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Deconvolution methods and their applications in the analysis of gamma-ray spectra

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Introduction and motivation

- one of the most delicate problems of any spectrometric method is that related to the extraction of the correct information out of the experimental spectra
- due to the limited resolution of the equipment, signals coming from various sources are overlapping
- deconvolution and decomposition 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 known resolution function
- the deconvolution methods are widely applied in various fields of data processing. Recently many applications have been found in various domains of experimental science, e.g. image and signal restoration, the determination of thickness of multilayer structures, tomography, magnetic resonance imaging, crystallography, geophysics, etc.
- deconvolution methods can be successfully applied also for the decomposition of multiplets and subsequently for the determination of positions and intensities of peaks in γ-ray spectra

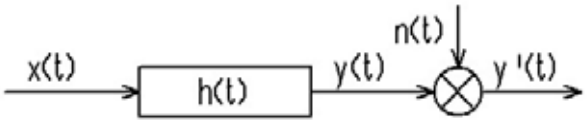
Theoretical background

Linear time (energy) invariant systems

- stationary system that satisfies the superposition principle can be described by convolution integral

$$y'(t) = \int_{-\infty}^{t} x(\tau) h(t-\tau) d\tau + n(t) = x(t) * h(t) + n(t),$$

where $x(t)$ is the input into the system, $h(t)$ is its impulse function (response), $y'(t)$ is the output from the system, $n(t)$ is additive noise and the mark $*$ denotes the operation of the convolution.



- analogously for discrete systems one can write

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

where N is the number of samples

- for two- and three-dimensional discrete convolution systems it holds

$$y'(i_1,i_2) = \sum_{k_1=0}^{i_1}\sum_{k_2=0}^{i_2} x(k_1,k_2)h(i_1-k_1,i_2-k_2) + n(i_1,i_2)$$

$i_1 = 0,1,...,N_1-1; i_2 = 0,1,...,N_2-1$,

and

$$y'(i_1,i_2,i_3) = \sum_{k_1=0}^{i_1}\sum_{k_2=0}^{i_2}\sum_{k_3}^{i_3} x(k_1,k_2,k_3)h(i_1-k_1,i_2-k_2,i_3-k_3) + n(i_1,i_2,i_3)$$

$i_1 = 0,1,...,N_1-1; i_2 = 0,1,...,N_2-1; i_3 = 0,1,...,N_3-1$, respectively

- in case we know the response function $h(t)$ and measured output signal and we want to determine the input signal we say about deconvolution.

Linear time (energy) dependent systems

- for time dependent continuous linear system one can write

$$y'(t) = \int_{-\infty}^{t} h(t,\tau)x(\tau)d\tau + n(t)$$

- Fredholm integral equation of the first kind is extremely ill-conditioned (posed) problem. Small changes in $y(t)$ cause enormous oscillations in the sought $x(t)$
- many different functions solve a convolution equation within error bounds of experimental data
- analogously for discrete system it holds

$$y'(i) = \sum_{k=0}^{i} h(i,k)x(k) + n(i)$$

- it represents general system of linear equations. In this case the columns of the system matrix are not simply shifted as it was in the above mentioned convolution systems. We say about decomposition or unfolding
- in general, this system can be in matrix form written

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

- the matrix H has dimension N x M, the vectors $\boldsymbol{y'}$, $\boldsymbol{n}$ have length N and vector $\boldsymbol{x}$ has length *M*, while $N \geq M$ (overdetermined system).

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

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

should be minimized

- unconstrained least squares estimate of vector $\boldsymbol{x}$ is

  $\hat{\boldsymbol{x}} = (H^T H)^{-1} \boldsymbol{H}^T \boldsymbol{y}$,
  where $H^T H$ is Toeplitz matrix

- when employing this algorithm to solve a convolution system small errors or noise can cause enormous oscillations in the result.

- the problem of finding $\boldsymbol{x}$ where H , $\boldsymbol{y'}$ are known, is a discrete ill-posed problem and requires regularization techniques to get adequate solution.

- several methods to regularize the solution of above given system were developed. Most methods used in inverse problems adopt both an extreme criterion to unfold data (for instance, those of least squares or the maximum entropy) and a regularization method to reduce the very large fluctuations of the unfolded spectrum.

- commonly used criteria for regularization are
  - smoothing
  - constraints imposition (for example only non-negative data are accepted)
  - choice of a prior information probability function - Bayesian statistical approach

Illustration of the sensitivity of the non-regularized solution of system of linear equations to noise

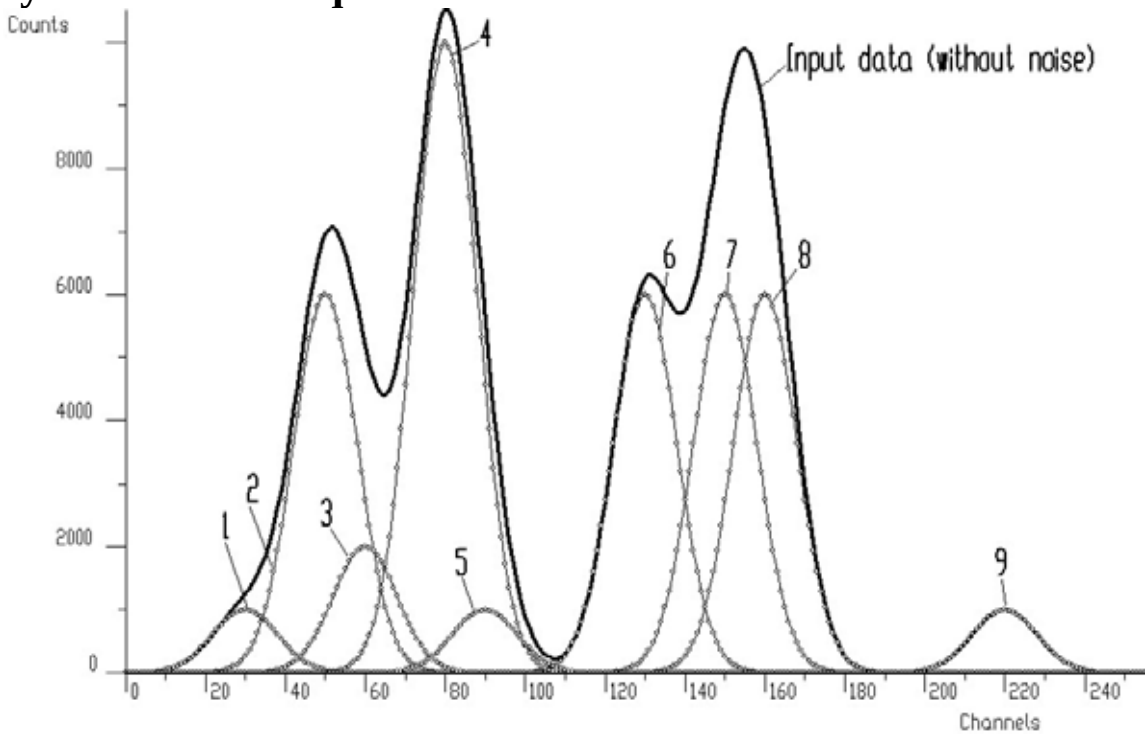


Figure 1 Example of synthetic spectrum (without noise) composed of 9 Gaussians

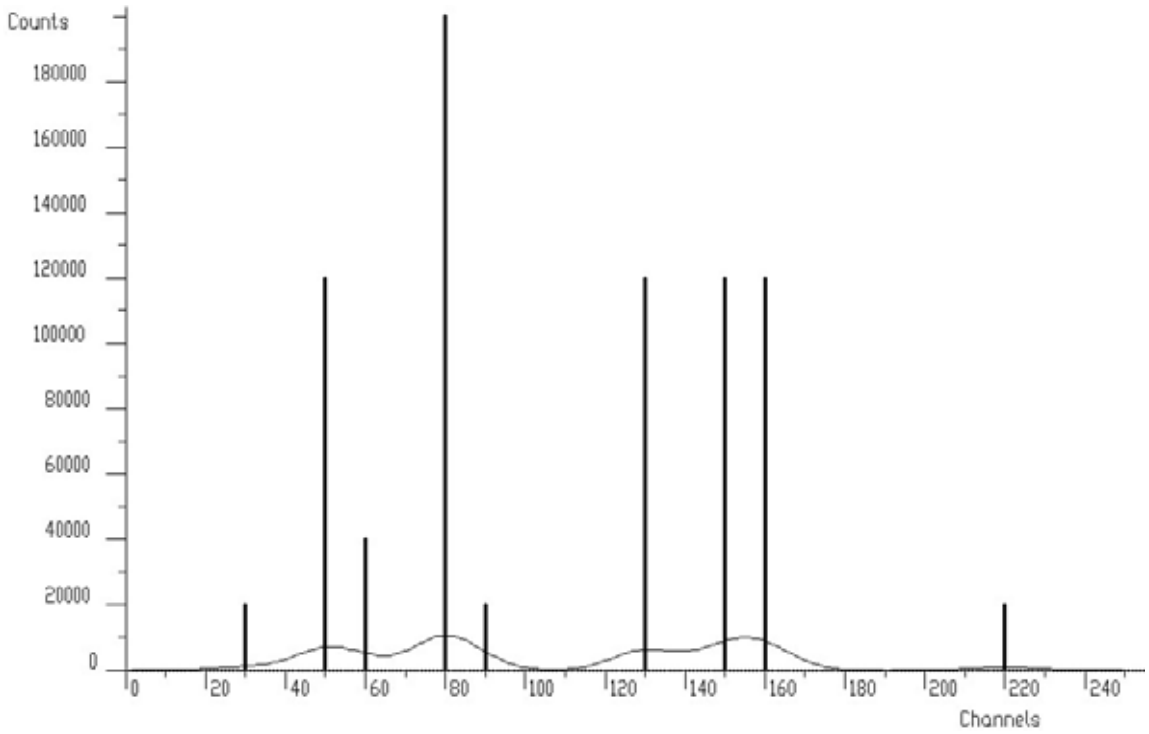


Figure 2 Original (thin line) and deconvolved spectrum (bars) using unconstrained solution of Toeplitz system of linear equations

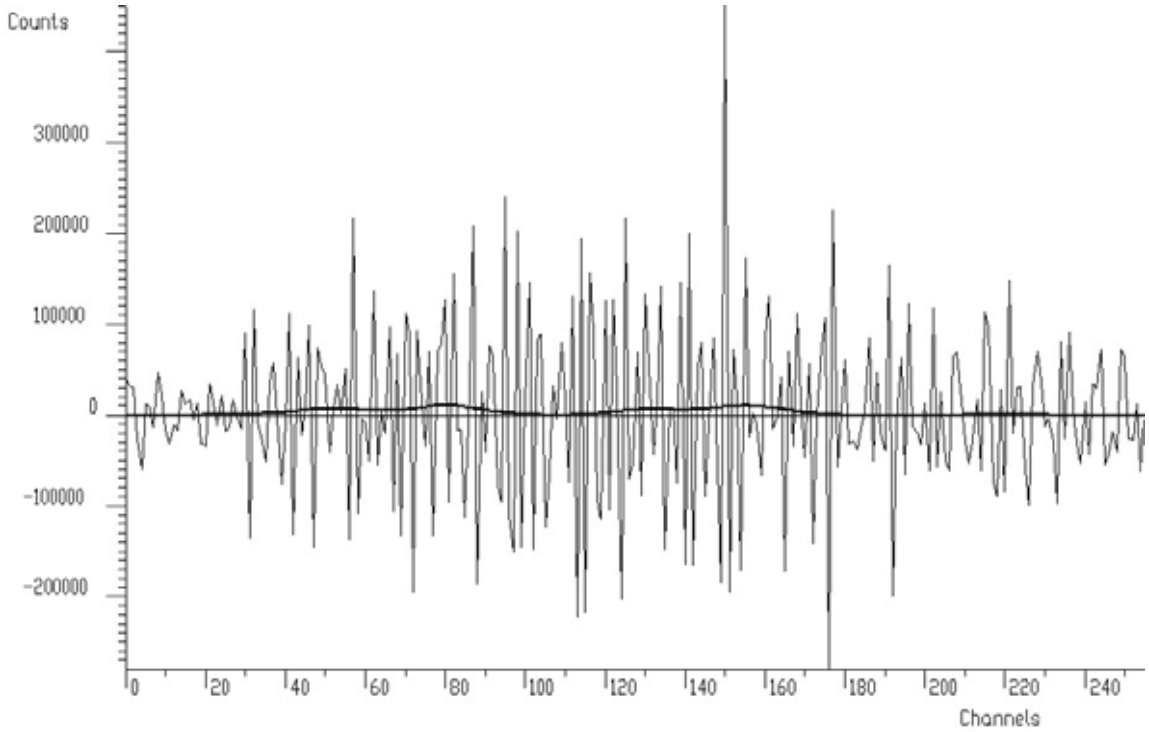


Figure 3 Original spectrum from Figure 1 + 1% of noise of the smallest peak # 9 (thick line) and deconvolved spectrum (strong oscillations) using unconstrained of Toeplitz system of system of linear equations

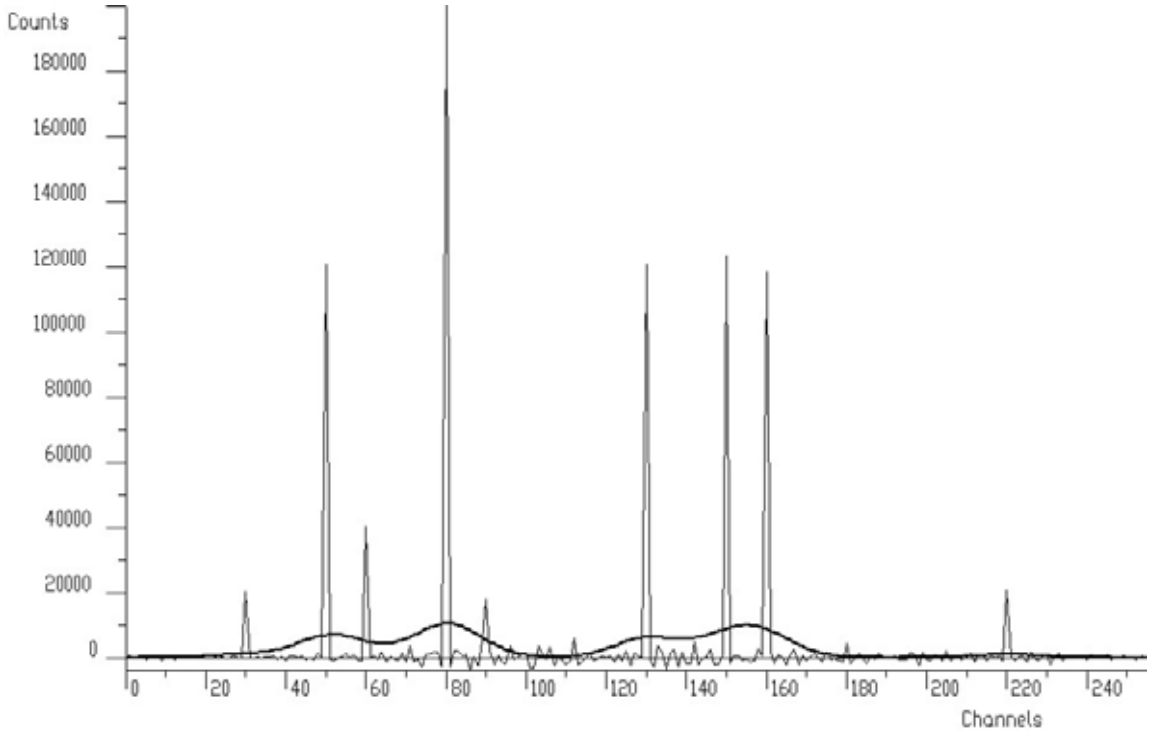


Figure 4 Original spectrum from Figure 1 + channel 80 increased by one (thick line) and deconvolved spectrum (thin line) using unconstrained solution of Toeplitz system of system of linear equations

Methods based on direct solution of system of linear equations.

Tikhonov-Miller regularization

- to find a regularized approximate solution of above given system of linear equations the functional

  $$\| H\hat{\boldsymbol{x}} - \boldsymbol{y} \|^2 + \alpha \| Q\hat{\boldsymbol{x}} \|^2$$

  is minimized, α being the regularization parameter. This solution can be obtained by solving the equation

  $$\hat{\boldsymbol{x}} = \left(H^T H + \alpha Q^T Q \right)^{-1} H^T \boldsymbol{y} ,$$

- for $Q = E$ - unit matrix we get so called zero-th order or Tikhonov regularization. Together with χ^2 also the sum of squares of elements of the estimated vector $\hat{\boldsymbol{x}}$ is minimized.
- an immediate generalization of zero-th order regularization is called linear regularization. The functional $\alpha \| Q\hat{\boldsymbol{x}} \|^2$ is replaced by more sophisticated measures of smoothness that derive from the first or higher derivatives. Suppose that ones a priori belief is that x_i is not too different from a constant, i.e., together with χ^2 one minimizes the sum of squares of differences of neighbouring points. Then the matrix Q is

  $$Q_1 = \begin{bmatrix} 1, & -1, & 0, & 0, & . & ., & 0, & 0 \\ 0, & 1, & -1, & 0, & . & ., & 0, & 0 \\ . & & & & & & & \\ . & & & & & & & \\ . & & & & & & & \\ 0, & 0, & 0, & 0, & . & ., & 1, & -1 \end{bmatrix}.$$

- anologously for quadratic or cubic approximation to x_i the matrices Q are

  $$Q_2 = \begin{bmatrix} -1, & 2, & -1, & 0, & . & ., & 0, & 0 \\ 0, & -1, & 2, & -1, & . & ., & 0, & 0, \\ . & & & & & & & \\ . & & & & & & & \\ . & & & & & & & \\ 0, & 0, & 0, & 0, & . & -1, & 2, & -1, \end{bmatrix},$$

  or

$$Q_3 = \begin{bmatrix} 1, & -3, & 3, & -1, & 0, & . & ., & 0, & 0, & 0, & 0 \\ 0, & 1, & -3, & 3, & -1, & . & ., & 0, & 0, & 0, & 0 \\ . & & & & & & & & & & \\ . & & & & & & & & & & \\ 0, & 0, & 0, & 0, & 0, & . & ., & 1, & -3, & 3, & -1 \end{bmatrix},$$

respectively. The extension to higher order differences is straightforward.

- there exist also some recommendations how to choose α $(0 < \alpha < \infty)$, e.g.

  $\alpha = Trace(H^T H) / Trace(Q^T Q).$

Riley algorithm

- this algorithm is commonly called iterated Tikhonov regularization. To obtain smoother solution one may use the above given formula with iterative refinement

  $$\boldsymbol{x}^{(n+1)} = \boldsymbol{x}^{(n)} + \left(H^T H + \alpha Q^T Q\right)^{-1}\left(\boldsymbol{y} - A\boldsymbol{x}^{(n)}\right)$$

  where $\boldsymbol{x}^{(0)} = 0$ and $n = 0,1,2,\ldots$.

Methods based on iterative solution of system of linear equations.

Van Cittert algorithm

- the basic form of Van Cittert algorithm for a general discrete system is

  $\boldsymbol{x}^{(n+1)} = \boldsymbol{x}^{(n)} + \mu\left(\boldsymbol{y} - A\boldsymbol{x}^{(n)}\right)$,

  where A is system Toeplitz matrix, n represents the number iterations and μ is the relaxation factor. The convergence condition of is that the diagonal elements of the matrix A satisfy

  $A_{ii} > \sum_{j=0, j\neq i}^{N-1} A_{ij}$, $i = 0,1,\ldots,N-1$.

- this deconvolution algorithm can be modified in a such way that it will satisfy the conditions of convergence. Hence

  $\boldsymbol{x}^{(n+1)} = \mu\boldsymbol{y} + \left(E - \mu A\right)\boldsymbol{x}^{(n)} = \mu\boldsymbol{y} + D\boldsymbol{x}^{(n)}$,

  where E is a unit matrix and

  $D = E - \mu A$.

  Let $\boldsymbol{x}^{(0)} = \boldsymbol{y}$, then we get

  $\boldsymbol{x}^{(n)} = \mu\left(E + D + \ldots + D^n\right)\boldsymbol{y}$.

- supposing that $\lambda_0,\ \lambda_1,\ldots,\lambda_{M-1}$ are eigenvalues of A, then $\left(1-\mu\lambda_0\right),\ldots,\left(1-\mu\lambda_{M-1}\right)$ are eigenvalues of D. If

$$\lim_{n\to\infty}\left(1-\mu\lambda_i\right)^n = 0, \qquad i = 0,1,...,M-1$$

then

$$\lim_{n\to\infty} D^n = [0]$$

and

$$\lim_{n\to\infty} \boldsymbol{x}^{(n)} = A^{-1}\boldsymbol{y} = \boldsymbol{x}\,.$$

- from this it implies that the necessary and sufficient conditions of convergence are

$$\left|1-\mu\lambda_i\right| < 1, \qquad i = 0,1,...,M-1$$

if we define λ_i and its conjugate λ_i^* as

$$\lambda_i = a_i + jb_i,\ \lambda_i^* = a_i - jb_i$$

we get

$$\mu\left[\mu\left(a_i^2 + b_i^2\right) - 2a_i\right] < 0,\ \ i = 0,1,,,.M-1.$$

- this inequality gives two bounds for μ

$$\mu = 0,\ \ \mu = \frac{2a_i}{a_i^2 + b_i^2},\quad i = 0,1,...,M-1\,.$$

M conditions that determine the bounds of μ coefficient.

- if the matrix A is positive definite the convergent solution always exists.
- matrix H^TH is symmetric, so its eigenvalues are real. The eigenvalues of matrix $\left(H^TH\right)\left(H^TH\right)$ are squares of the eigenvalues of matrix $\left(H^TH\right)$ and therefore positive. The iterative algorithm of deconvolution becomes

$$\boldsymbol{x}^{(n+1)} = \boldsymbol{x}^{(n)} + \mu\left[\left(H^THH^T\right)\boldsymbol{y} - \left(H^THH^TH\right)\boldsymbol{x}^{(n)}\right]$$

or

$$\boldsymbol{x}^{(n+1)} = \boldsymbol{x}^{(n)} + \mu\left[\boldsymbol{y'} - H'\boldsymbol{x}^{(n)}\right]$$

- eigenvalues λ_i are real, positive numbers, so then for μ one can write

$$0 < \mu < 2/\lambda_{\max}\ ,$$

where $\lambda_{\max}$ is the greatest eigenvalue of H'.

- for eigenvalues of $\left(H^THH^T\right)\boldsymbol{y} = \left(H^THH^TH\right)\boldsymbol{x}$ we can write

$$H'\boldsymbol{x} = \lambda_i\boldsymbol{x} \quad i = 0,1,...,M-1\,.$$

- if x_j is the greatest absolute element in $\boldsymbol{x}$ then we get

$$\lambda_i = \frac{\sum_{m=0}^{M-1} H'_{jm}x_m}{x_j}\,.$$

- as we do not know the greatest element in x we estimate it from the condition

$$\lambda_i \le \sum_{m=0}^{M-1} \left| H'_{jm} \right|, \quad i = 0,1,...,M-1 \ .$$

- from these conditions we can estimate μ .

Reference:
Van Cittert P.H., Zum Einfluss der Spaltbreite auf die Intensitätverteilung in Spektralinien II, Z. Physik (1933) 298.

Janson algorithm

- local variable relaxation factor μ_i is introduced into Van Cittert algorithm

$$x^{(n+1)}(i) = x^{(n)}(i) + \mu_i \left[y'(i) - \sum_{m=0}^{M-1} H'_{im} x^{(n)}(k) \right] .$$

where

$$\mu_i = r \left(1 - \frac{2}{b-a} \right) \left| x^{(n)}(i) - \frac{a+b}{2} \right| ,$$

and r is usually about 0.2, a is usually 0 and b must be greater than the ultimate height of the highest peak in the data

Reference:
Coote G.E., Iterative smoothing and deconvolution of one- and two-dimensional elemental distribution data, NIM B 130 (1997) 118.

