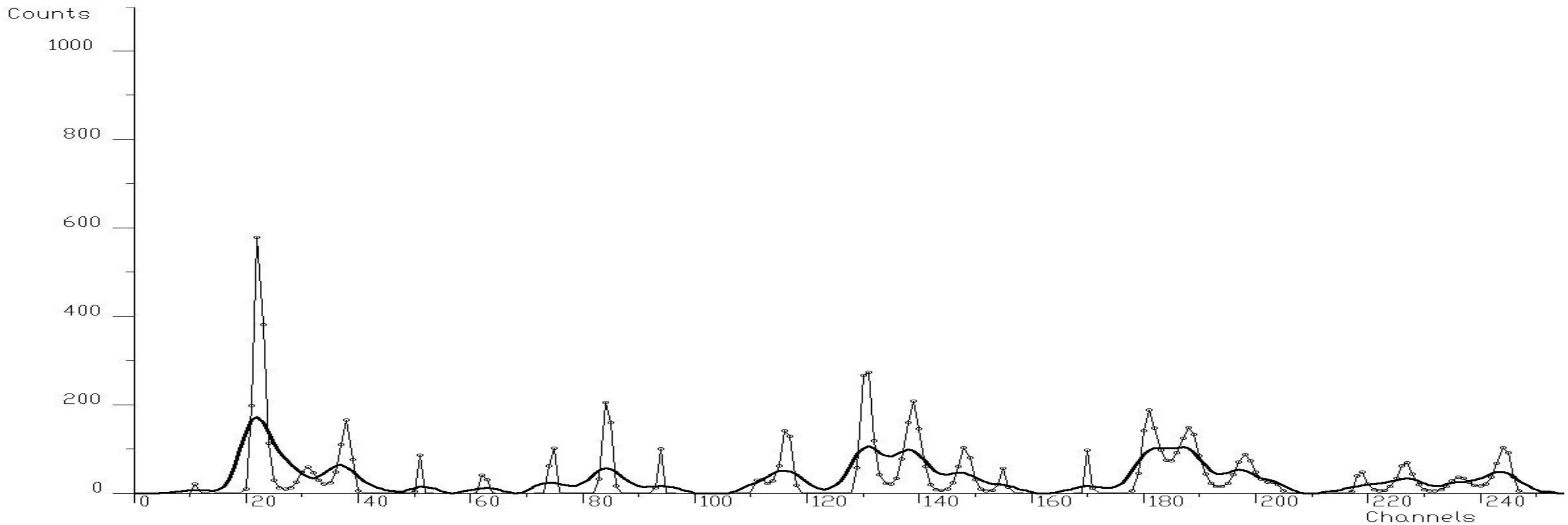


Fig. Original gamma-ray spectrum (thick line) and deconvolved spectrum using classic Gold algorithm (thin line) after 10 000 iterations.

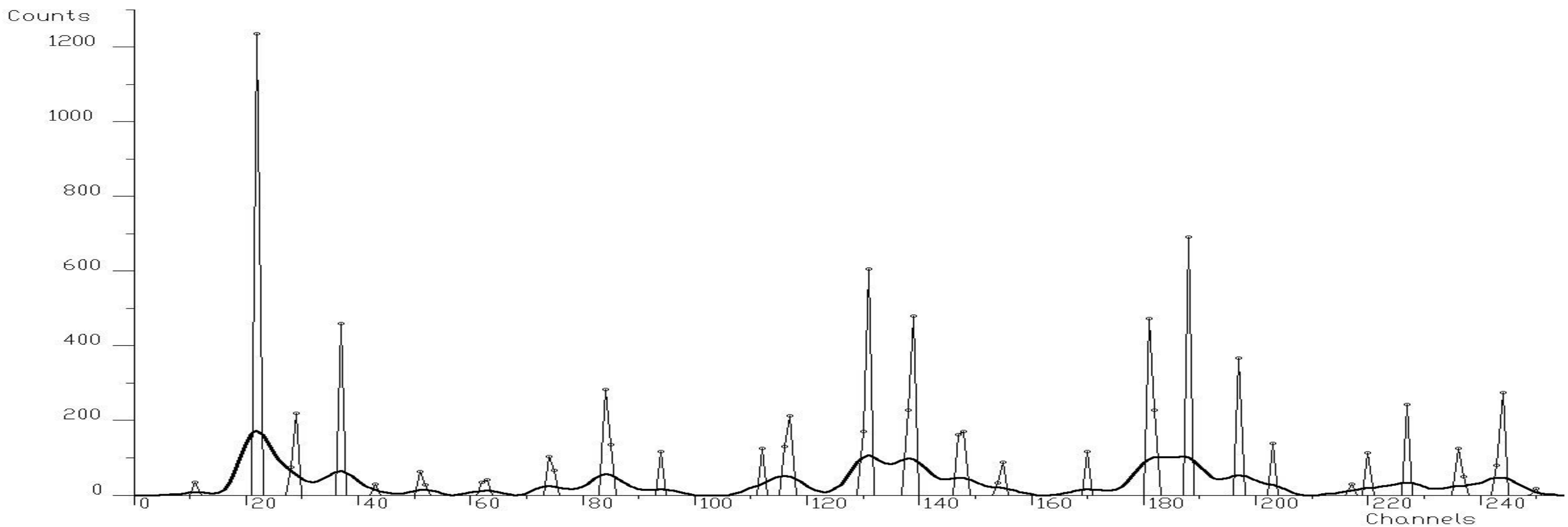


Fig.: Gamma-ray spectrum (thick line) and deconvolved spectrum using boosted Gold algorithm (thin line) after 200 iterations and 50 repetitions (p=1.2)