Gold algorithm

- if we choose a local variable relaxation factor

$$\mu_i = \frac{x^{(n)}(i)}{\sum_{m=0}^{M-1} H'_{im} x^{(n)}(m)}$$

and we substitude it into Van Cittert algorithm we get

$$x^{(n+1)}(i) = \frac{y'(i)}{\sum_{m=0}^{M-1} H'_{im} x^{(n)}(m)} x^{(n)}(i)$$

- this is the Gold deconvolution algorithm. Its solution is always positive when both the elements of input data and response matrix are positive
- the algorithm is suitable for use with histograms, e.g. in γ-ray spectroscopy.

Reference:
Gold R., ANL-6984, Argonne National Laboratories, Argonne III, 1964.

Richardson-Lucy algorithm

- in formal way one can express the output of the continuous linear system in the form of probabilities

  $y(t) = \int h(t|\tau)\, x(\tau)\, d\tau$.

- from this one can write

  $x(\tau) = \int q(\tau|t)\, y(t)\, dt$,

  where $q(\tau|t)$ is related to $h(t|\tau)$ via Bayes theorem

  $$q(\tau|t) = x(\tau)\frac{h(t|\tau)}{y(t)} \ .$$

- to solve this problem $q(\tau|t)$ is calculated using an iteration approach

  $$q^{(n)}(\tau|t) = x^{(n)}(\tau)\frac{h(t|\tau)}{y^{(n)}(t)}$$

  and

  $$x^{(n)}(\tau) = \int q^{(n-1)}(\tau|t)\, y^{(0)}(t)\, dt = \int x^{(n-1)}(\tau)\frac{h(t|\tau)}{y^{(n-1)}(t)}\, y^{(0)}(t)\, dt$$

  with $y^{(0)}(t)$ being the measured data $y(t)$ and

  $y^{(n-1)}(t) = \int h(t|\tau)\, x^{(n-1)}(\tau)\, d\tau$.

- finally in discrete form we have

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

  $i \in \langle 0, M-1 \rangle$. For positive input data and response matrix this iterative method forces the deconvoluted spectra to be non-negative.

- the Richardson-Lucy iteration converges to the maximum likelihood solution for Poisson statistics in the data.

References:

Abreu M.C. et al., A four-dimensional deconvolution method to correct NA38 experimental data, NIM A 405 (1998) 139.
Lucy L.B., A.J. 79 (1974) 745.
Richardson W.H., J. Opt. Soc. Am. 62 (1972) 55.

Muller algorithm

- setting the probability to have Gauss statistics another deconvolution algorithm based on Bayes formula was derived by Muller (1997)

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

$i \in \langle 0, M-1 \rangle$. This algorithm again applies the positivity constraint.

Modifications and extensions of the deconvolution algorithms

Minimization of squares of negative values

- while in the classic Tikhonov algorithm we minimize the sum of squares of contents of all channels, in this case we do not care about channels with positive values. The objective of the method is to minimize the sum of squares, but only negative elements of the vector $\boldsymbol{x}$.
- let us define the regularization algorithm

  $\hat{\boldsymbol{x}}^{(k)} = \left(H^T H + \alpha Q_0^{(k)T} Q_0^{(k)} \right)^{-1} H^T \boldsymbol{y}^{(k)}$,

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

  where

  $$Q_0^{(k)}(i,j) = \begin{cases} 1 \text{ if } x^{(k)}(i) < 0 \text{ and } i = j, \\ 0 \text{ else,} \end{cases}$$

  k is the iteration step and $\boldsymbol{y}^{(0)} = \boldsymbol{y}$.

- the combinations of negative values are changing and therefore we have to solve the full general system of linear equations in each iteration step.

Efficient one-fold Gold deconvolution

- above we have presented the basic algorithm of the Gold deconvolution. We started from the overdetermined system of linear equations

  $\boldsymbol{y} = H \cdot \boldsymbol{x}$.

- multiplying both sides by H^T we get

  $H^T \cdot \boldsymbol{y} = H^T H \cdot \boldsymbol{x}$.

- with the respect to the above given reasons for Van Cittert algorithm in original Gold algorithm we multiplied both sides by $H^T H$

$$H^T H H^T \cdot \boldsymbol{y} = H^T H H^T H \cdot \boldsymbol{x}$$

- in practice, we have revealed that the second multiplication by the matrix $H^T H$, for Gold deconvolution, is redundant. On the contrary, its omitting gives result with better resolution in γ-ray spectra. Then let us have the system of linear equations in the form

$$\boldsymbol{z} = T \cdot \boldsymbol{x} \ ,$$

where T is Toeplitz matrix $H^T H$. By its substitution into the iterative formula to solve systems of linear equations we get

$$\boldsymbol{x}^{(k+1)} = \boldsymbol{x}^{(k)} + \mu\left(\boldsymbol{z} - T\boldsymbol{x}^k\right).$$

- now instead of common coefficient μ let us introduce a local variable relaxation factor μ_i for every element of the vector $\boldsymbol{x}$

$$\mu_i = \frac{x^{(k)}(i)}{d(i)}$$

where

$$\boldsymbol{d} = T \cdot \boldsymbol{x}^{(k)}$$

and consequently, the resulting formula is

$$x^{(k+1)}(i) = \frac{z(i)\,x^{(k)}(i)}{d(i)};\ i \in \langle 0, N-1 \rangle .$$

- hereafter this algorithm will be called one-fold Gold deconvolution.
- if we take the initial solution

$$\boldsymbol{x}^{(0)} = [1, 1, ..., 1]^T$$

and if all elements in the vectors $\boldsymbol{h}$, $\boldsymbol{y}$ are positive (this requirement is fulfilled for nuclear spectra), this estimate is always positive. It converges to the least square estimate in the constrained subspace of positive solutions.

Boosted deconvolution

- in practice, we have observed that the positive definite deconvolutions (Gold, Richardson-Lucy, Muller etc.) converge to stable states. Then it is useless to increase the number of iterations, the result obtained does not change.
- however sometimes we are not satisfied with the resolution achieved and want to continue in decreasing the sigma of peaks.
- we have found out that when the solution reaches its stable state it is necessary to stop iterations, then to change the particular solution $\boldsymbol{x}^{(L)}$ in a way and repeat again the deconvolution. To change the relations among elements of the particular solution we need to apply non-linear boosting function to it.
- the power function proved to give the best results. Then, e.g. the algorithm of boosted Gold deconvolution is:
  1. Set the initial solution $\boldsymbol{x}^{(0)} = [1,1,...,1]^T$.
  2. Set required number of repetitions R and iterations L
  3. Set the number of repetitions $r = 1$.
  4. According to Gold deconvolution algorithm for $k = 0,1,...,L-1$ find solution $\boldsymbol{x}^{(L)}$.
  5. If $r = R$ stop calculation, else
     a. apply boosting operation, i.e., set
        $x^{(0)}(i) = \left[x^{(L)}(i) \right]^p$; $i = 0,1,...,N-1$
        and p is boosting coefficient >0
     b. $r = r + 1$
     c. continue in 4.

Problems

We can conclude that there exist many problems inherent to the solution of the problem of deconvolution and decomposition in general :

- ill conditionality of systems
- influence of the errors due to the measured noise
- rounding-off errors or truncation errors due to the finite length of computer word
- resolution
- computational complexity
- convergence speed
- robustness to noise

Results

- the principal results of the deconvolution operation with invariant response (independent on energy) were presented in

Reference:
Morháč M., Kliman J., Matoušek V., Veselský M., Turzo I., Efficient one and two dimensional Gold deconvolution and its application to gamma-ray spectra decomposition, NIM A 401 (1997) 385.

- the deconvolution was applied to the experimental results from investigation of the prompt γ-ray emission of the fission fragments from spontaneous fission of ^{252}Cf collected with the Gammasphere spectrometer. In the paper, we employed the Gold deconvolution method, which proved to be stable with good results. Its basic property is that the solution is always nonnegative. We have extended and applied the method to the two-dimensional γ-ray spectra as well.

- later we have optimized the Gold deconvolution algorithm that allowed to carry out the deconvolution operation much faster and to extend it to three-dimensional spectra. The results of the optimized Gold deconvolution for all one-, two-, and three-dimensional data are given in

References:
Morháč M., Matoušek V., Kliman J., Efficient algorithm of multidimensional deconvolution and its application to nuclear data processing, Digital Signal Processing 13 (2003) 144.
Morháč M., Matoušek V., Kliman J., Optimized multidimensional nonoscillating deconvolution, Journal of Computational and Applied Mathematics 140 (2002) 639.

One-fold Gold deconvolution and boosting

a. One-dimensional spectra

- let us now study the properties of improvements, modifications and extensions of the Gold deconvolution algorithm.
- we shall investigate decomposition capabilities of deconvolution algorithms, i.e., the ability to concentrate the area of peaks in the deconvolved spectrum to as few channels as possible.
- first let us take the synthetic one-dimensional spectrum consisting of 3 peaks (σ=2) and added noise. Two of them were positioned very close to each other (channels 445 and 447) and one in the position 531.
- we have applied classic two-fold Gold deconvolution to these data.

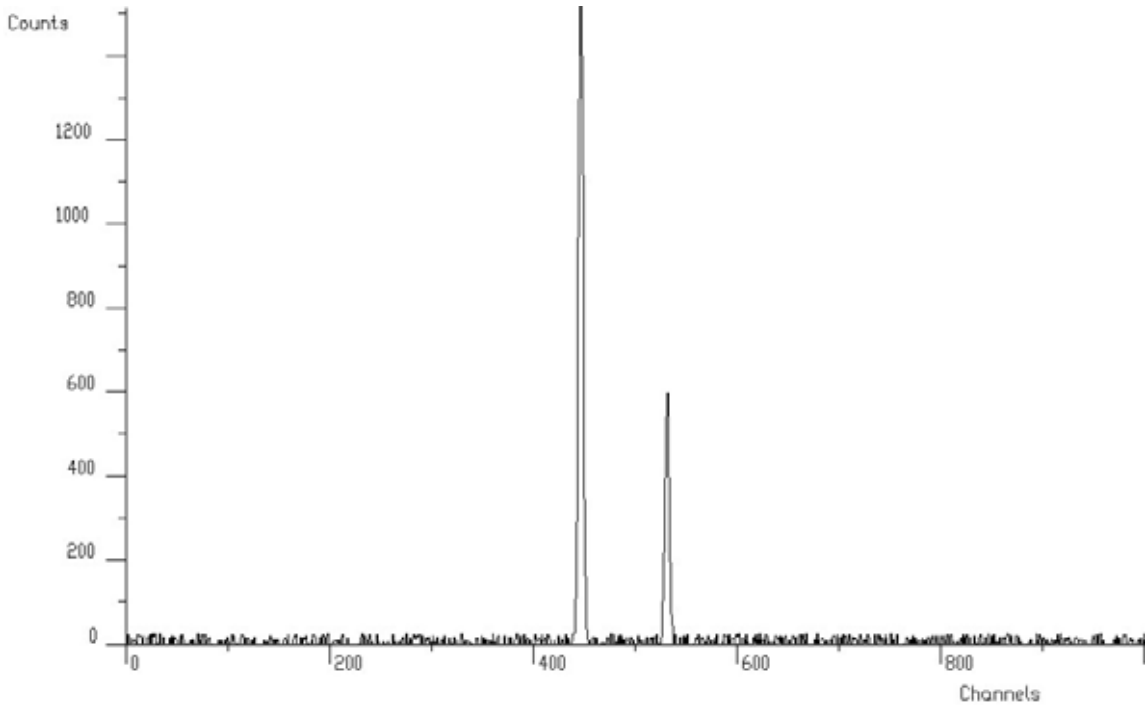


Figure 5 Synthetic one-dimensional spectrum

- the result (detail containing peaks in the spectrum) after 10000 iteration steps is shown in next Figure (thick line original spectrum, thin line deconvolved spectrum).

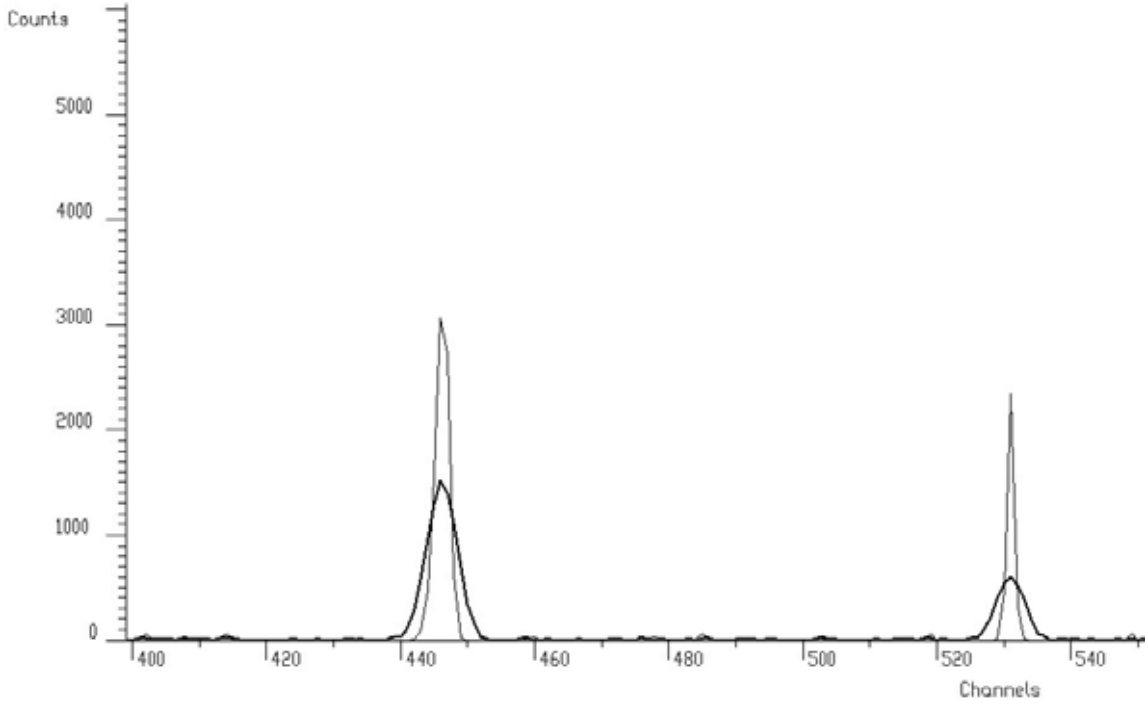


Figure 6 Detail of the spectrum from Figure 5 (thick line) and after (thin line) two-fold Gold deconvolution (10000 iterations)

- the resolution is improved but apparently, the method is unable to decompose the doublet.

- γ-ray spectrum can be thought of being composed of shifted response (instrument) functions.

- so at the input of the detector and electronic system it can be imagined as a sum of δ - functions.

- at the output of the system the spectrum represents a linear combination of the δ-functions with various amplitudes positioned in various channels, which are blurred by the system response function.

- our endeavor in the deconvolution operation is to remove the influence of the response function to the utmost, i.e., to deblur the data and in ideal case to obtain a spectrum consisting of δ-functions like "peaks".

- therefore, we continued in the investigations of more efficient deconvolution methods. Let us continue with the above presented example.

- when we apply one-fold Gold deconvolution algorithm (again 10000 iterations) we can observe an outline of two peaks in the region of channels 440-450

In TSpectrum class the function "Deconvolution1"

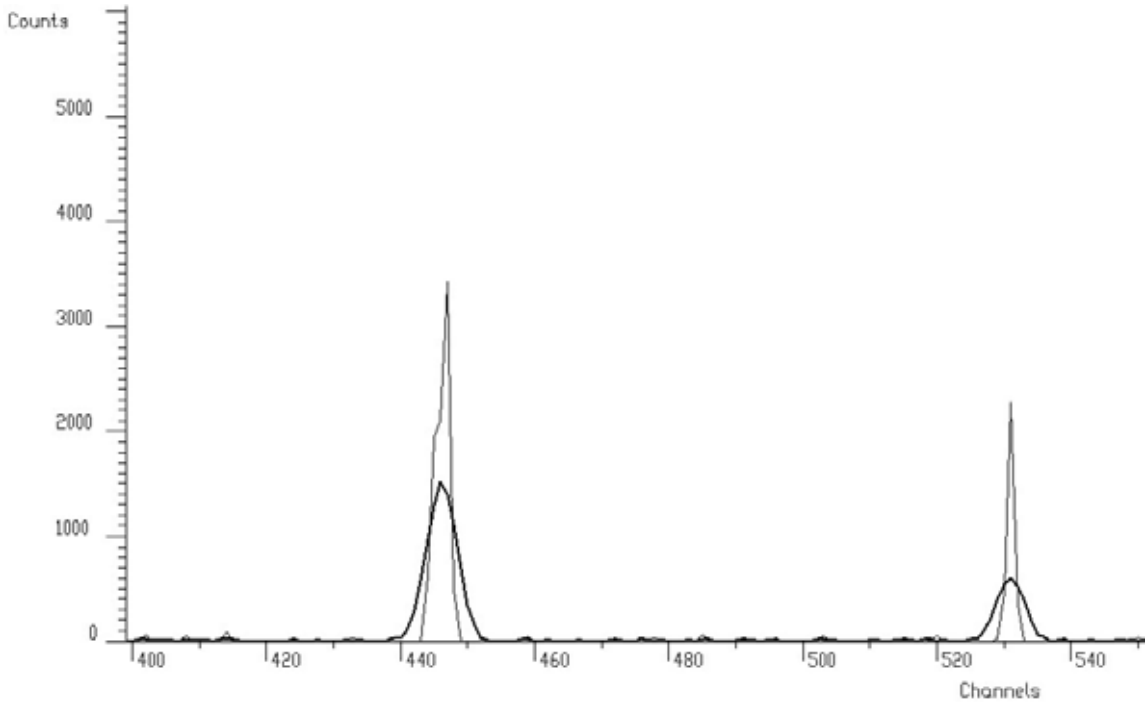


Figure 7 Detail of the spectrum from Figure 5 before (thick line) and after (thin line) one-fold Gold deconvolutions (10000 iterations)

- to see and judge the course of the deconvolution procedure we recorded the sum of weighted squares of errors per channel, denoted by letter Q, after each iteration step in the form of graph.

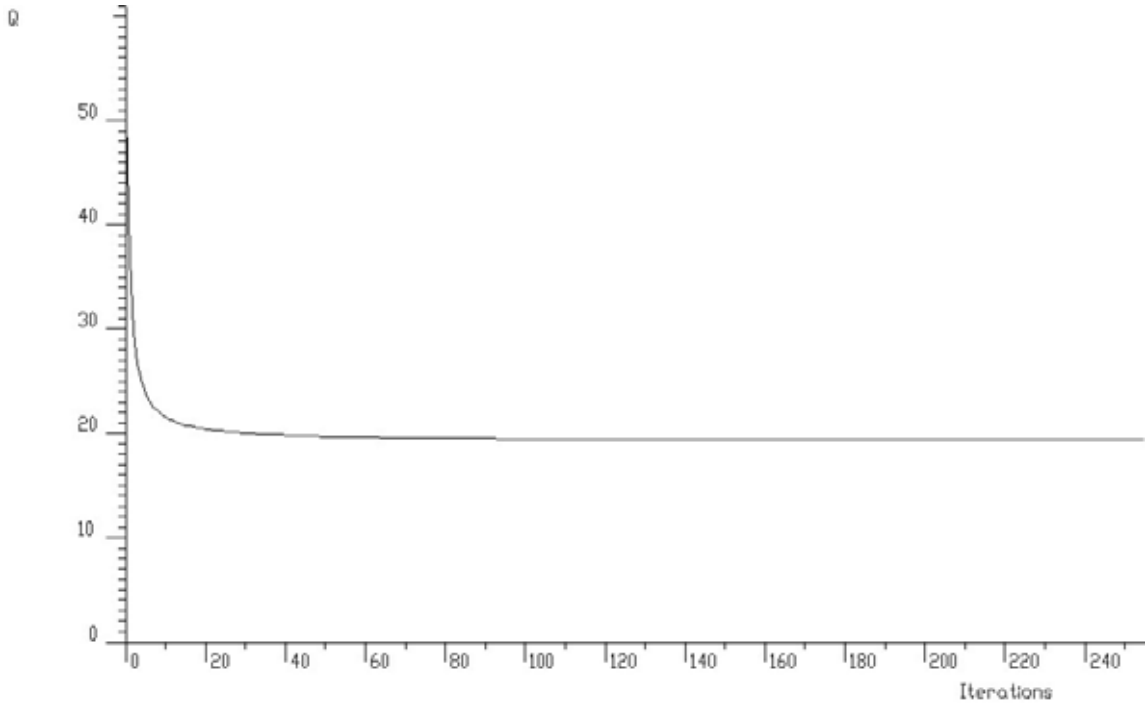


Figure 8 Sum of weighted squares of errors per one channel in dependence on number of iterations

- obviously, after initial decrease of Q at the beginning of the deconvolution operation during the following iteration steps it remains constant. Consequently, the deconvolved spectrum does not change.
- therefore, it is useless to continue in the iterations. We stopped the iterations after each 200 steps, applied boosting operations according to the above proposed algorithm and repeated this procedure 50 times. Entirely it gives also 10000 iteration steps.
- the result of the boosted one-fold Gold deconvolution is shown in next two figures in both polyline and bars display mode, respectively.

In TSpectrum class the function "Deconvolution1HighResolution"

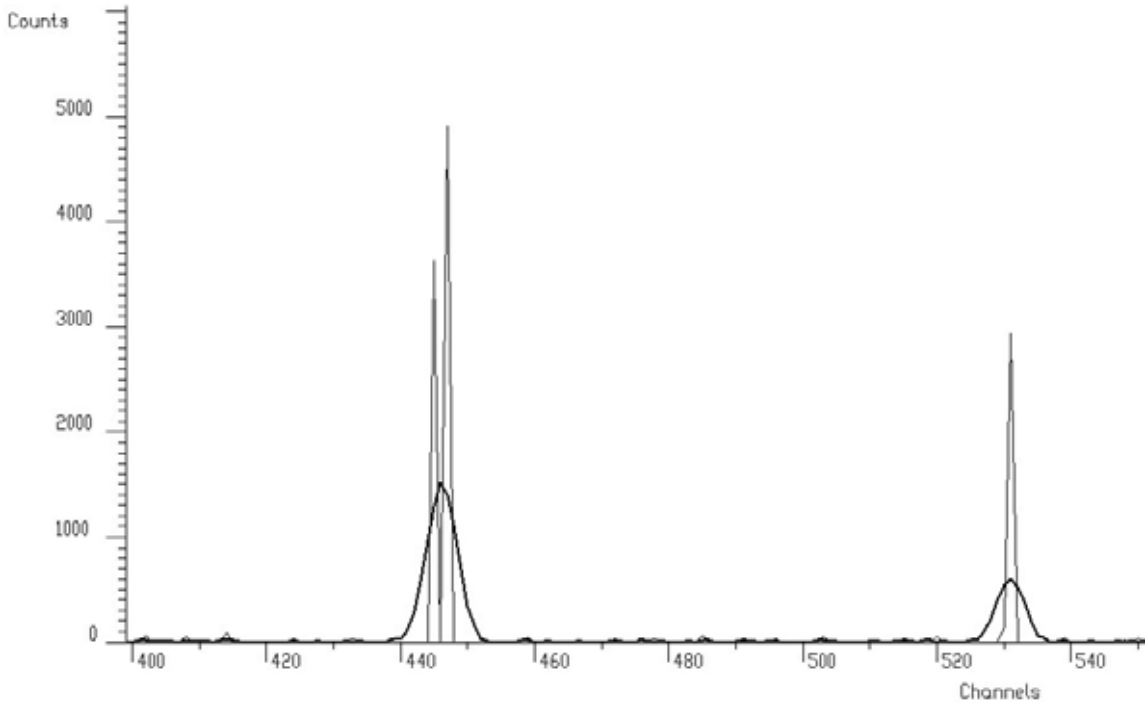


Figure 9 Detail of the spectrum from Figure 5 before (thick line) and after boosted one-fold Gold deconvolution (shown in polyline display mode - thin line)

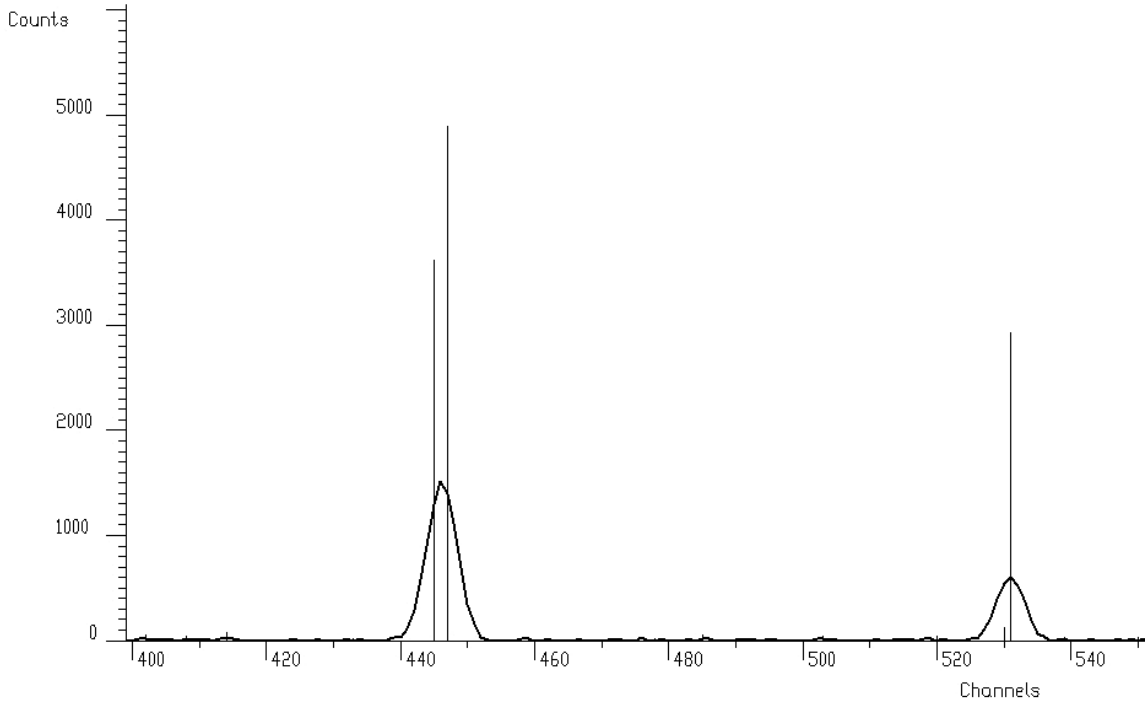


Figure 10 The same like Figure 9 only the deconvolved spectrum is shown in bars display mode

- the method decomposes completely the doublet in channels 445 and 447, while preserving the ratio of amplitudes of both peaks.