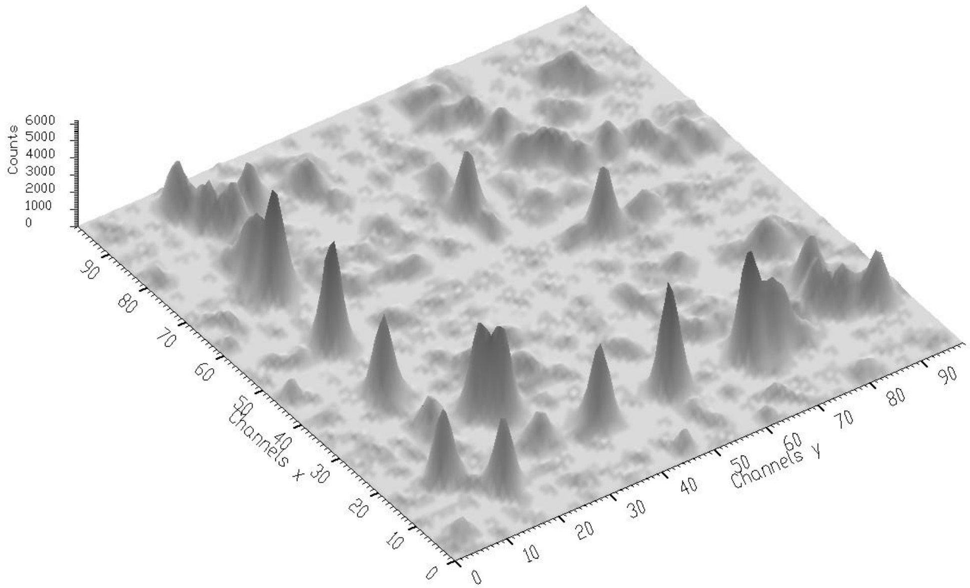


Fig.: Experimental gamma-gamma-ray spectrum (after background elimination).

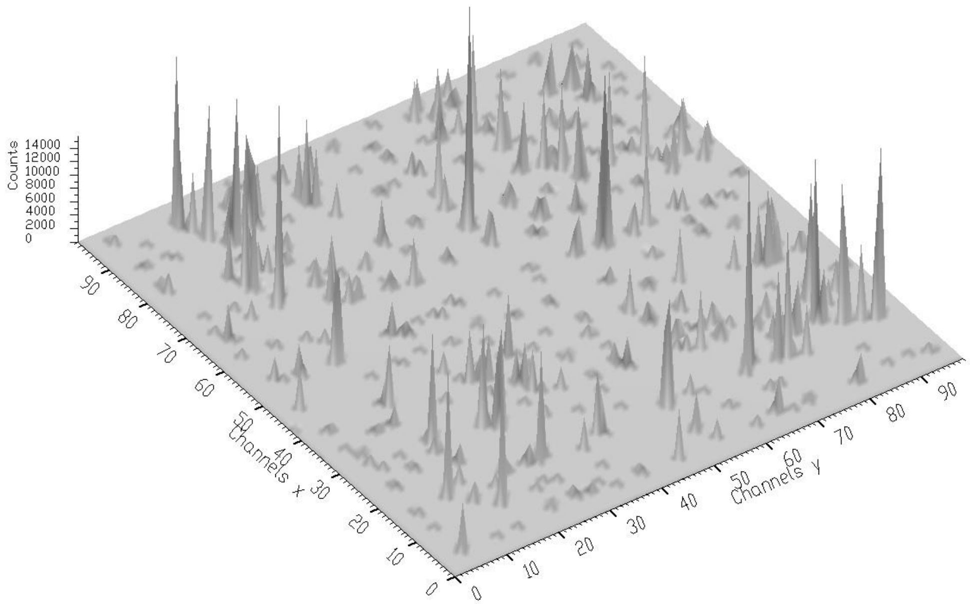


Fig.: Spectrum after boosted Gold deconvolution (50 iterations repeated 20 times).

Conclusions

- We have discussed and analyzed a series of deconvolution methods. There exists immense number of variations of deconvolution algorithms applied in various scientific fields. We have introduced only basic classes of deconvolution algorithms that can be easily employed and implemented for the processing of spectrometric data.
- The classical positive definite methods of deconvolution improve substantially the resolution in the gamma-ray spectra, but they are not efficient enough to decompose closely positioned peaks.
- We have presented the robustness of the deconvolution methods in respect to increasing level of noise. It has been shown, that the methods are insensitive to the noise enough.
- Though the procedures are fully automatic, due to large variability of the data, some intervention of the user and tuning of some parameters are required.
- Several algorithms were also implemented in ROOT system in the form of TSpectrum, TSpectrum2 and TSpectrum3 classes, developed in collaboration with CERN.

Some relevant publications:

1. M. Morháč , V. Matoušek: Multidimensional Experimental Data Processing in Nuclear Physics, In:Computer Physics, Eds.: S. Doherty and A. Molloy, Book Series, Nova Science Publishers, Inc., ISBN: 978-1-61324-790-7, 2012, pp. 1 - 236.
2. M. Morháč, V. Matoušek, High-resolution boosted deconvolution of spectroscopic data, Journal of Computational and Applied Mathematics, 235 (2011) 1629–1640.
3. M. Morháč, V. Matoušek: Complete positive deconvolution of spectrometric data. Digital Signal Processing, Volume 19, Issue 3, May 2009, Pages 372-392.
4. M. Morháč, V. Matoušek: Applied Spectroscopy 62, 91 (2008).
5. M. Morháč: Deconvolution methods and their applications in the analysis of gamma-ray spectra, Nucl. Instrum. Methods Phys. Res., Sect. A 559 (1) (2006), pp. 119-123.