- the question is the choice of the boosting coefficient p. Apparently when we want to boost peaks in the spectrum it should be greater than 1.
- otherwise, the peaks would be suppressed (smoothed) and consequently the resolution decreased. On the other hand, according to our experience, it should not be too big (greater than 2).
- when choosing it too big, small peaks will disappear from spectrum at the expense of big ones. Empirically we have found that good results are obtained with the boosting coefficient p=1.2.
- further we have applied the sequence of above mentioned methods also to experimental γ-ray spectra. However, before application of the deconvolution procedure we removed background from the spectrum using the background elimination algorithm presented in

Reference:

Morháč M., Kliman J., Matoušek V., Veselský M., Turzo I., Background elimination methods for multidimensional coincidence gamma-ray spectra, NIM A 401 (1997) 113.

In TSpectrum class the function "Background1" or "Background1General"

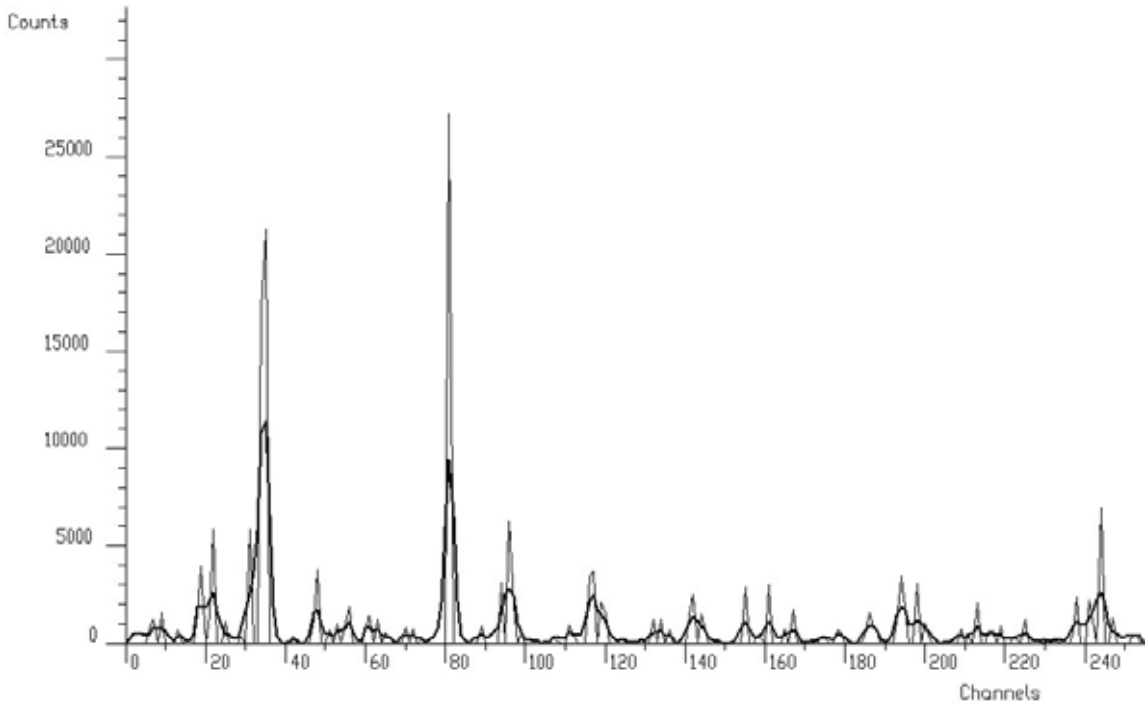


Figure 11 Experimental γ-ray spectrum before (thick line) and after (thin line) boosted one-fold Gold deconvolution

- again, boosted one-fold Gold deconvolution decomposes the spectrum practically to δ functions.

b. Two-dimensional spectra

- we have done analogous experiment with two-dimensional spectra. Let us take two-dimensional synthetic spectrum containing 17 peaks and added noise.
- there are 5 overlapped peaks concentrated in a cluster (positions x-y, 14-40, 17-37, 19-39, 19-46, 22-43) and 2 overlapped peaks in a doublet (44-46, 48-46).

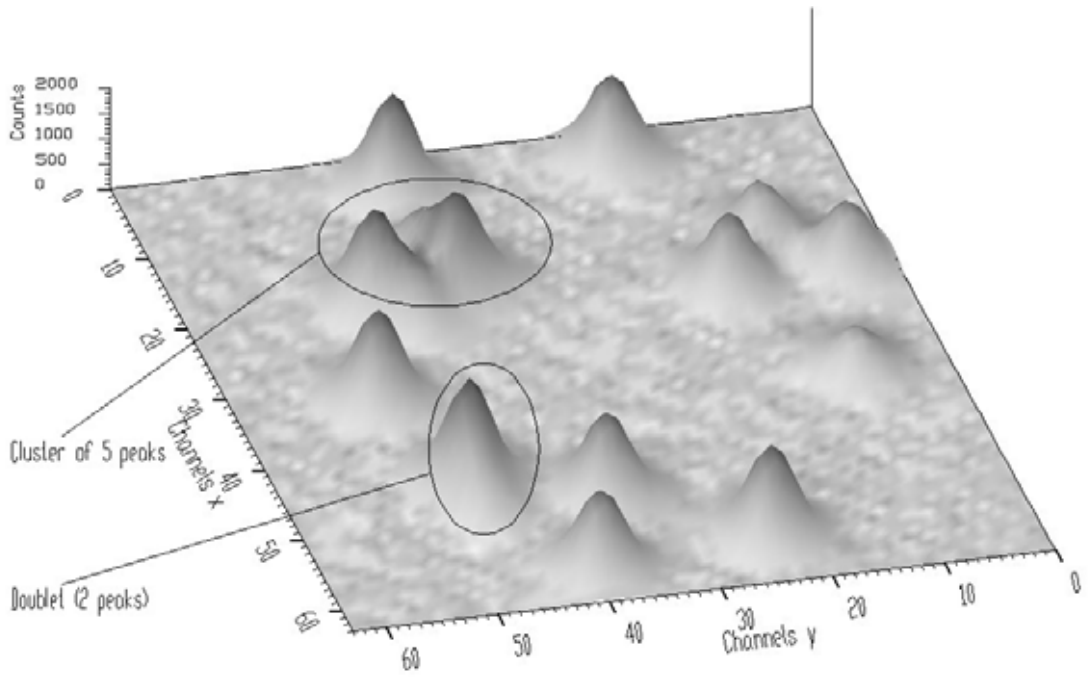


Figure 12 Two-dimensional original synthetic spectrum

- after two-fold Gold deconvolution (1000 iteration steps), we get the result with better resolution than in original data, however the overlapped peaks remained unresolved.

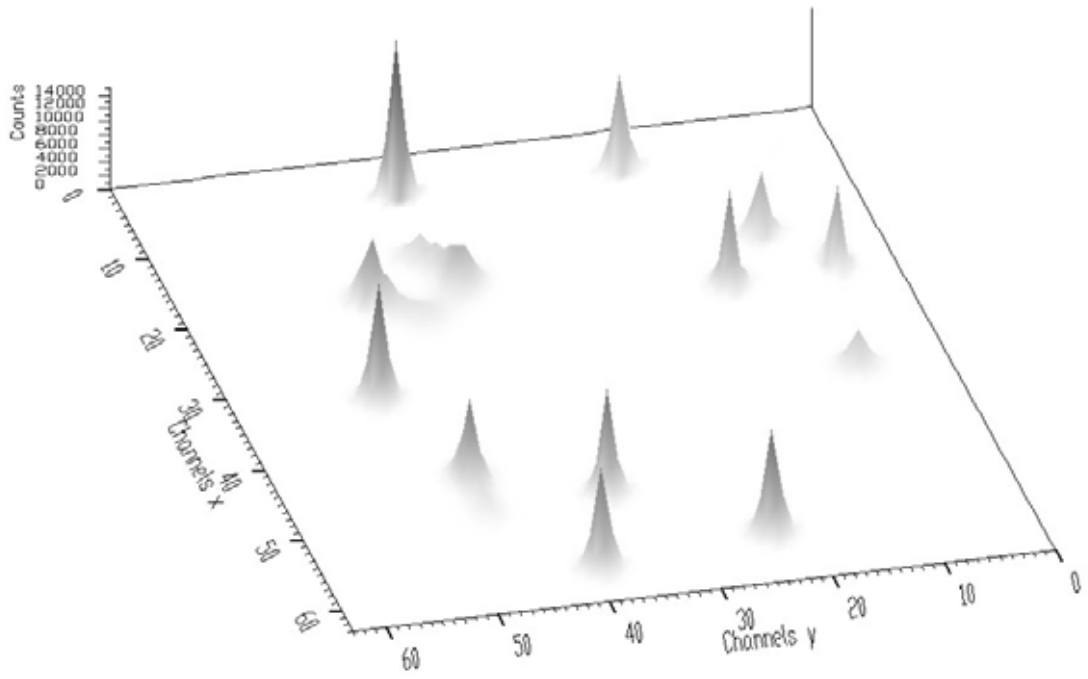


Figure 13 Spectrum from Figure 12 after two-fold Gold deconvolution (1000 iterations)

- the result is slightly better after application of one-fold Gold deconvolution (1000 iterations).

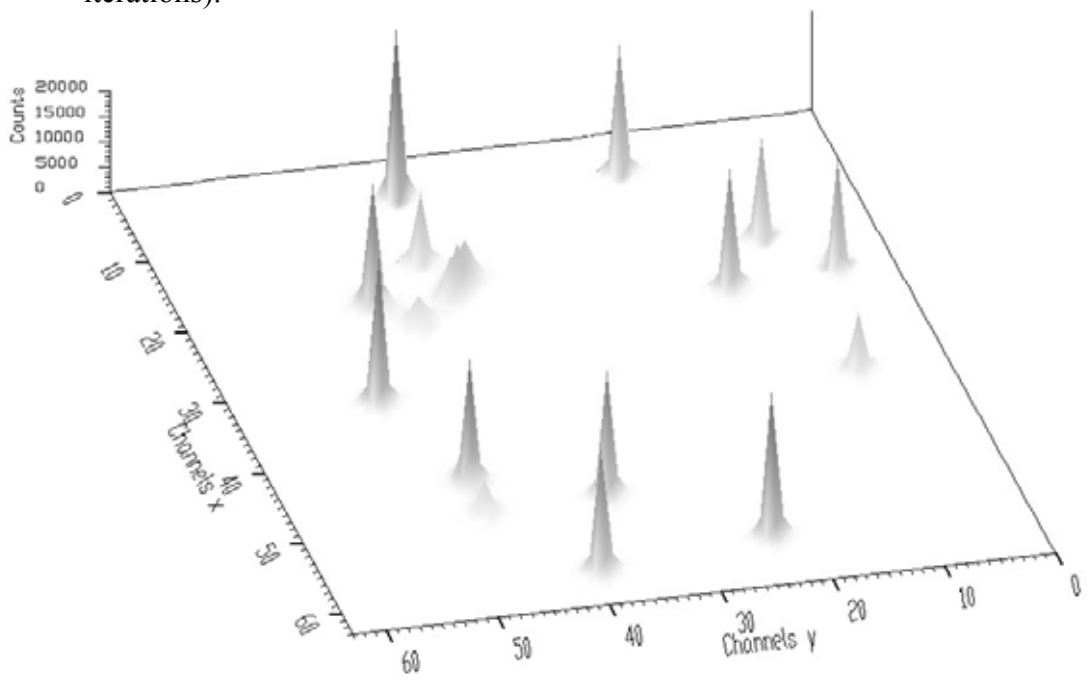


Figure 14 Spectrum from Figure 12 after one-fold Gold deconvolution (1000 iterations)

- when applying one-fold boosted deconvolution (50 iterations, repeated 20 times with boosting coefficient p=1.2) we get the result presented in both shaded and bars display modes in next two figures.
- even the close positioned peaks from cluster and doublet are practically completely decomposed to one-channel "peaks". The positions in the deconvolved spectrum coincide with the positions of peaks in the original data.

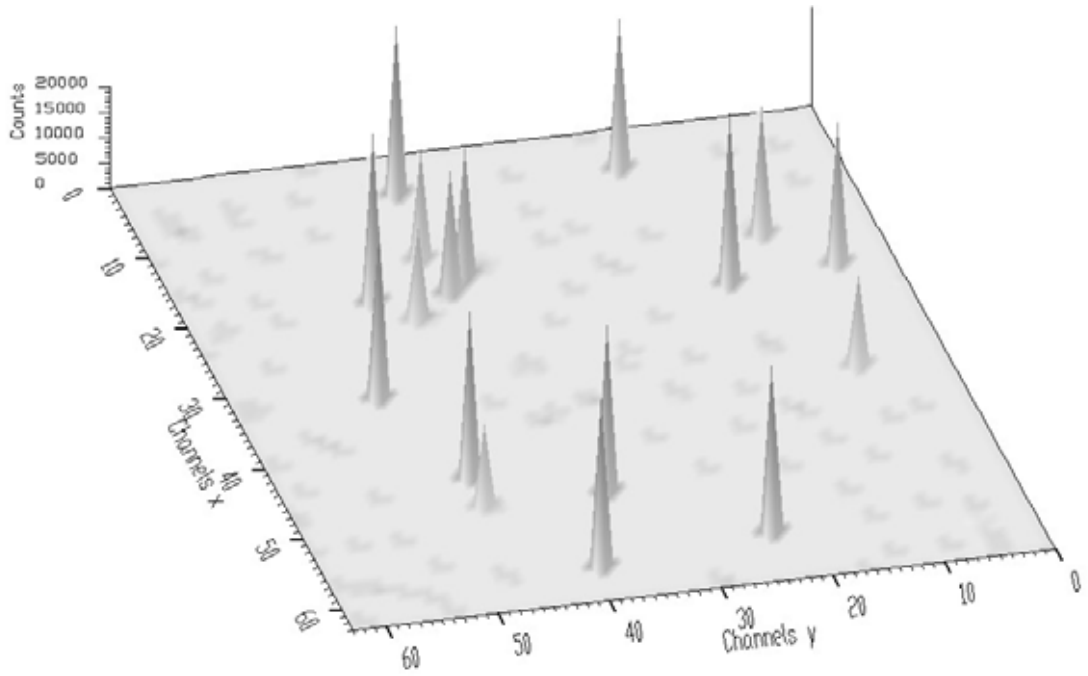


Figure 15 Spectrum from Figure 12 after boosted one-fold Gold deconvolution (50 iterations repeated 20 times)

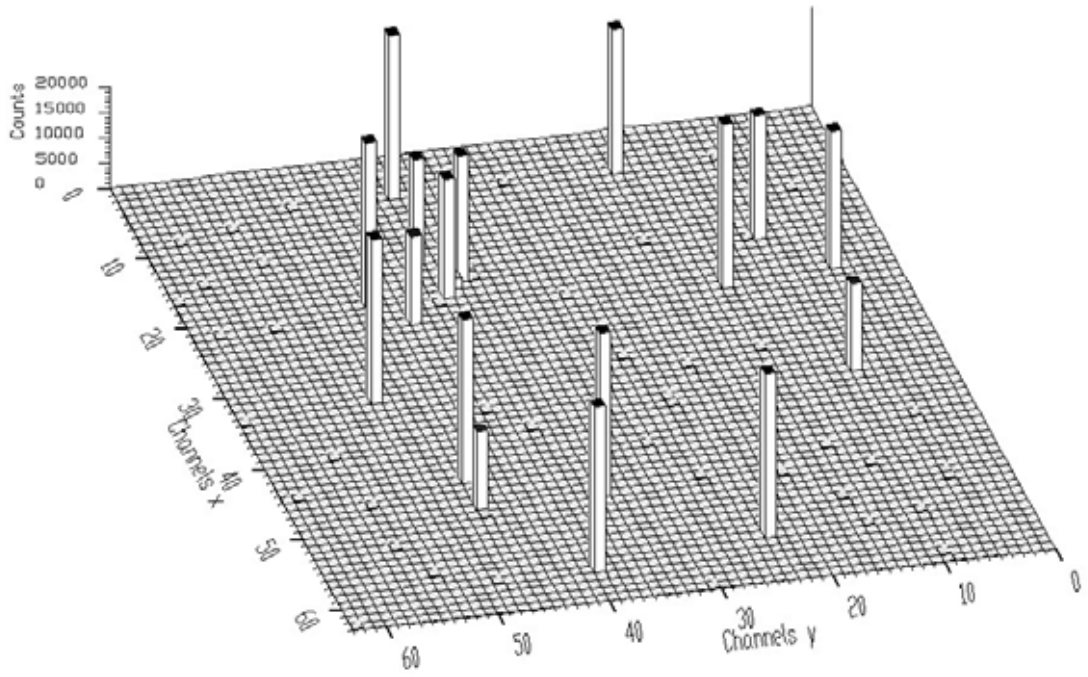


Figure 16 The same like in Figure 15 displayed in bars display mode

- analogously to one-dimensional data, we applied the deconvolution methods also to experimental $\gamma - \gamma$ coincidence two-dimensional spectra (256x256 channels).
- in next two Figures we show a part (128x128 channels) of original two-dimensional spectrum and after one-fold boosted Gold deconvolution (50 iterations, with boosting coefficient p=1.2 repeated 20 times).

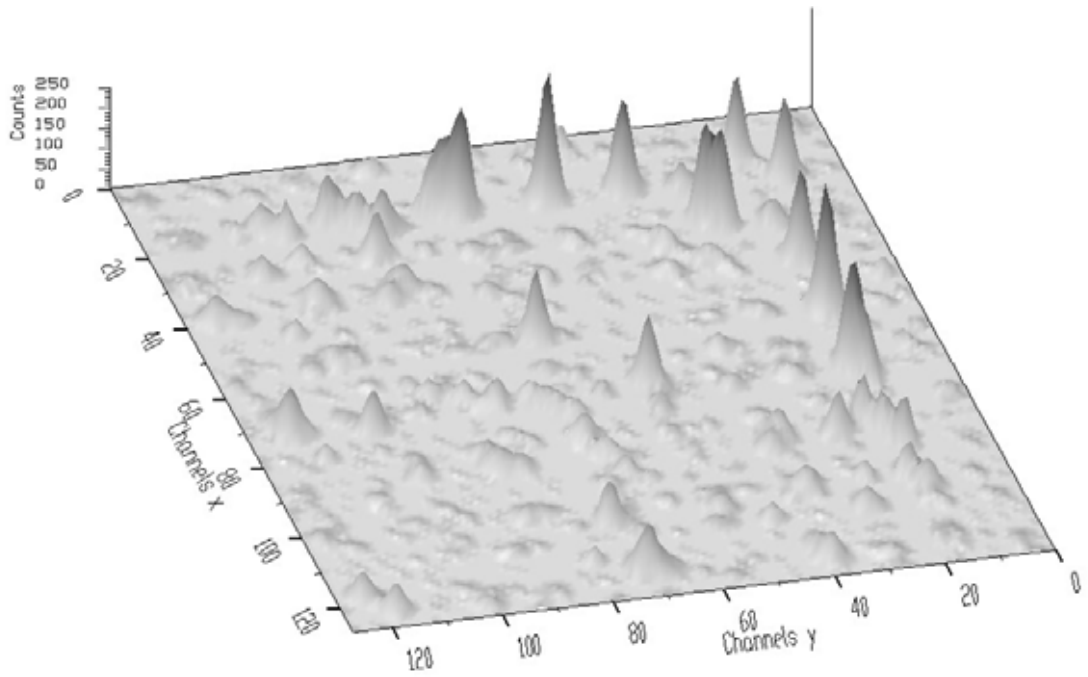


Figure 17 Part of original experimental two-dimensional $\gamma - \gamma$ coincidence spectrum

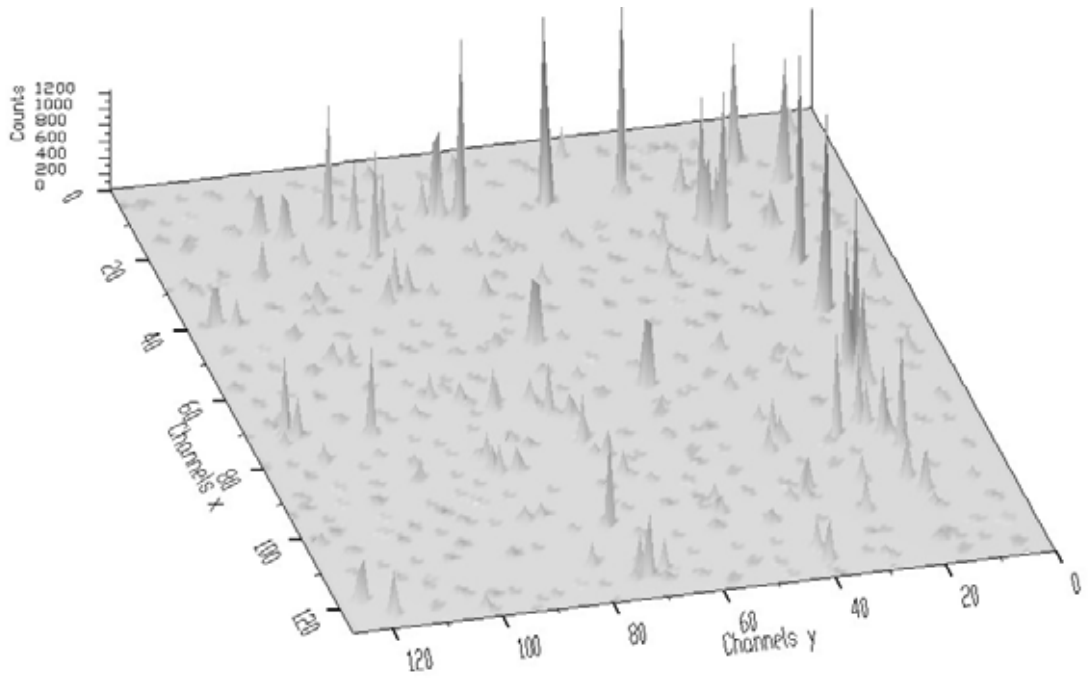


Figure 18 Spectrum from Figure 17 after boosted one-fold deconvolution (50 iterations repeated 20 times)

c. Three-dimensional spectra

- finally, we have implemented the above mentioned variations of the Gold deconvolution method also for three-dimensional data.
- the original three-dimensional synthetic spectrum consisting of 4 peaks positioned close to each other (positions x-y-z, 15-15-15 with amplitude A=100, 12-12-18, A=250, 14-19-12, A=150, 20-20-13 A=50) is shown in next Figure.

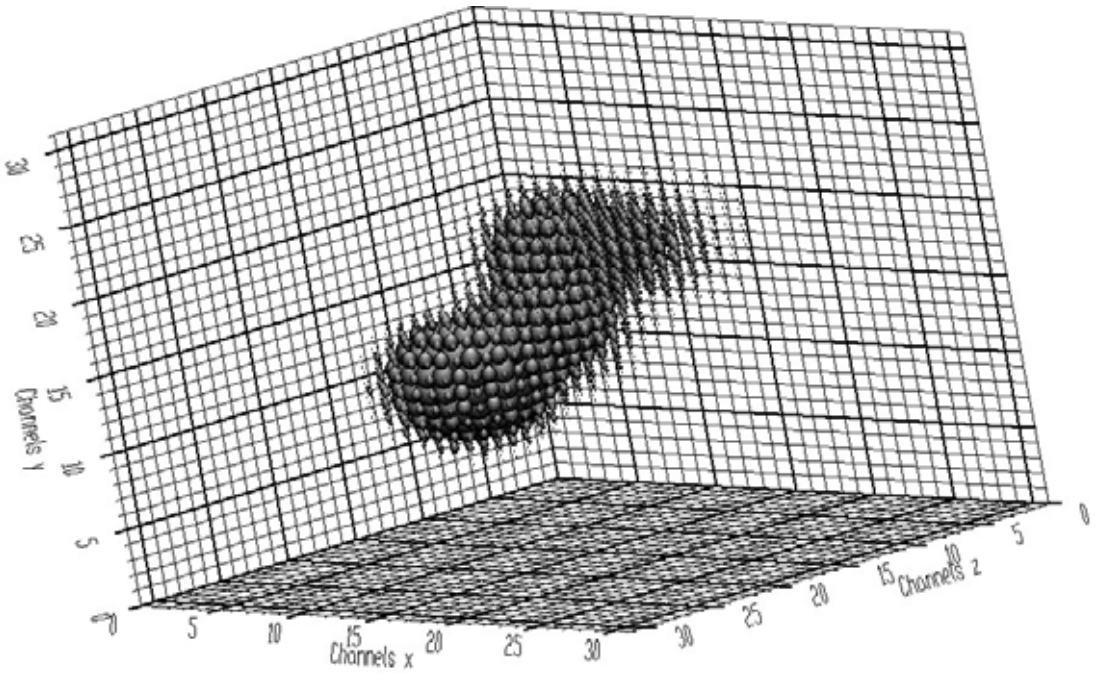


Figure 19 Three-dimensional synthetic spectrum

- in next Figure we give the same spectrum after one-fold boosted Gold deconvolution (50 iterations, with boosting coefficient p=1.2, repeated 20 times).
- the volumes of peaks are concentrated separately practically into one channel each. The positions of peaks coincide with the peaks positions in original spectrum.
- the relations among amplitudes of peaks are also approximately preserved. The counts scales in both Figures are different (1-250, 1-20000).

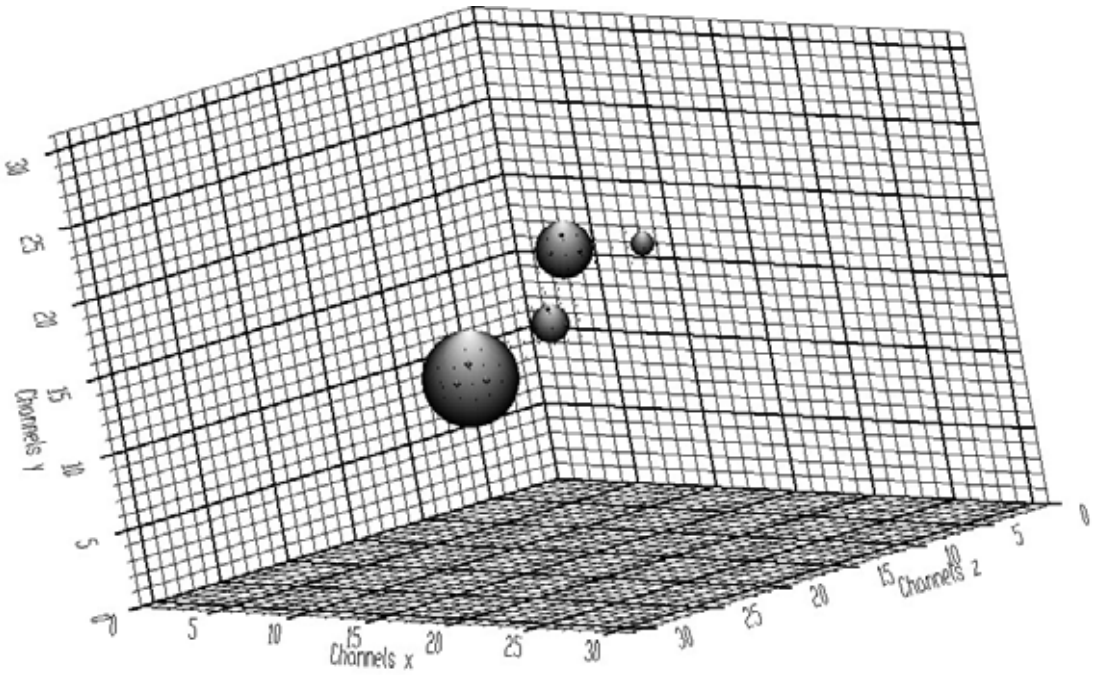


Figure 20 Spectrum from Figure 19 after boosted one-fold Gold deconvolution (50 iterations repeated 20 times)

Linear systems with changing response

- so far we assumed to have a linear system with constant response (independent of the energy in nuclear spectra). It means that the shape of the response function is the same in all range of processed data and the spectrum can be considered to be a composition of shifted responses with different amplitudes.
- if the change of the shape of the response function can be expressed either analytically or in any other way, we can make a benefit of this knowledge in generation of the system matrix.
- an example of employing this technique was applied in the decomposition of electron spectra. In the next example we present the processed electron spectrum.

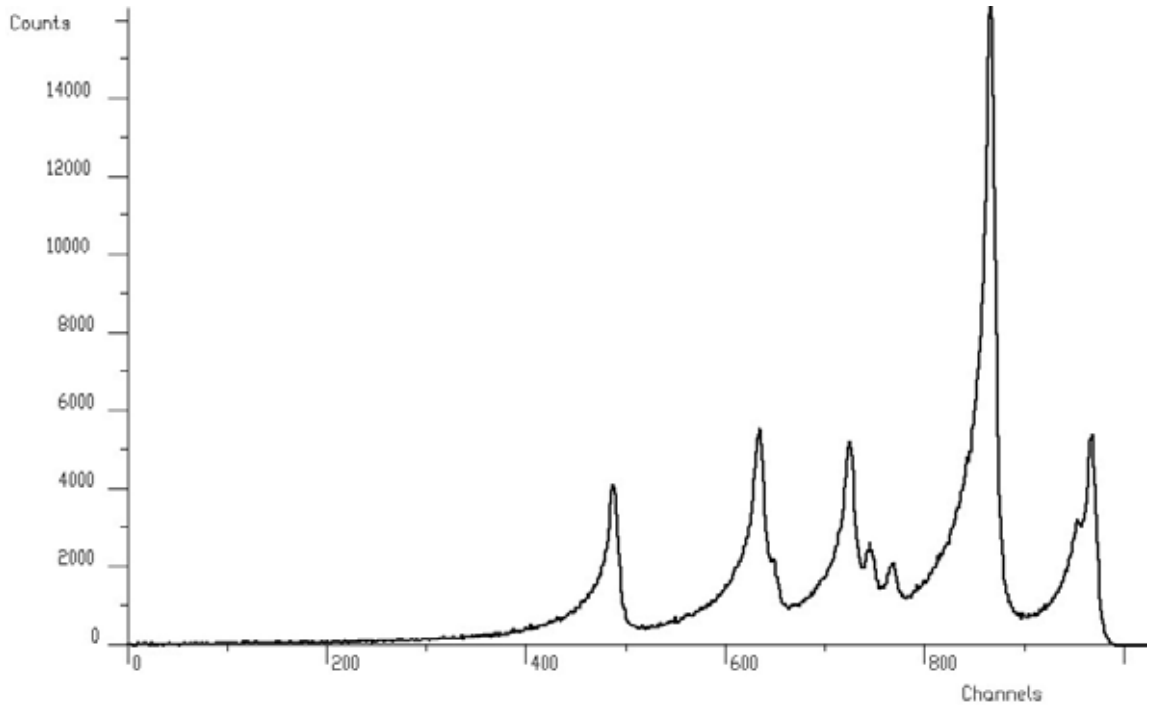


Figure 21 One-dimensional electron spectrum

- first few responses at the beginning of the coordinate system are shown in next Figure. The shape of the responses is changing with increasing energy (number of the response). It should reflect the left-side tail typical for this kind of data.

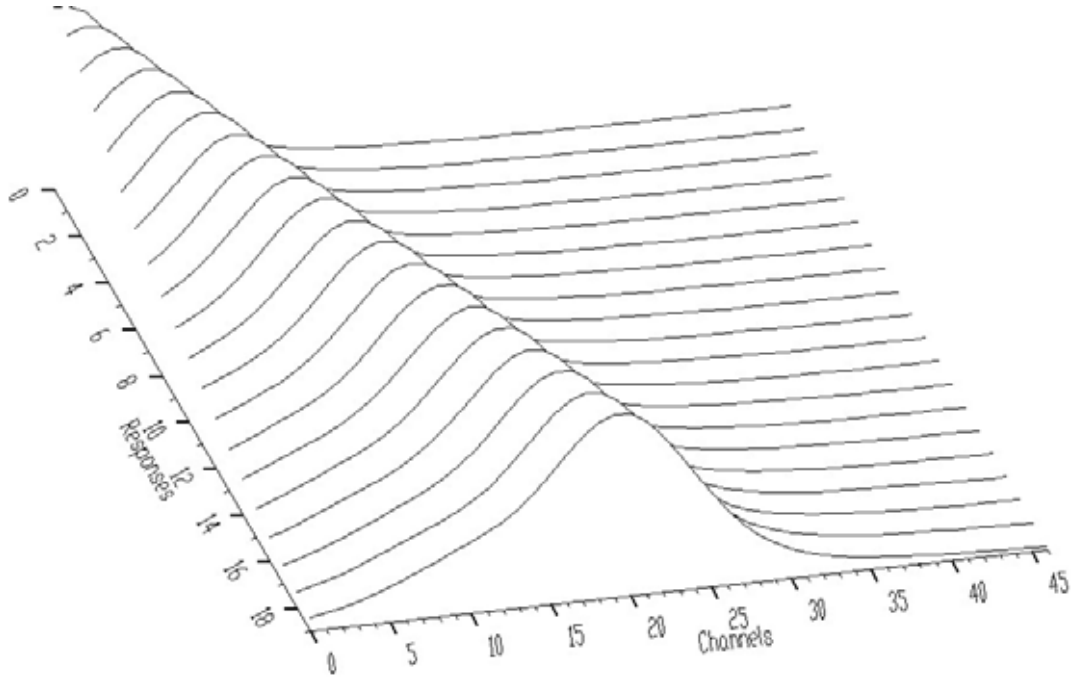


Figure 22 Part of response matrix composed of response electron spectra

- using the system matrix, we applied the Gold decomposition algorithm to the original electron spectrum (again with boosting).
- the result of the decomposition (thin line) together with the original data (thick line) in log scale is given in the next Figure.

In TSpectrum class the function "Deconvolution1Unfolding"

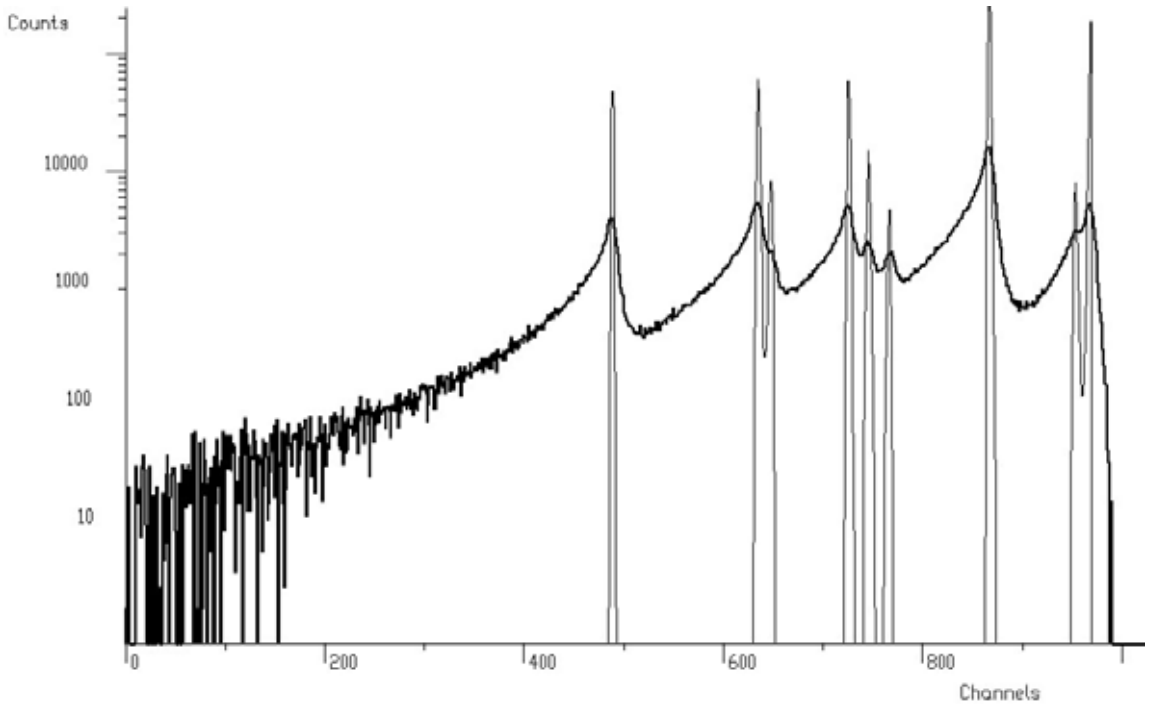


Figure 23 Original electron spectrum (thick line) and deconvolved (boosted one-fold deconvolution - thin line)

- to see details close to the baseline we introduce the same spectra in linear scale.

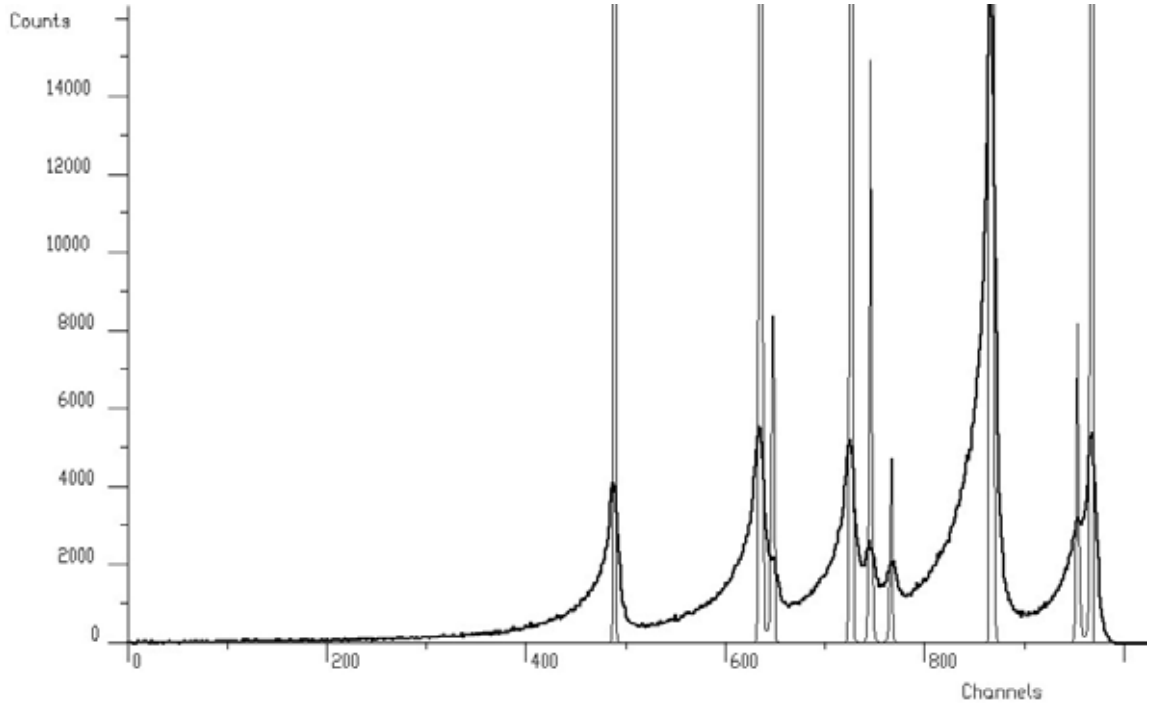


Figure 24 Detail of the spectrum from Figure 23

- the results prove in favor of the method in the deconvolution operation. The method finds correctly also overlapped small peaks positioned close to the big ones.

- the decomposition of continuum γ-ray spectra is another example of linear system with changing response and was described in

Reference:
Jandel M., Morháč M., Kliman J., Krupa L., Matoušek V., Hamilton J. H., Ramaya A. V., Decomposition of continuum gamma-ray spectra using synthetized response matrix, NIM A 516 (2004) 172.

Study of deconvolution methods and regularization techniques

- so far, to process experimental data we have employed and studied the Gold deconvolution algorithm.
- for relatively narrow peaks (in the above given examples σ=2) the one-fold Gold deconvolution method combined with boosting operation is able to decompose spectra practically to δ - functions.
- in what follows, we shall study the properties of other methods and regularization techniques as well. We shall compare their decomposition capabilities. To make these investigations we have chosen a synthetic data (spectrum, 256 channels) consisting of 5 very closely positioned, relatively wide peaks (σ=5), with added noise (Figure 25).

- thin lines represent pure Gaussians; thick line is a resulting spectrum with additive noise (10% of the amplitude of small peaks).
- one can notice that the smaller peaks are not observable by eye. It should be emphasized that this is an extremely difficult task. The positions, amplitudes and areas are given in the following Table1.

Peak #	Position	Height	Area
1	50	500	10159
2	70	3000	60957
3	80	1000	20319
4	100	5000	101596
5	110	500	10159

Table 1 Positions, heights and areas of peaks in the spectrum shown in Figure 25

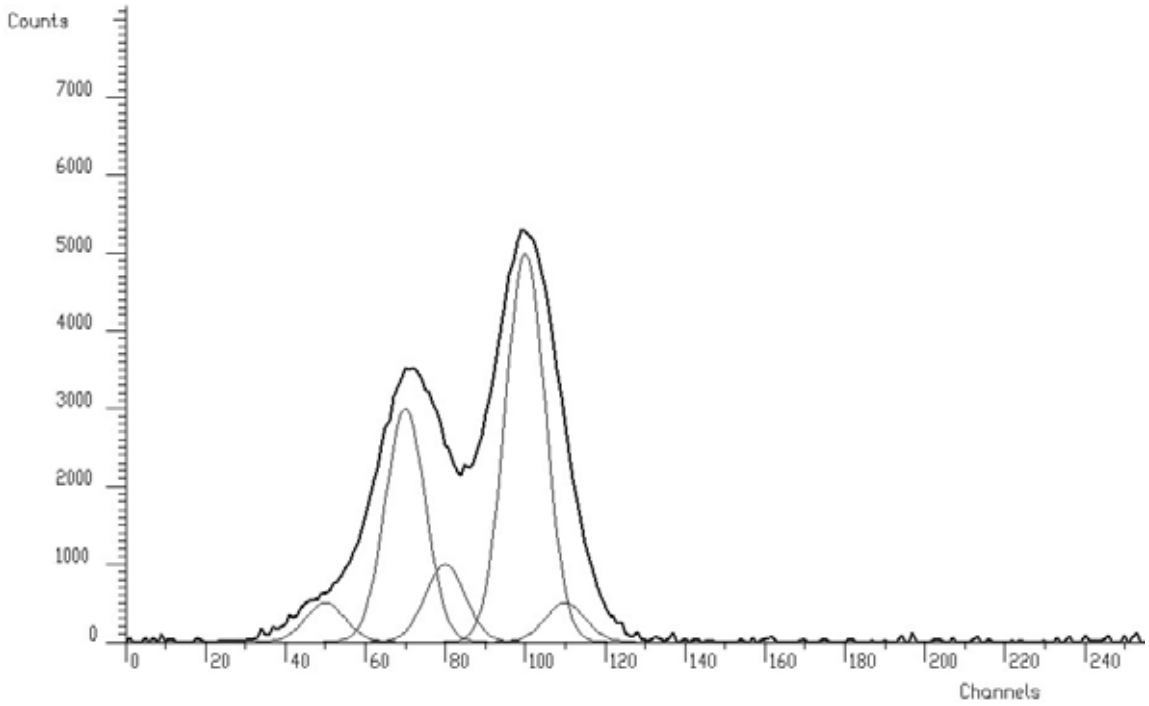


Figure 25 Testing example of synthetic spectrum composed of 5 Gaussians with added noise

- in ideal case, we should obtain the result given in Figure 26. The areas of the Gaussian components of the spectrum are concentrated completely to δ-functions.

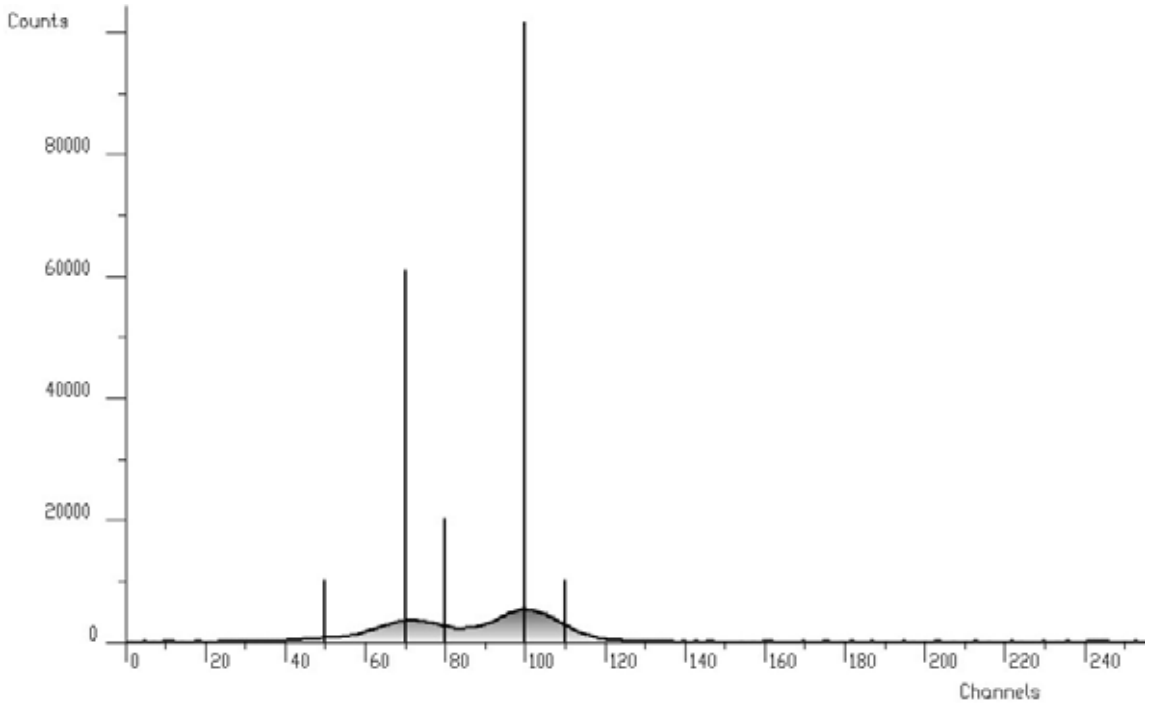


Figure 26 The same spectrum like in Figure 25, outlined bars show the contents of present components (peaks)

- when solving the overdetermined system of linear equations with data from Figure 25 in the sense of minimum least squares criterion without any regularization or constraints we obtain the result with large oscillations (Figure 27).
- from mathematical point of view, it is the optimal solution in the unconstrained space of independent variables. From physical point of view we are interested only in a meaningful solution, i.e., the contents of channels should be non-negative.
- therefore, we have to employ regularization techniques and/or to confine the space of allowed solutions to subspace of positive solutions.

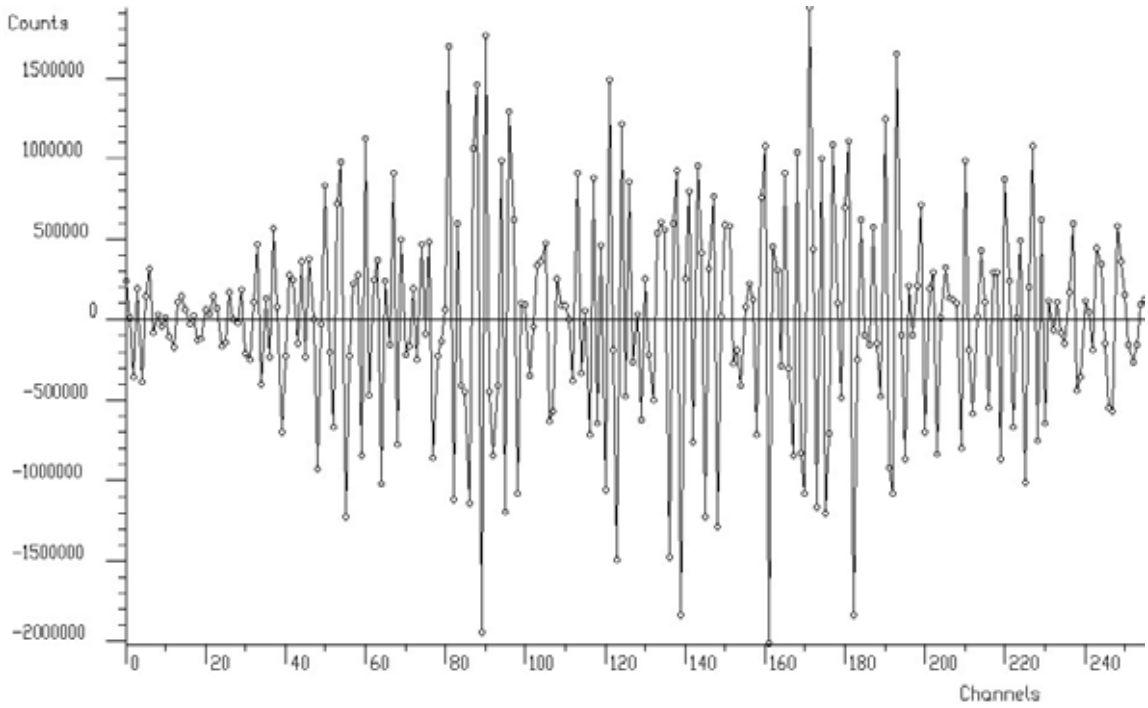


Figure 27 Least squares solution of the system of linear equations without regularization

Methods based on direct solution of system of linear equations.

a. Tikhonov regularization

- let us apply this algorithm to our data from Figure 25. In Figure 28 we see the original spectrum (thick line), the result of the deconvolutions for α=10 000 (thin line) and α=100 000 (thin line with circle marks).
- some outlines of the present peaks are visible (two side small peaks being in incorrect positions) but in both cases one can observe oscillations even outside of the peak region of the spectrum.
- with increasing α the oscillations are softened, but on the other hand, the outline of the peak at the position 80 disappears. The deconvolved spectra contain non-realistic negative values.

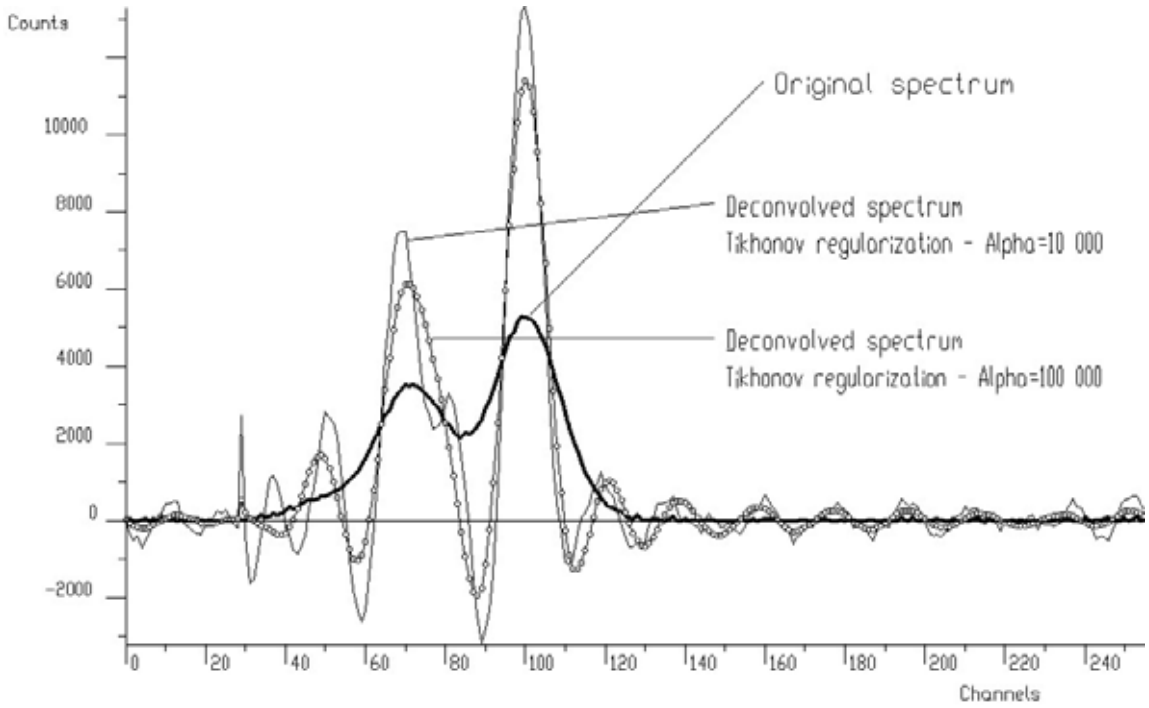


Figure 28 Solution obtained using Tikhonov method of regularization

- instead of classic 0-th order regularization operator, we can apply also operator of the 1-st or 2-nd order differences. The order of the operator influences the result. The resolution of peaks for higher orders is slightly better but anyway there are the same problems like in the previous example.

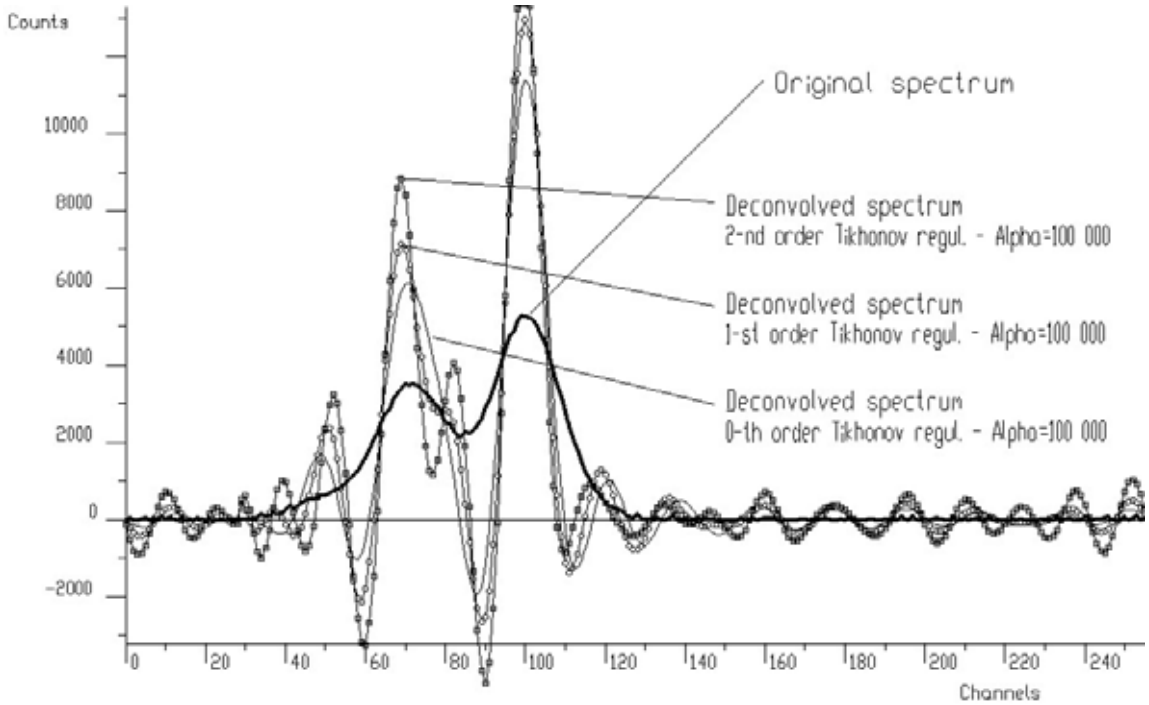


Figure 29 Illustration of the influence of the order of regularization operator

b. Riley algorithm

- this method is sometimes called iterated Tikhonov method. Non-regularized is of little importance as it leads practically always to oscillating solution. When regularized (e.g. employing 0-order regularization operator) we get the result similar to classic Tikhonov algorithm.
- an example of application of Riley algorithm for our testing spectrum is given in Figure 30 (1000 iterations, α =25 000 000).

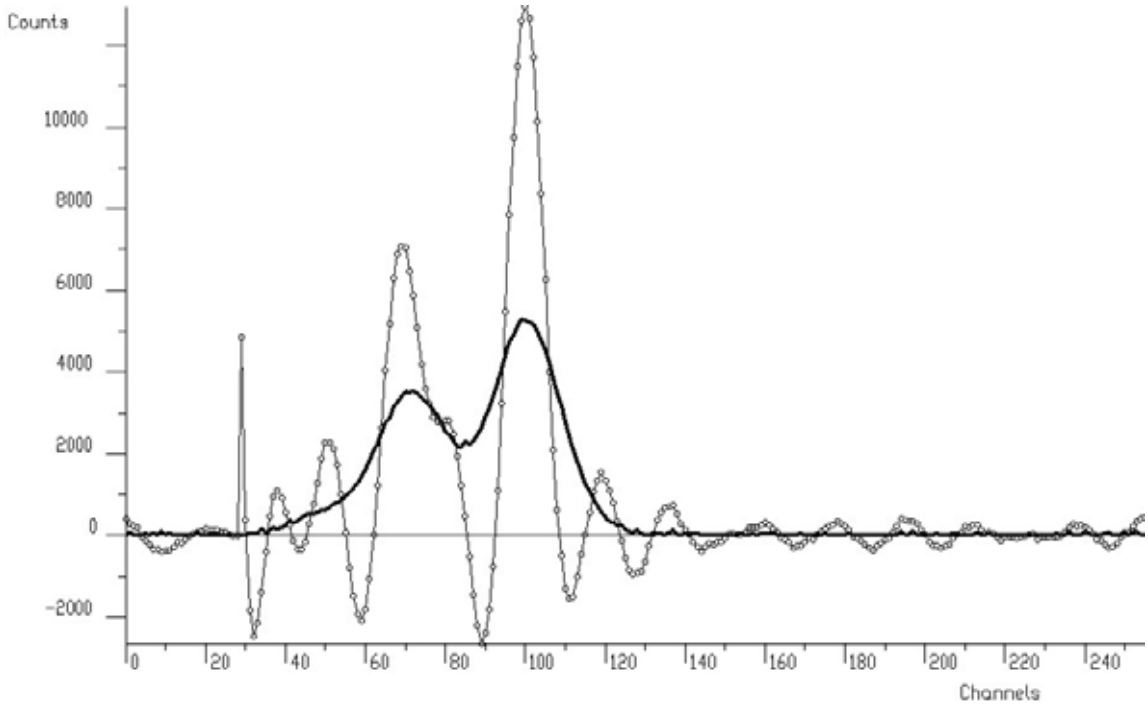


Figure 30 Illustration of Riley algorithm of deconvolution

- however, because of its iterative nature, the algorithm lends itself to another kind of regularization, so called Projections on Convex Sets - POCS. A projection onto the positive $\hat{x}$'s simply means to set all negative elements to zero after each iteration.

References:

Backus G.E., Gilbert F., Geophysical Journal of the Royal Astronomical Society, 16 (1968) 169.

Backus G.E., Gilbert F., Philosophical Transactions of the Royal Society of London, 266 (1970) 123.

Sanchez-Avila C., Behavior of nonlinear POCS higher order algorithms in the deconvolution problem, Nonlinear Analysis, Theory, Methods & Applications 30 (1997) 4909.

- when applying it to our example we get the result given in Figure 31 (1000 iterations, α=10 000 000). Due to POCS regularization negative values disappeared from the solution.

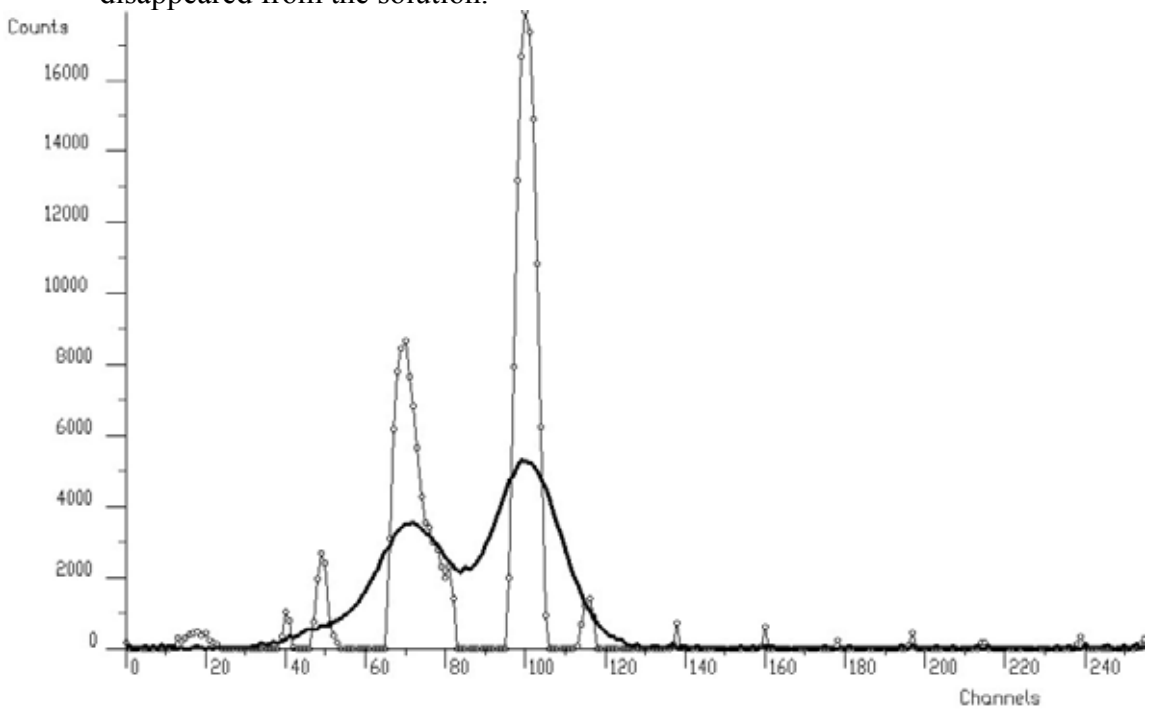


Figure 31 Riley deconvolution with POCS regularization

- let us go on and let us apply the boosting operation in the same way as in the previous examples. For boosting coefficient 1.2, we get the result given in Figure 32. Dominant two peaks at positions 70 and 100 are well resolved. Though visible, there are still problems with both side peaks and with the peak at position 80.

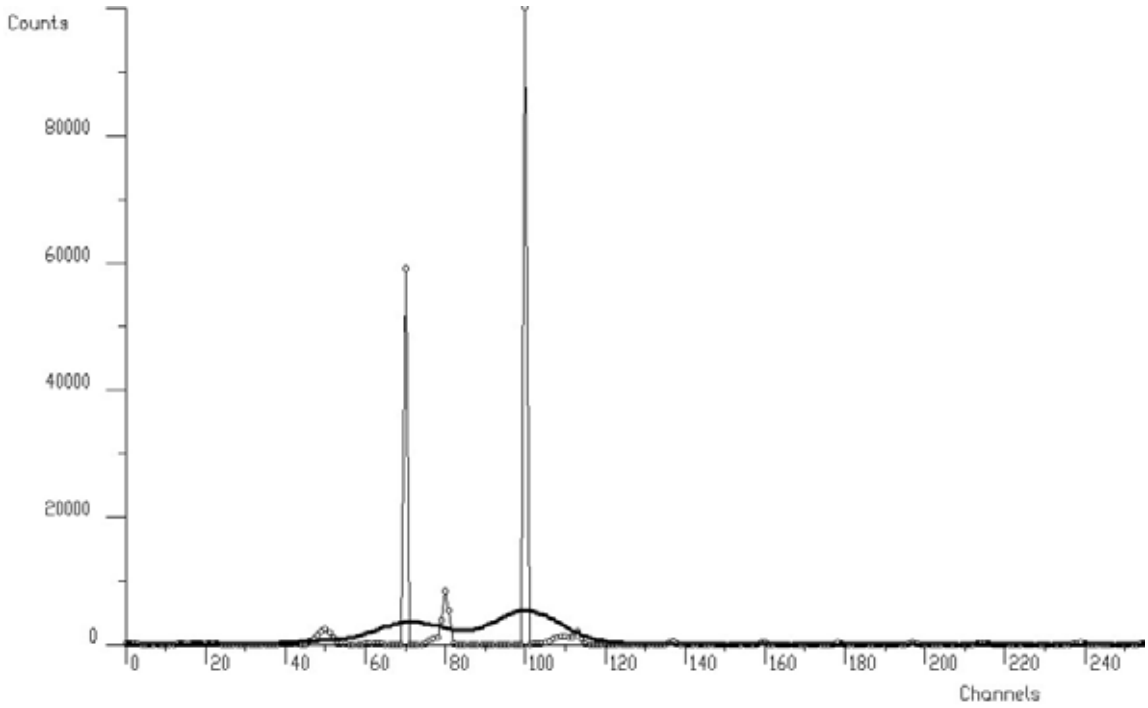


Figure 32 Riley deconvolution with POCS regularization and boosting

c. Minimization of squares of negative values

- we have proposed a new method of regularization. While in the classic Tikhonov algorithm we minimize the sum of squares of contents of all channels, in this case we do not care about channels with positive values. We minimize only the channels with the negative values.
- the result of this algorithm after 100 iteration steps for α=1000 is given in Figure 33. One can see that it well estimates the positions of peaks. Though small, there are still present negative values and oscillations outside of the peaks region. The results in peaks regions are presented in Table 2.

Peak #	Original/Estimated (max) position	Original/Estimated area
1	50/50	10159/10406
2	70/70	60957/59119
3	80/80	20319/21721
4	100/100	101596/102443
5	110/111	10159/8600

Table 2 Results of the estimation of peaks in spectrum shown in Figure 33

- in the next example (Figure 34), we increased number of iteration steps to 1000. The negative values as well as oscillations became smaller. The contents of peaks channels have changed only slightly.

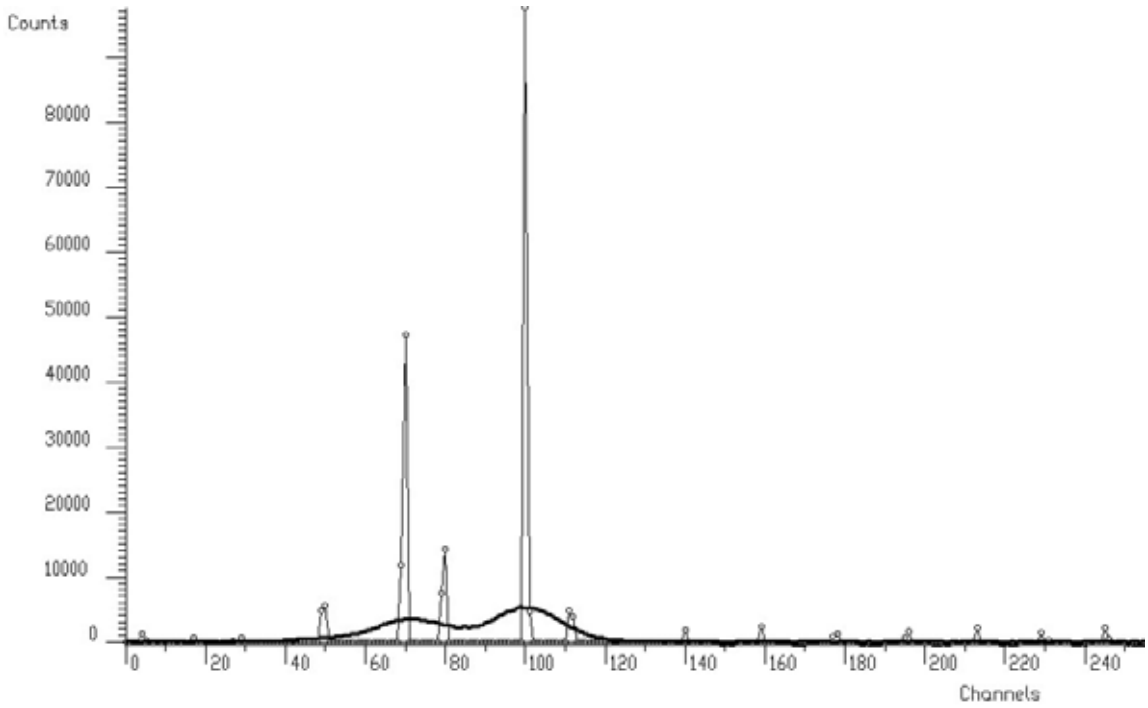


Figure 33 New algorithm of deconvolution with minimization of squares of negative values (100 iteration steps)

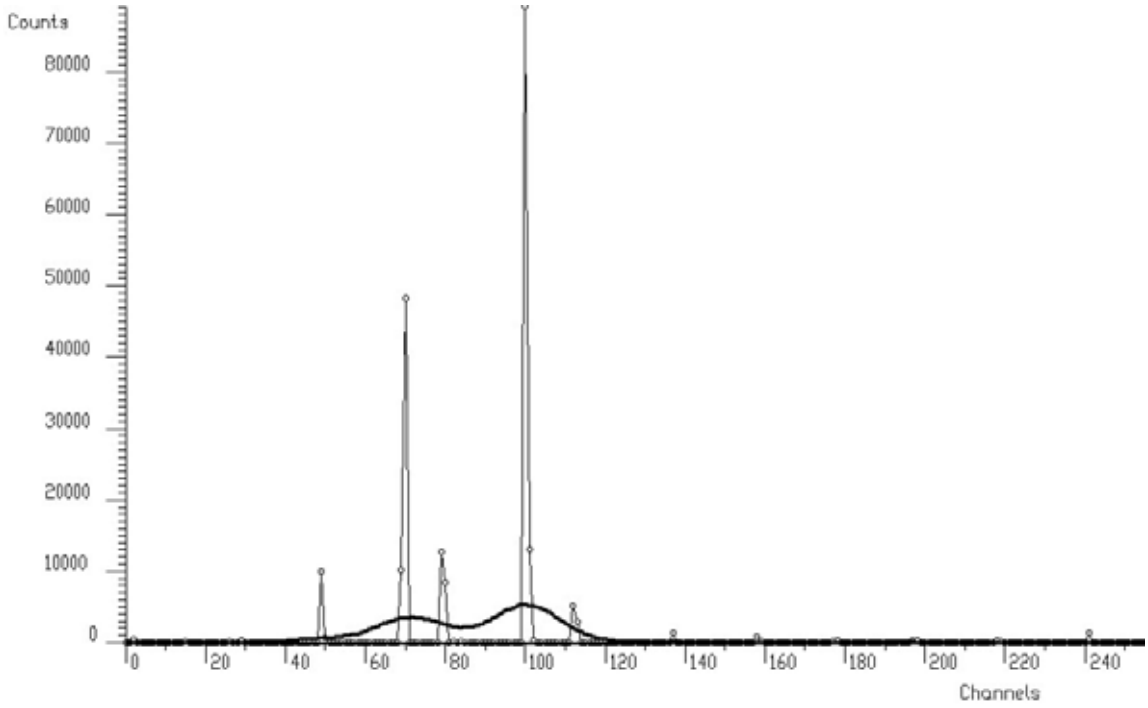


Figure 34 The same like in Figure 33 but number of iteration steps was 1000

- the method works well and gives pretty results. Its disadvantage consists in the necessity to solve the full system of linear equations in every iteration step.

Therefore, it is not applicable for big systems of linear equations (large spectra) and for multidimensional data.

Methods based on iterative solution of system of linear equations.

a. Van Cittert algorithm

- it represents the basic method of this class of deconvolution algorithms. Let us continue in our previous example in the study of the properties of various deconvolution algorithms. The result achieved by the classic Van Cittert algorithm does not differ too much from that obtained by the Tikhonov algorithm.
- again, it oscillates and gives negative values in clusters of channels. However when applying POCS regularization after every iteration step the oscillations as well as negative values disappear. In Figure 35 we present original spectrum (thick line), spectrum deconvolved through the use of classic Van Cittert algorithm and regularized (via POCS method) deconvolved spectrum (1000 iterations).
- though better, nevertheless, the small peak at the position 110 and peak between two strong peaks (position 80) could not be disclosed even by POCS regularization of the Van Cittert algorithm.

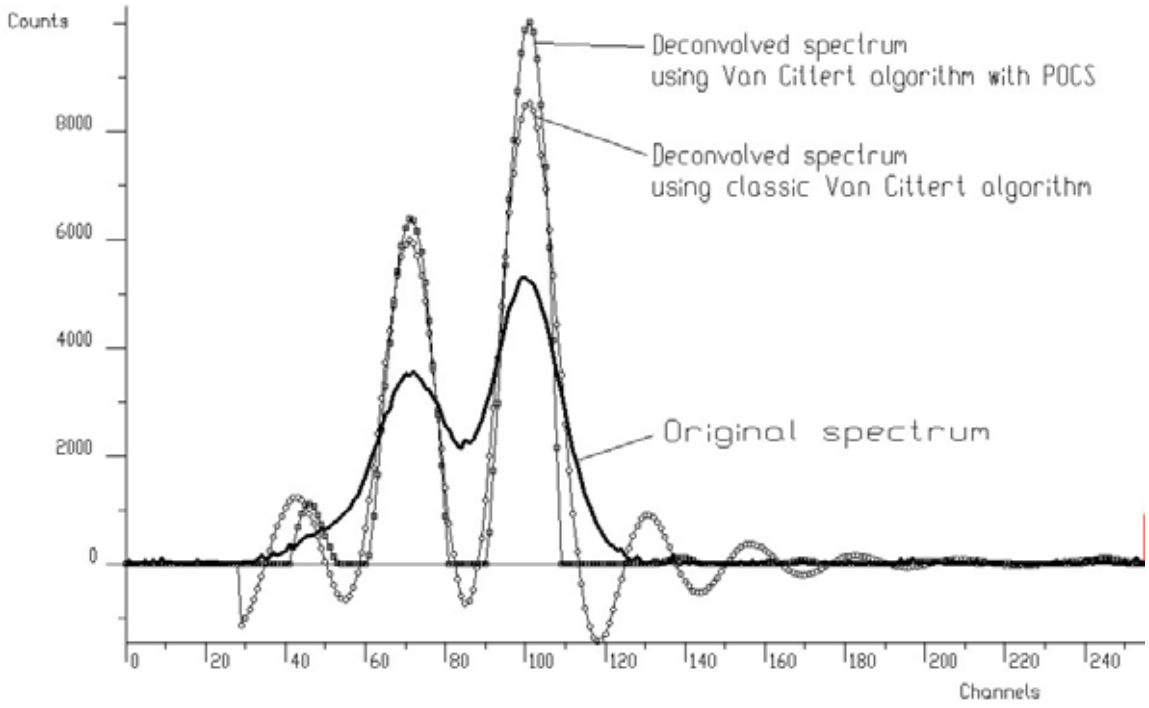


Figure 35 Original spectrum (thick line), deconvolved using Van Cittert algorithm (without regularization) and deconvolved using Van Cittert algorithm and regularized via POCS method

b. Gold algorithm

- in contradiction to Van Cittert algorithm, the Gold deconvolution (for positive response and output data) gives always positive result. The result of Gold deconvolution is intrinsically constrained to the subspace of positive solutions.
- let us apply it to our example. In Figure 36 we give original spectrum and deconvolved spectrum using one-fold Gold algorithm (10 000 iterations). We see that the peak at the position 80 cannot be resolved and that there is only an indication of the right-side small peak at position 110.

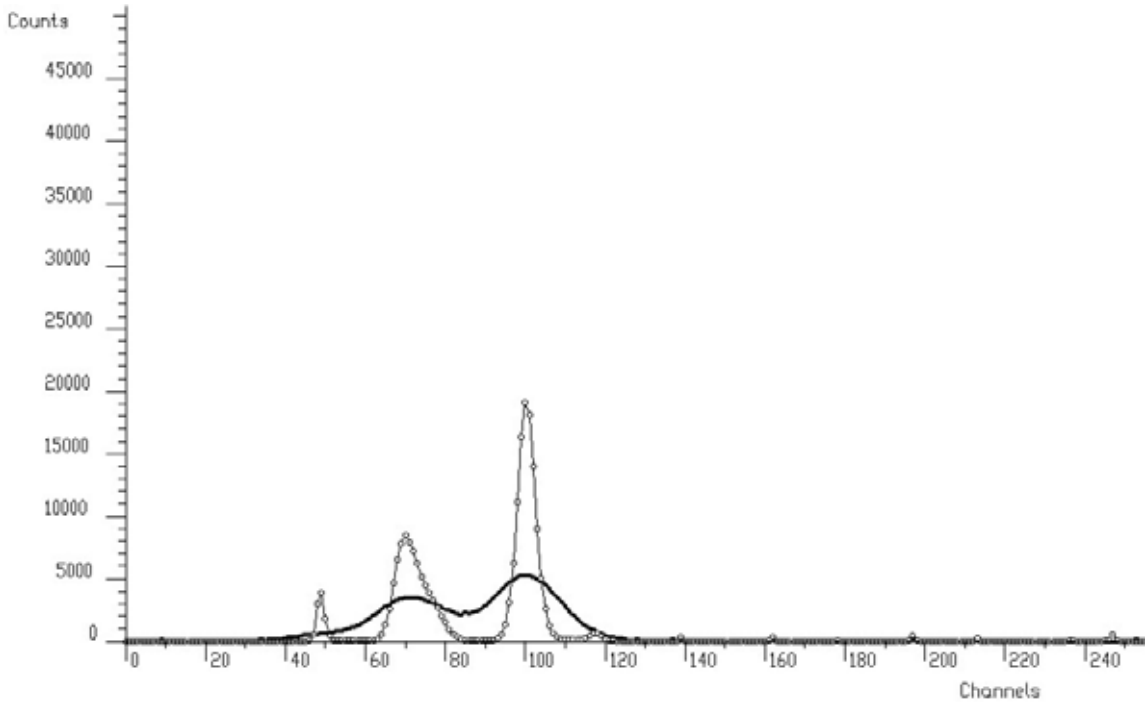


Figure 36 Original spectrum (thick line) and deconvolved spectrum using one-fold Gold algorithm (10000 iterations, thin line)

- good result for Gold deconvolution is obtained by employing boosting operation (Figure 37). It concentrates areas of peaks practically into one channel.

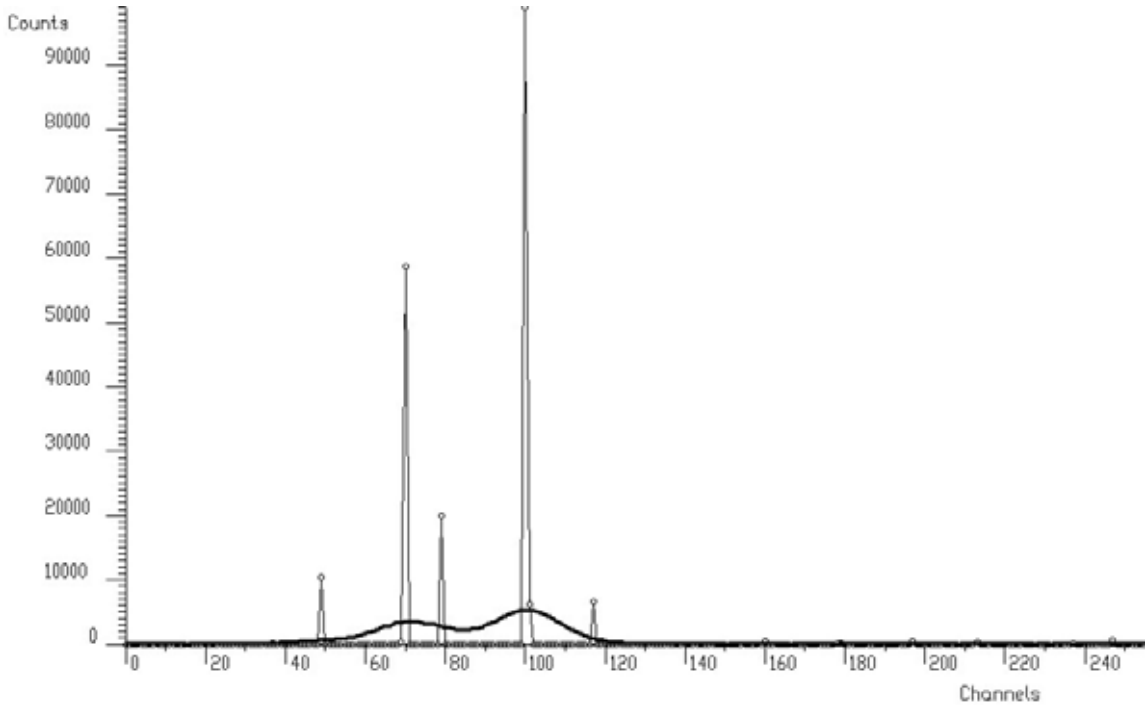


Figure 37 Illustration of deconvolution via boosted Gold deconvolution

- the results in peaks regions are presented in Table 3. Anyway, there still remains the problem in the positions of estimated peaks. Mainly the estimate of the small peak at position 110 is quite far from reality.

Peak #	Original/Estimated (max) position	Original/Estimated area
1	50/49	10159/10419
2	70/70	60957/58933
3	80/79	20319/19935
4	100/100	101596/105413
5	110/117	10159/6676

Table 3 Results of the estimation of peaks in spectrum shown in Figure 37

c.Richardson-Lucy algorithm

- the method is based on Bayes theorem of maximum probability. Like in the case of Gold deconvolution the method is positive definite.
- when applied to our example it exhibits very good properties. On the other hand, it converges slowly and its implementation is not so simple like in Gold deconvolution.
- Figure 38 illustrates its decomposition capabilities. In the deconvolved spectrum (after 10 000 iterations) we can see indications even of small peaks # 3 and 5.

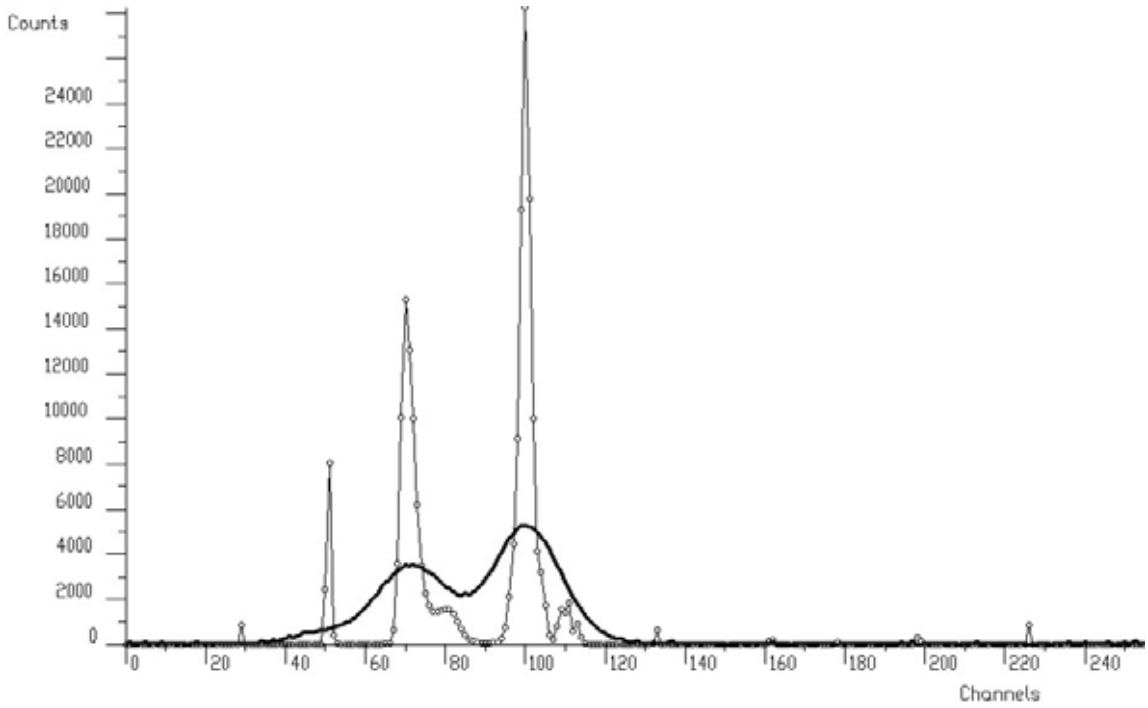


Figure 38 Illustration of application of Richardson-Lucy algorithm of deconvolution

- in Figure 39 we present the result of boosted Richardson-Lucy algorithm (50 iterations, repeated 20 times with boosting coefficient p=1.2). It decomposes completely (to one channel) the multiplet.

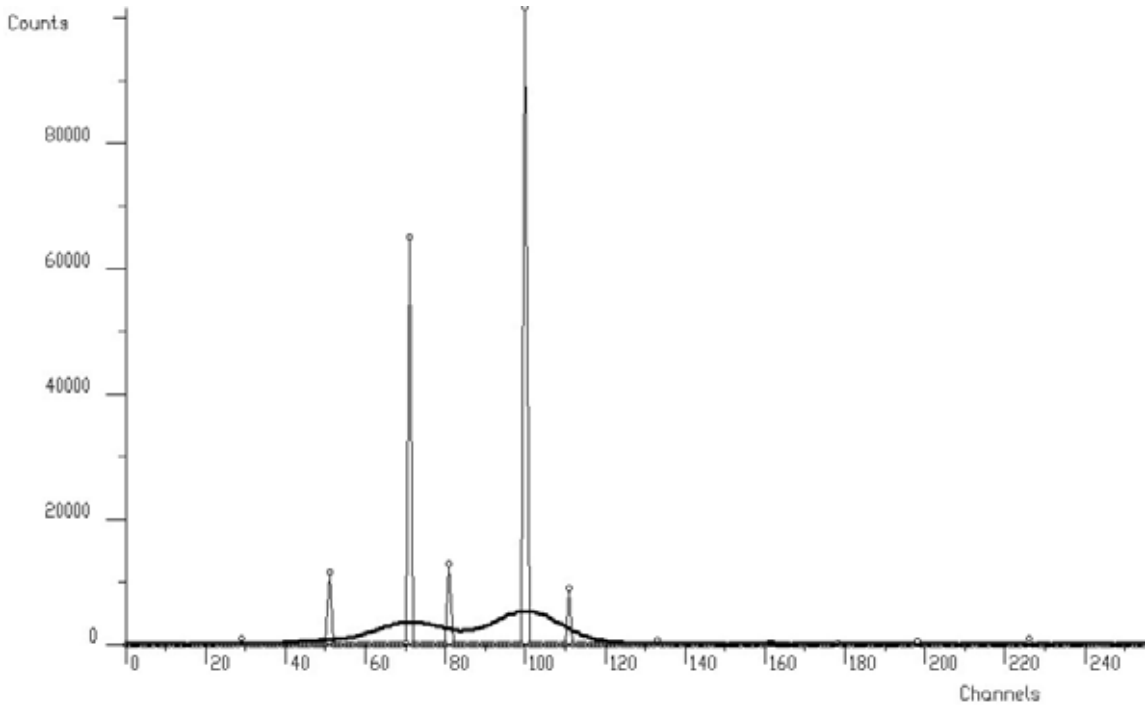


Figure 39 Spectrum deconvolved using boosted Richardson-Lucy algorithm of deconvolution

- the results in peaks regions are presented in Table 4. The errors in positions estimation do not exceed one channel. From this point of view, the algorithm gives the best result. There is a considerable error in the area estimation of the peak # 3.

Peak #	Original/Estimated (max) position	Original/Estimated area
1	50/51	10159/11426
2	70/71	60957/65003
3	80/81	20319/12813
4	100/100	101596/101851
5	110/111	10159/8920

Table 4 Results of the estimation of peaks in spectrum shown in Figure 39

d. Muller algorithm

- for completeness' sake, we briefly present also results of obtained by application of Muller algorithm of deconvolution. Again, it is positive definite algorithm. It gives smoother result similar to that obtained by Gold deconvolution.

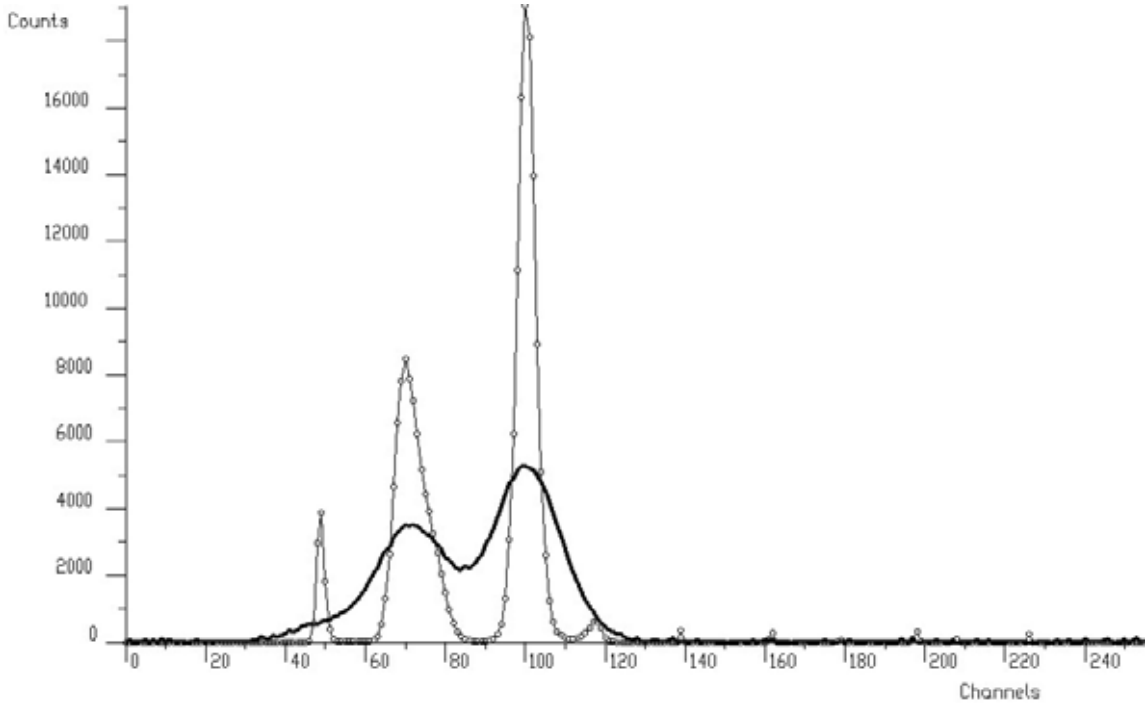


Figure 40 Illustration of Muller algorithm of deconvolution

- in Figure 41 we give the result obtained by including boosting operation into the Muller deconvolution.

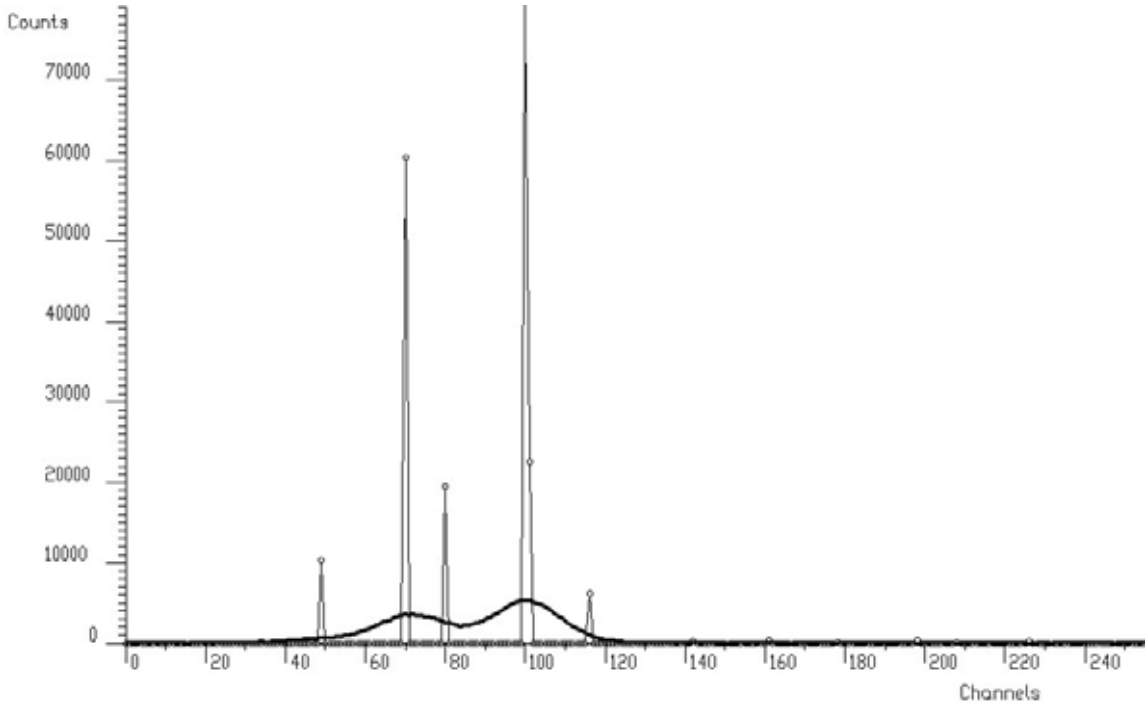


Figure 41 Illustration of Muller algorithm of deconvolution with boosting

- the results are slightly better than in Gold deconvolution. However, the algorithm is more time consuming and its implementation more complicated.

Robustness of deconvolution methods

Original synthetic spectrum

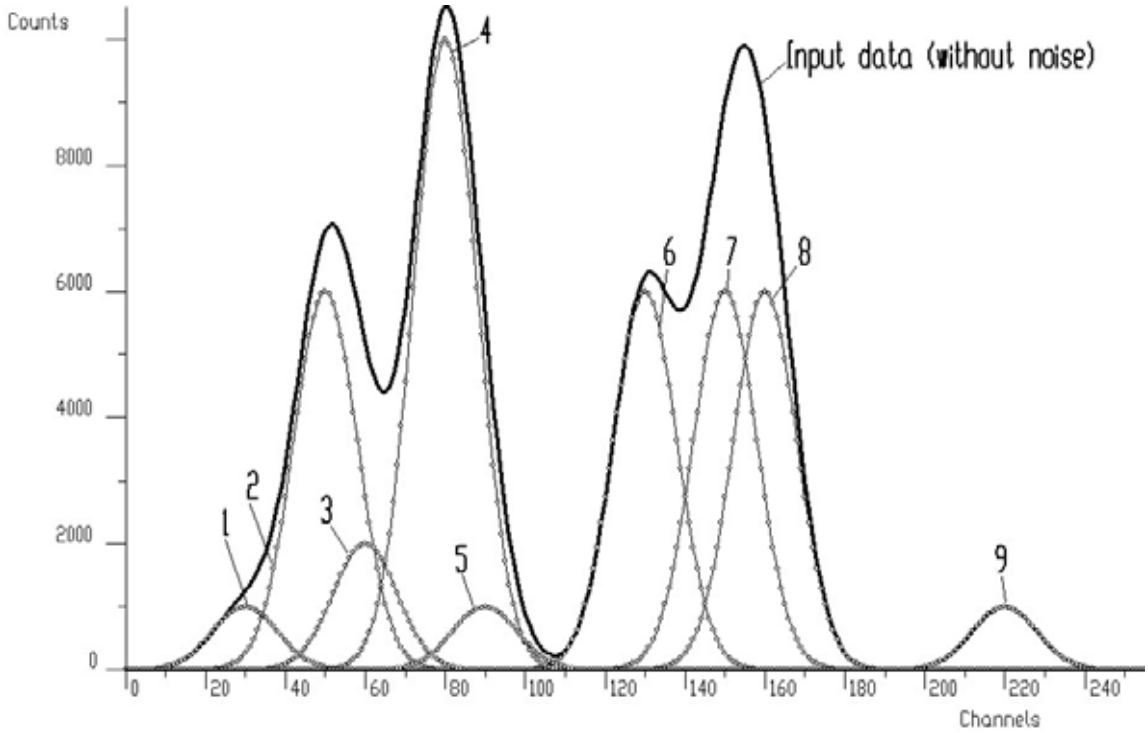


Figure 42 Original spectrum composed of 9 Gaussians

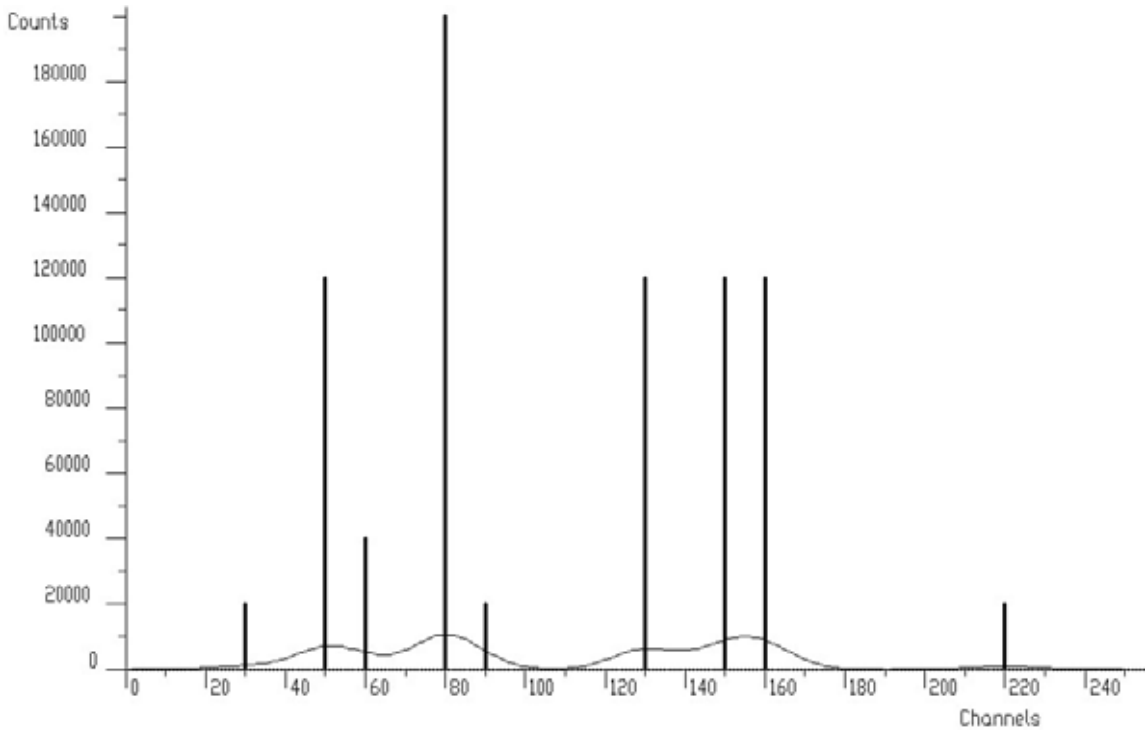


Figure 43 Original synthetic spectrum (thin lines) and the ideal solution (thick bars)

Original matrix

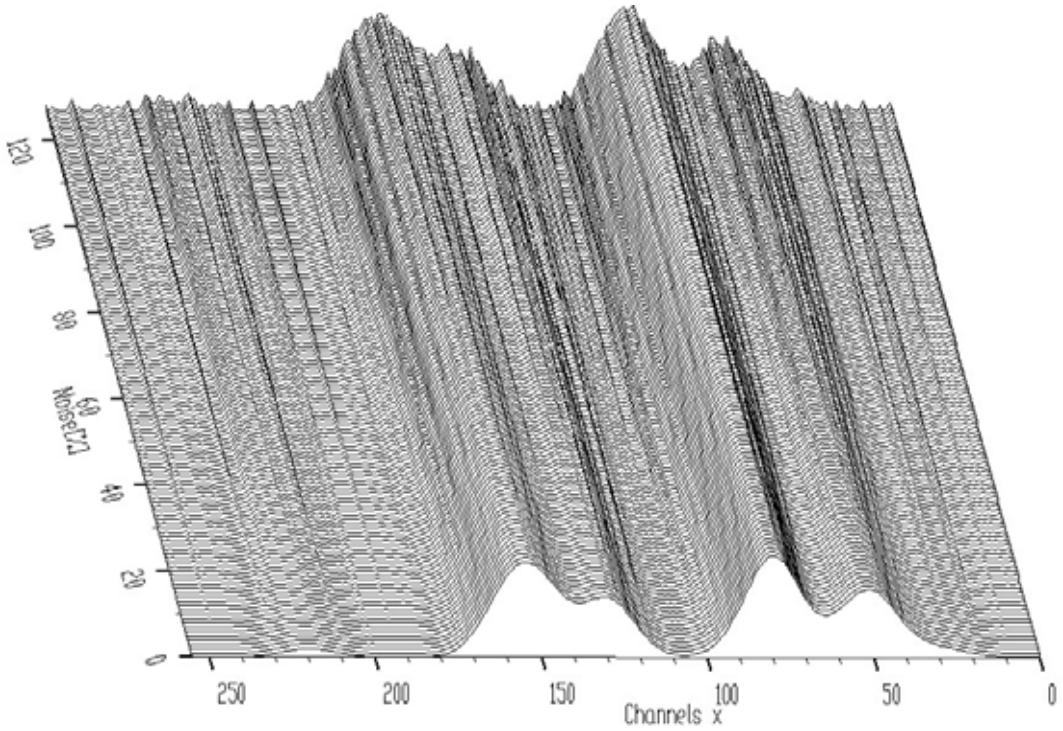


Figure 44 Original spectrum with increasing added noise (in % of the amplitude of smallest peak in the spectrum)

Classic Gold deconvolution

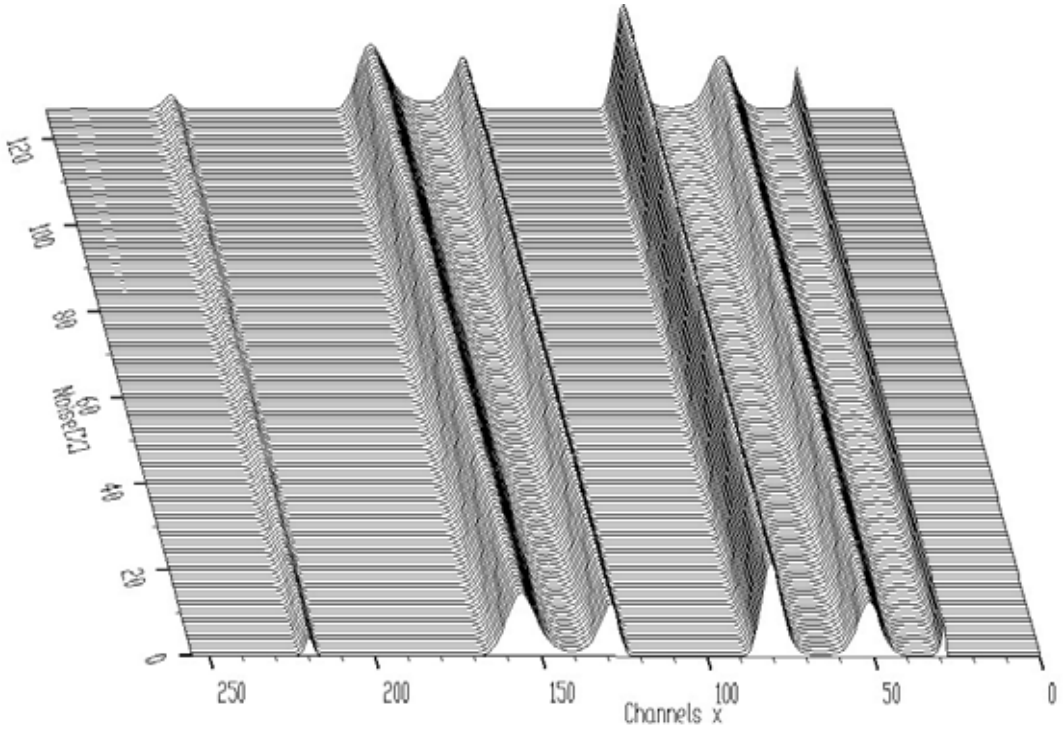


Figure 45 Result of classic Gold deconvolution for increasing level of noise

One-fold Gold deconvolution

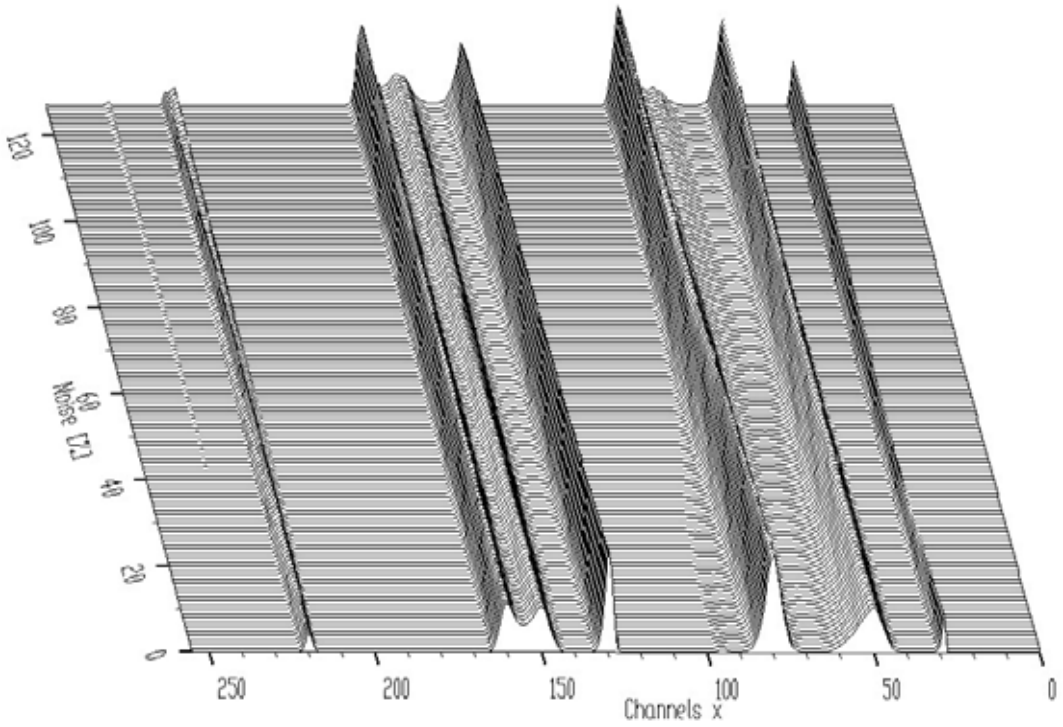


Figure 46 Result of one-fold Gold deconvolution for increasing level of noise

Gold boosted deconvolution

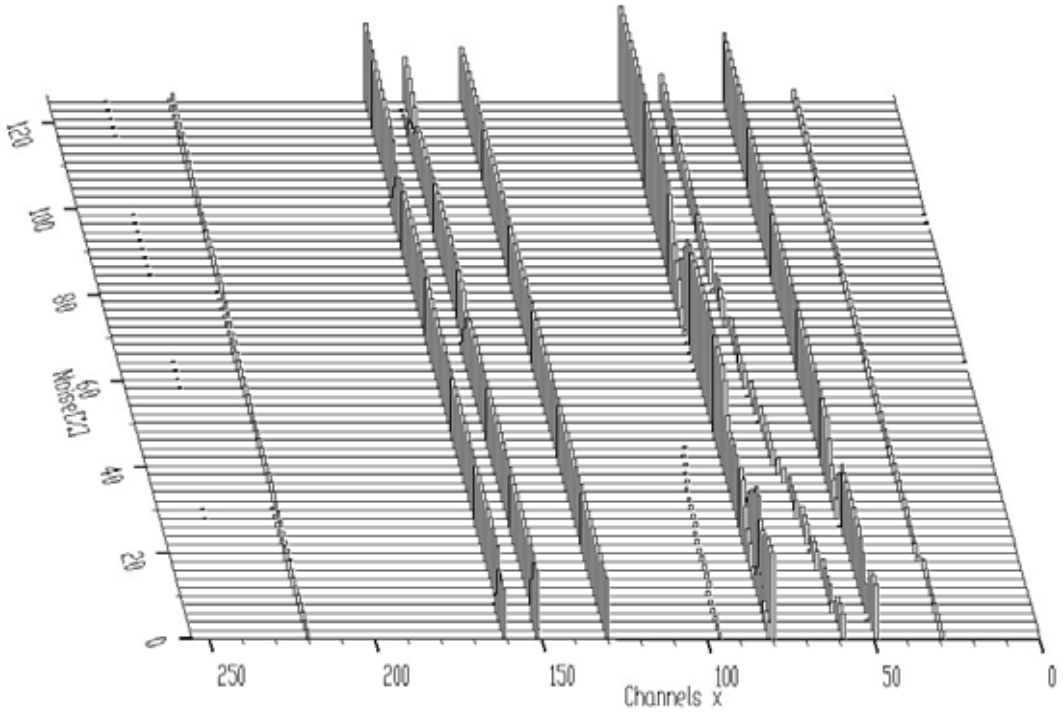


Figure 47 Result of boosted Gold deconvolution for increasing level of noise

Richardson-Lucy deconvolution

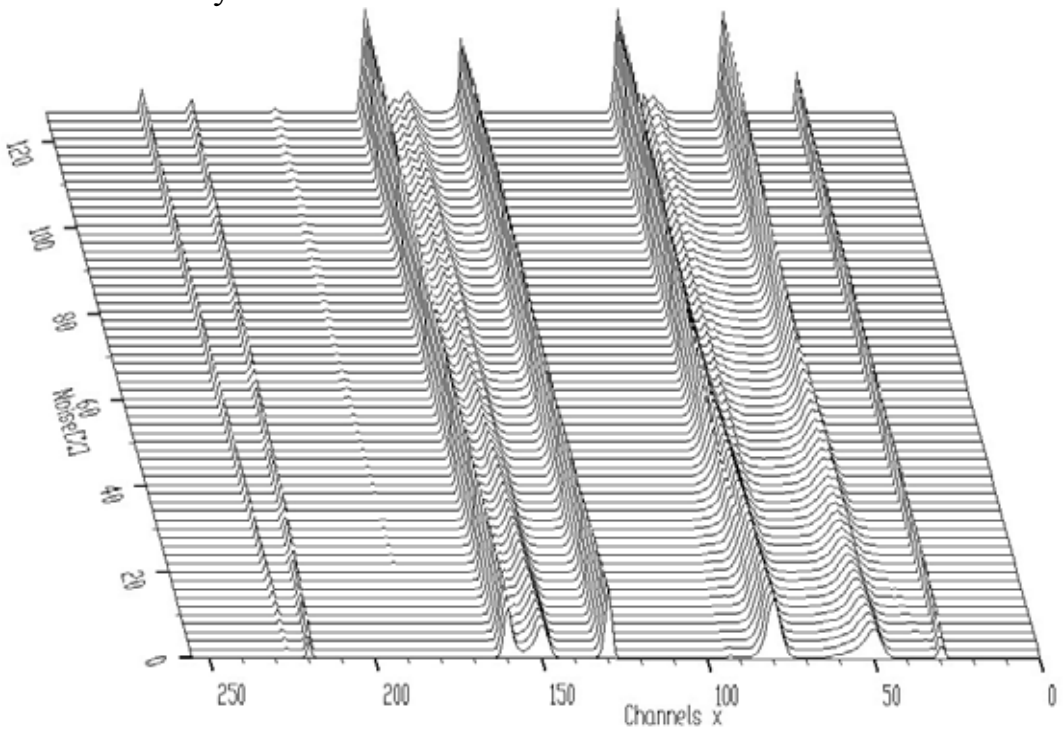


Figure 48 Result of Richardson-Lucy deconvolution for increasing level of noise

Richardson-Lucy boosted deconvolution

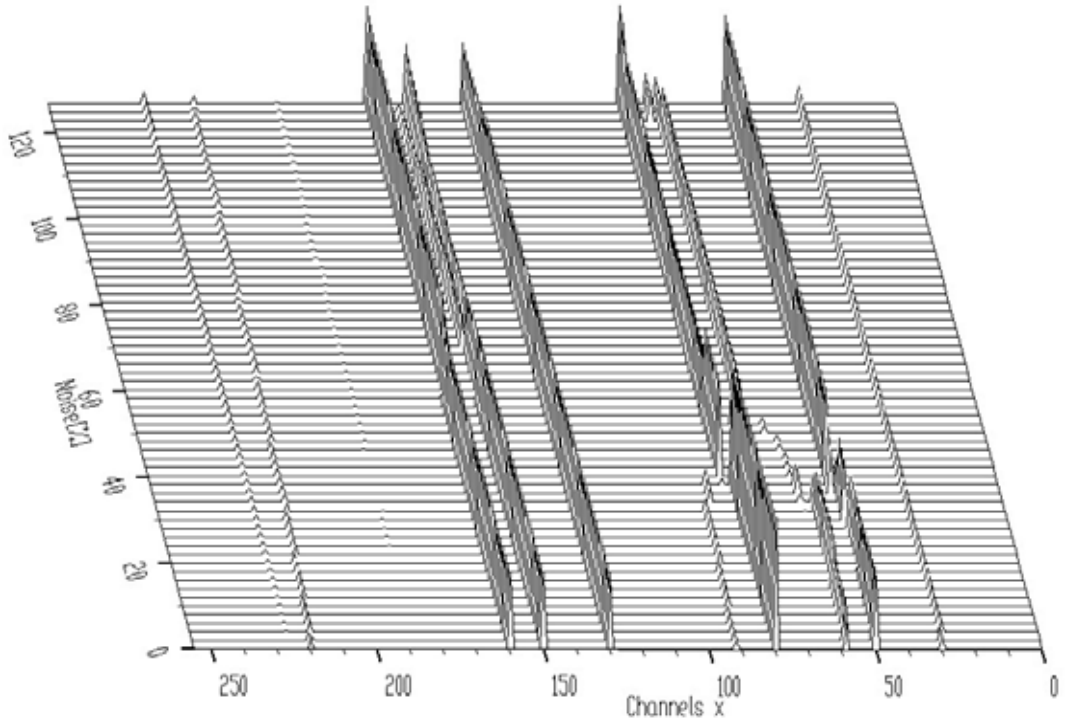


Figure 49 Result of boosted Richardson-Lucy deconvolution for increasing level of noise

Movies

Peak identification

- the basic aim of one-dimensional peak searching procedure is to identify automatically the peaks in a spectrum with the presence of the continuous background and statistical fluctuations - noise.
- the common problems connected with correct peak identification are
  - non-sensitivity to noise, i.e., only statistically relevant peaks should be identified.
  - non-sensitivity of the algorithm to continuous background.
  - ability to identify peaks close to the edges of the spectrum region. Usually peak finders fail to detect them.
  - resolution, decomposition of doublets and multiplets. The algorithm should be able to recognize close positioned peaks.
  - ability to identify peaks with different σ.

General peak searching algorithm based on smoothed second differences

- the essential one-dimensional peak searching algorithm is based on smoothed second differences (SSD) that are compared to its standard deviations.

Reference:
Mariscotti M.A., A method for automatic identification of peaks in the presence of background and its application to spectrum analysis, NIM 50 (1967) 309.

- we have extended the above presented SSD based method of peak identification for two-dimensional and in general for multidimensional spectra. In addition to the above given requirements now the algorithm must be insensitive to the lower-fold coincidences peak-background (ridges) and their crossings.
- the multidimensional peak searching algorithm based on sophisticated technique employing SSD was derived and described in detail in

Reference:
Morháč M., Kliman J., Matoušek V., Veselský M., Turzo I., Identification of peaks in multidimensional coincidence gamma-ray spectra, NIM A 443 (2000) 108.

High resolution peak searching algorithm

One-dimensional spectra

- to improve the resolution capabilities we have proposed a new algorithm based on Gold deconvolution.
- however, unlike SSD algorithm before applying the deconvolution algorithm we have to remove the background using one of the background elimination algorithm
- let us apply the high resolution algorithm to the synthetic spectrum with several peaks located very close to each other. The result for σ=2 and threshold=4% is shown in next Figure.
- the method discovers all 19 peaks in the spectrum. It finds also small peak at the position 200 and decomposes the cluster of peaks around the channels 551-568. In the bottom part of the Figure, we present the deconvolved spectrum.

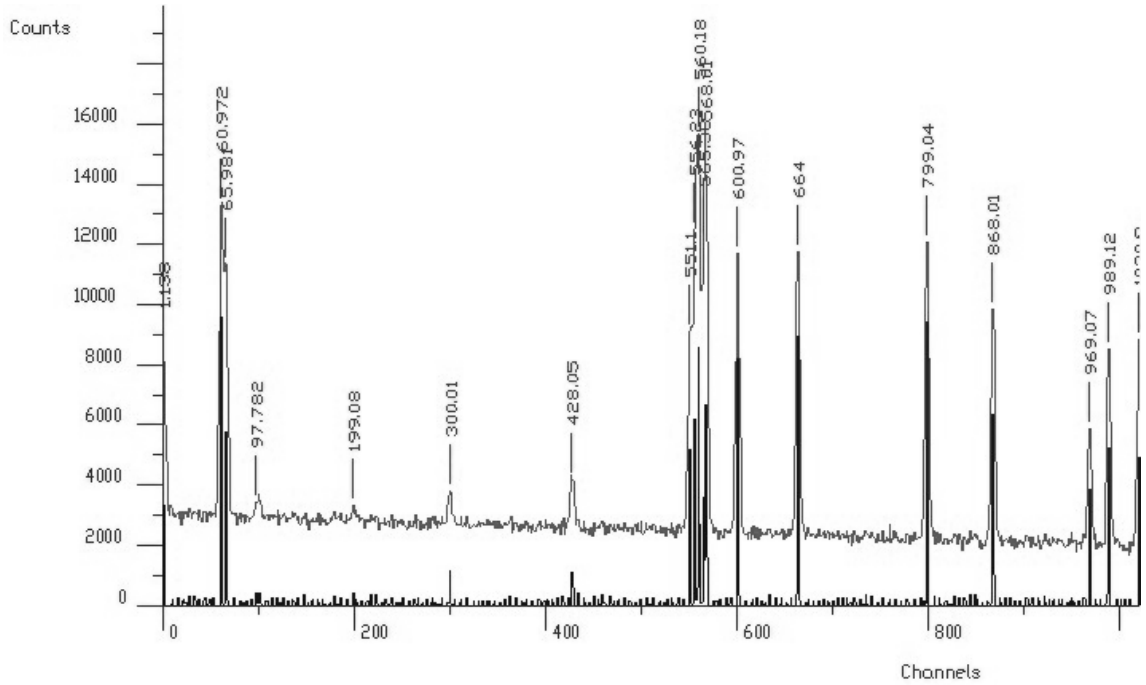


Figure 50 Example of synthetic spectrum with doublet and multiplet and its deconvolved spectrum (in bottom part of picture)

- the detail of peaks in cluster is shown in the following Figure. In the upper part of the Figure one can see original data and in the bottom part the deconvolved data.
- the method finds also the peaks about existence of which it is impossible to guess from the original data.

In TSpectrum class the function "Search1HighRes"

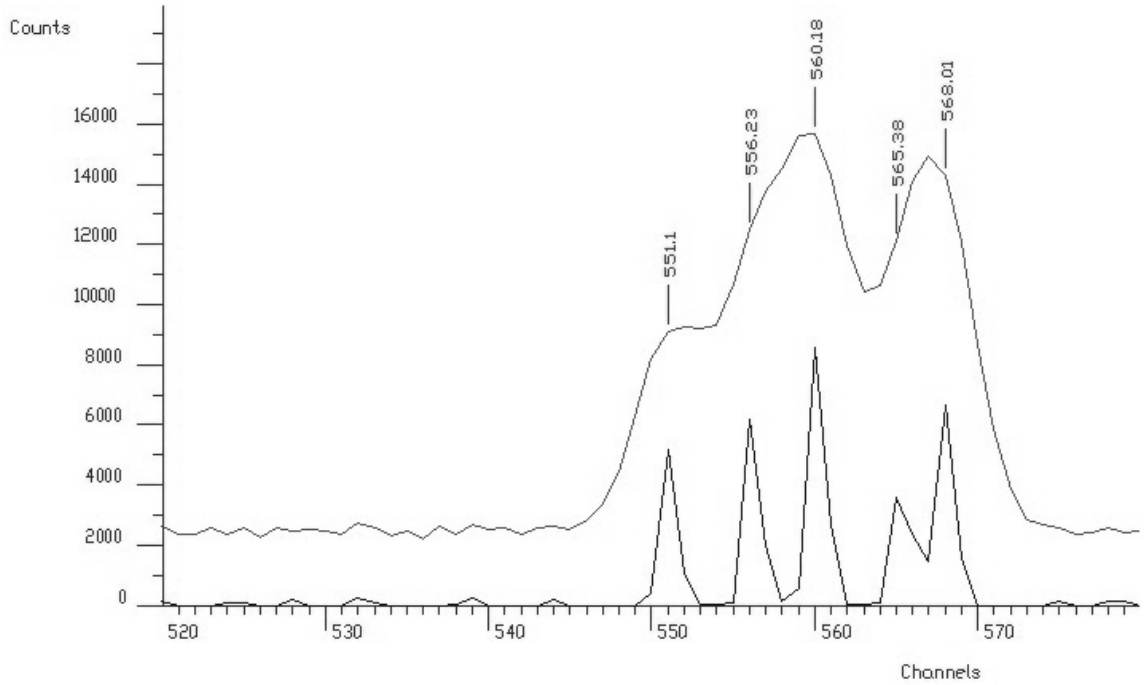


Figure 51 Detail of multiplet from Figure 50

Two-dimensional spectra

- analogously to one-dimensional case to treat the resolution problem one has to employ the high resolution method based on the Gold deconvolution.
- the result of the search using the high resolution algorithm for σ=2 and threshold=5% applied to the previous example is shown in next Figure and its appropriate deconvolved spectrum in Figure 53. It discovers correctly all peaks including the small peak (position 46, 48) in the doublet.

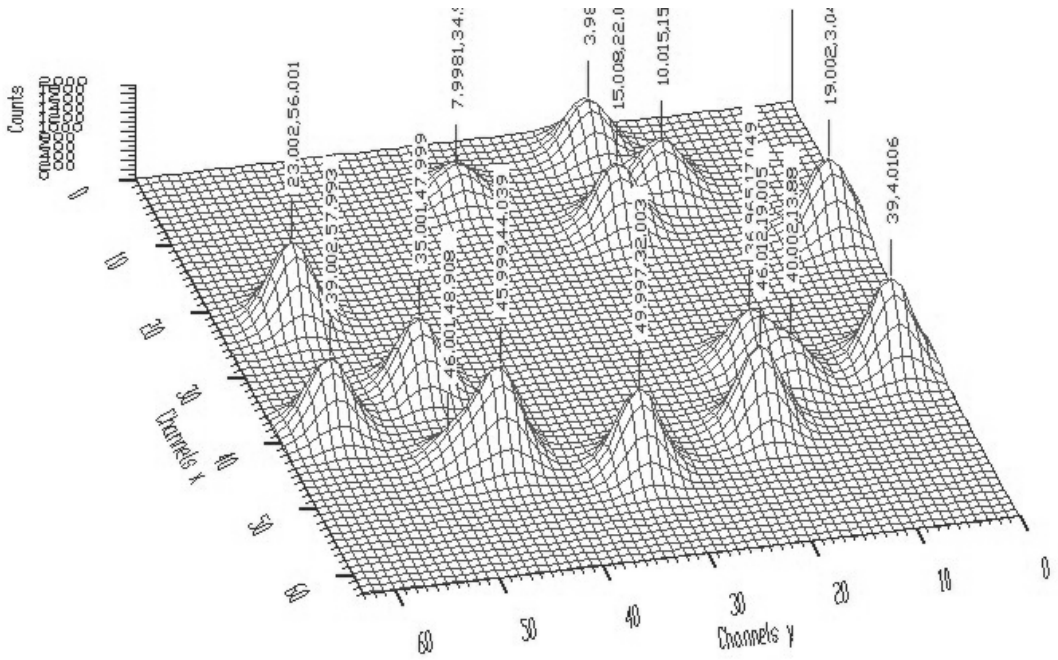


Fig 52 Result of the search using high resolution method based on Gold deconvolution

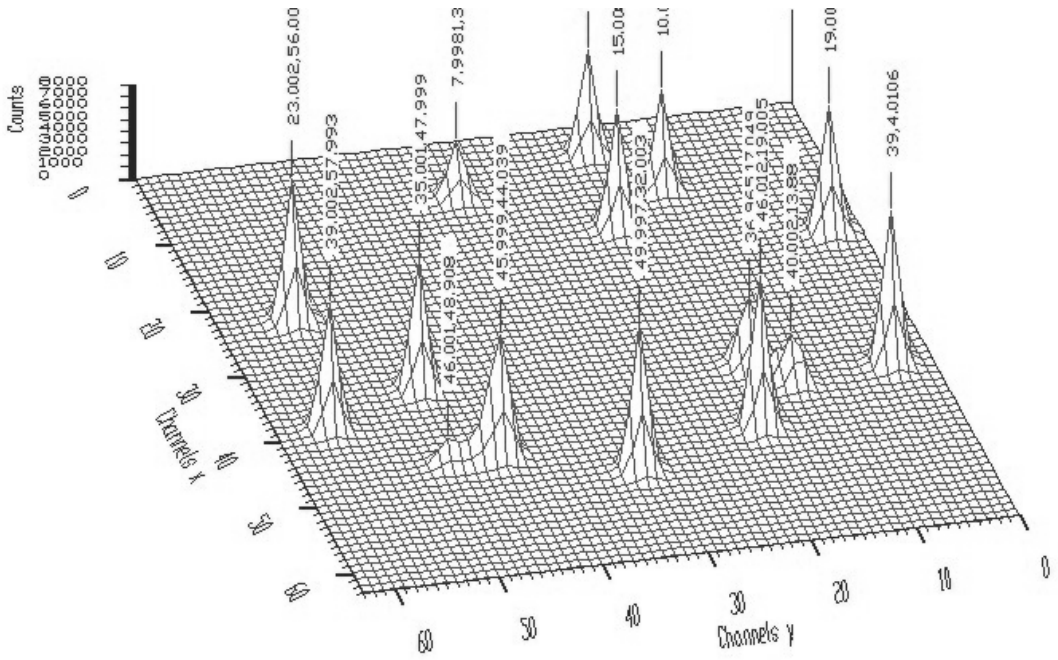


Figure 53 Deconvolved spectrum of the data from Figure 52

Sigma range peak search algorithm

- in previous sections we have demonstrated the ability of the peak searching algorithms to identify peaks with different σ. To some extent, the algorithm is robust to the variations of this parameter.
- however, for large scale of the range of σ and for poorly resolved peaks both previously designed algorithms fail to work properly. This is the case, e.g. for high energy spectra.

Outline of the algorithm

For every σ the algorithm comprises two deconvolutions. The principle of the method is as follows:

a. for $\sigma_i = \sigma_1$ up to σ_2
b. we set up the matrix of response functions (Gaussians) according to next Figure. All peaks have the same $\sigma = \sigma_i$. The columns of the matrix are mutually shifted by one position. We carry out the Gold deconvolution of the investigated spectrum.

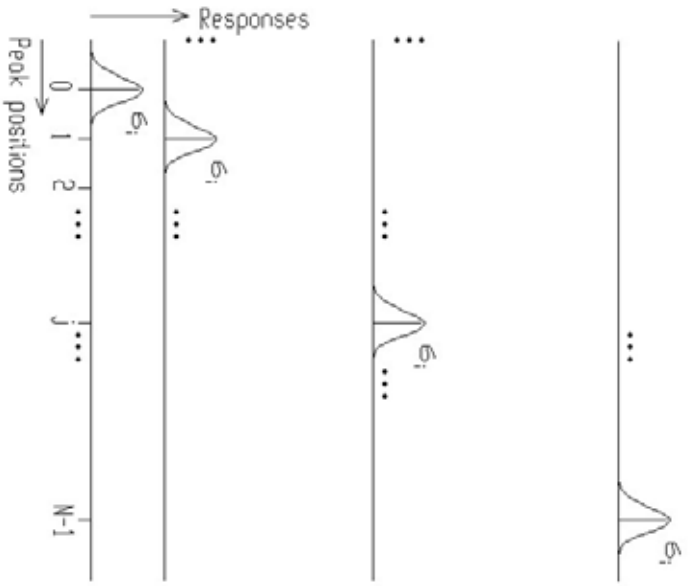


Figure 54 Response matrix consisting of Gaussian functions with the same σ

c. In the deconvolved spectrum, we find local maxima higher than given threshold value and include them into the list of 1-st level candidate peaks.
d. Next, we set up the matrix of the response functions for the 2-nd level deconvolution.
   There exist three groups of positions:

- positions where the 1-st level candidate peaks were localized. Here we generate response (Gaussian) with σ_i.
- positions where the 2-nd level candidate peaks were localized in the previous steps $\sigma_1 \le \sigma_k < \sigma_i$ (see next step). For each such a position, we generate the peak with the recorded σ_k.
- for remaining free positions where no candidate peaks were registered, we have empirically found that the most suitable functions are the block functions with the width $\pm 3\sigma_i$ from the appropriate channel.

The situation for one 2-nd level candidate peak in position j_2 with σ_k and for one 1-st level candidate peak in the position j_1 (σ_i) is depicted in next Figure. We carry out the 2-nd level Gold deconvolution.

e. Further, in the deconvolved spectrum we find the local maxima greater than given threshold value.

We scan the list of the 2-nd level candidate peaks:

- if in a position from this list there is not local maximum in the deconvolved spectrum, we erase the candidate peak from the list.

We scan the list of the 1-st level candidate peaks

- if in a position from this list there is the local maximum in the deconvolved spectrum, we transfer it to the list of the 2-nd level candidate peaks.

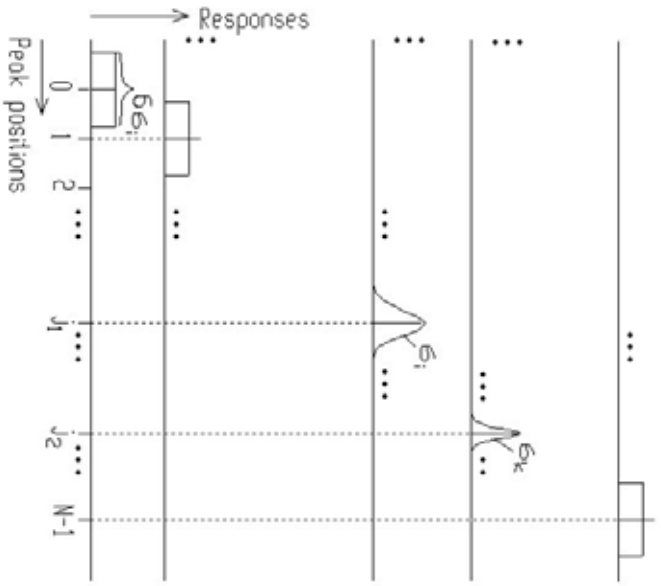


Figure 55 Example of response matrix consisting of block functions and Gaussians with different σ

f. Finally peaks that remained in the list of the 2-nd level candidate peaks are identified as found peaks with recorded positions and σ.

- the method is rather complex as we have to repeat two deconvolutions for the whole range of σ.

- in what follows we illustrate in detail practical aspects and steps during the peak identification. The original noisy spectrum to be processed is shown in next Figure. The σ of peaks included in the spectrum varies in the range 3 to 43. It contains 10 peaks with some of them positioned very close to each other.

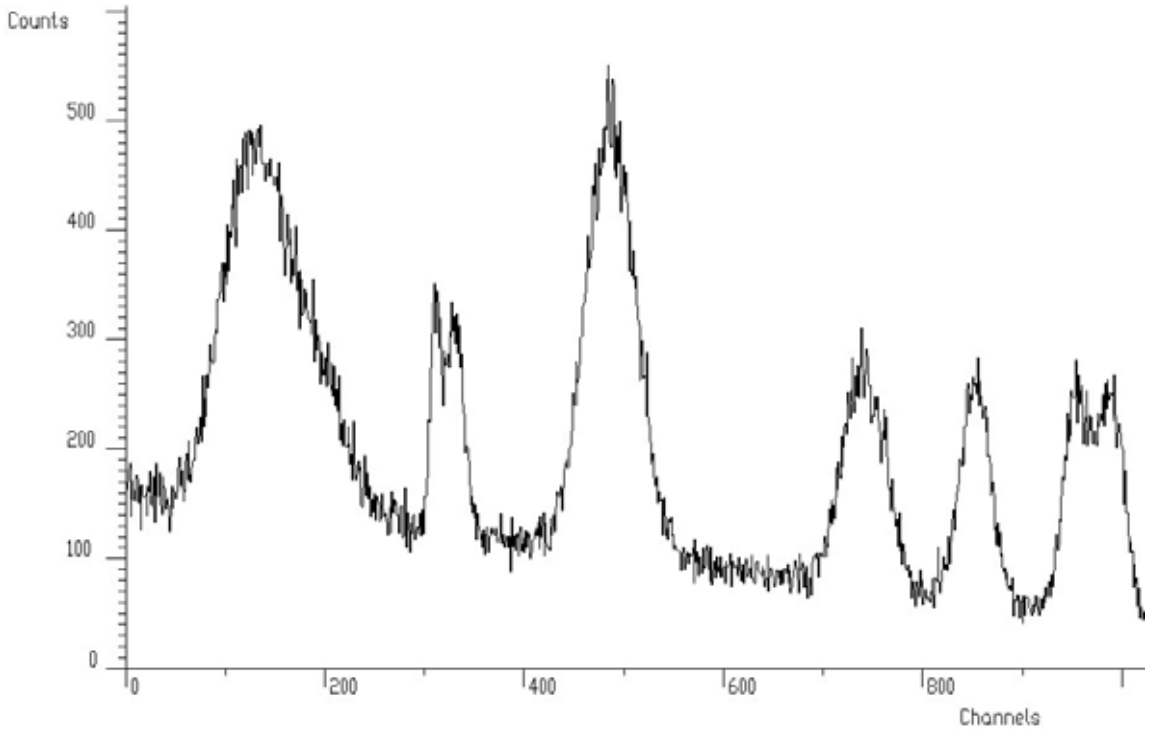


Figure 56 Noisy spectrum containing 10 peaks of rather different widths

- as the SRS algorithm is based on the deconvolution in the first step we need to remove background.

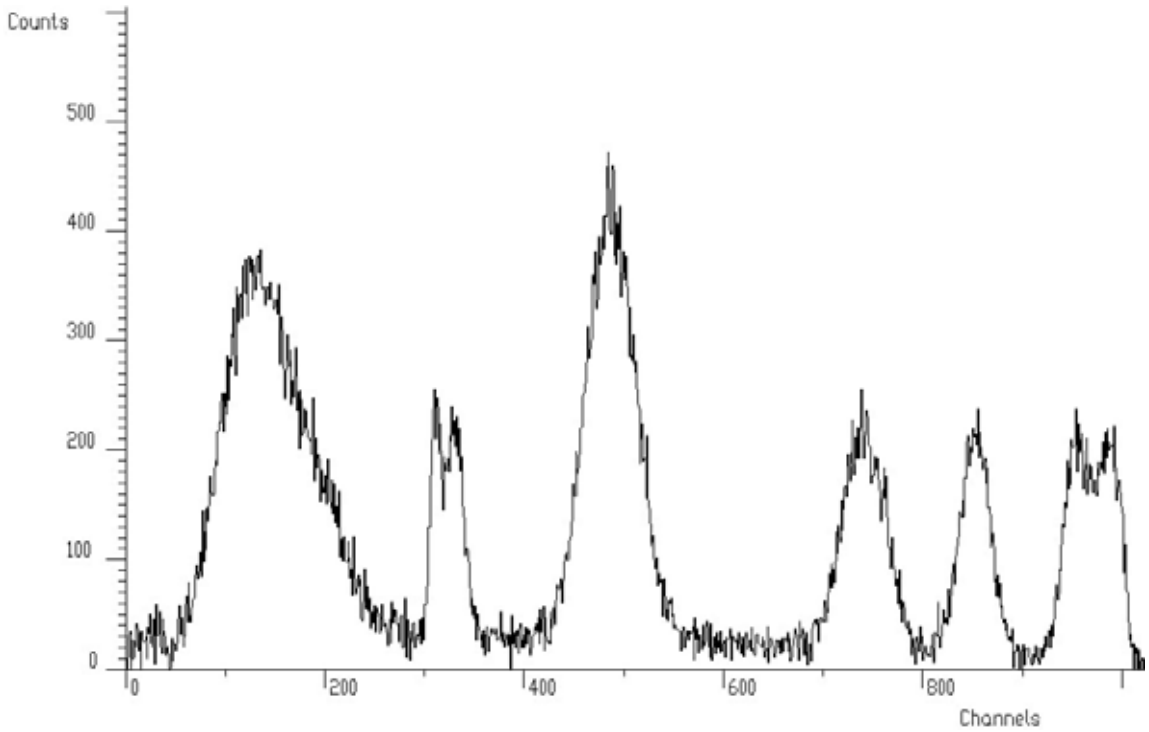


Figure 57 Spectrum from Figure 56 after background elimination

- at every position, we have to expect any peak from the given σ range (3, 43). To confine the possible combinations of positions and σ we generated inverted positive SSD of the spectrum for every σ from the range.
- we get matrix shown in next Figure. We consider only the combinations with non-zero values in the matrix.

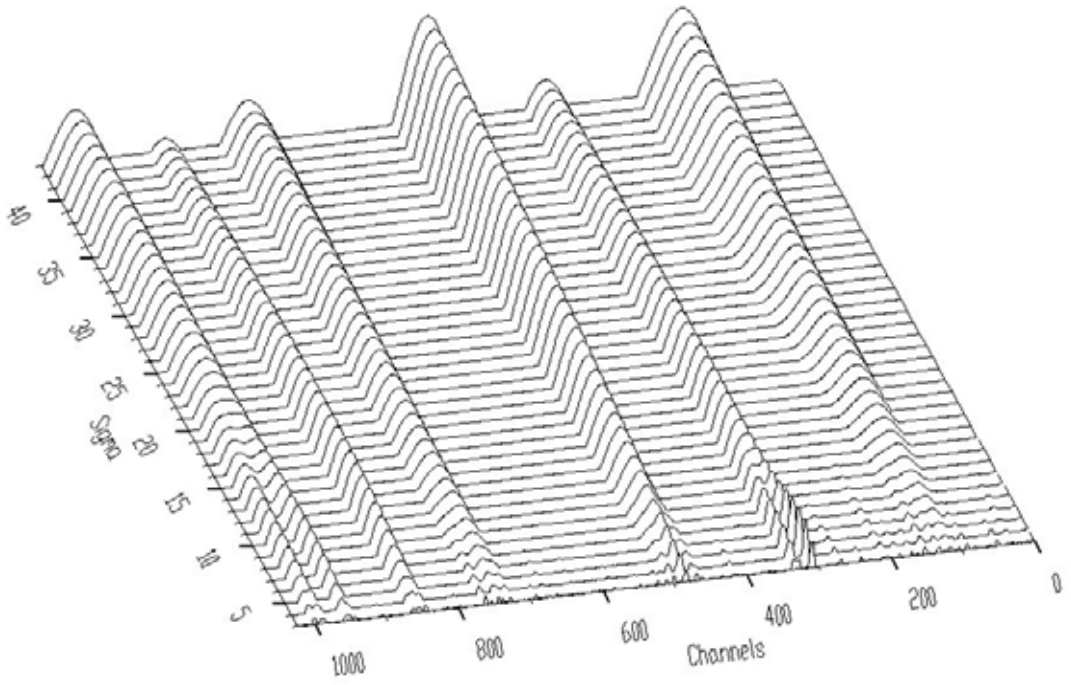


Figure 58 Matrix of inverted positive SSD

- the SRS algorithm is based on two successive deconvolutions. In the first level deconvolution, we look for peak candidates. We changed σ from 3 up to 43.
- for every σ we generated response matrix and subsequently we deconvolved spectrum from Figure 57. Again, we arranged the results in the form of matrix given in Figure 59.

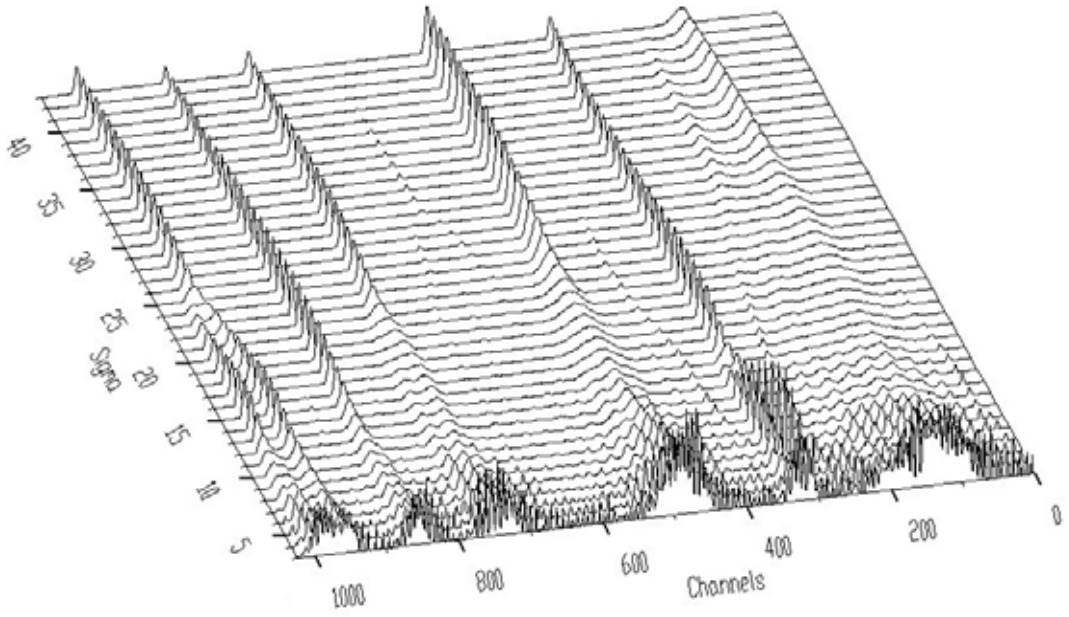


Figure 59 Matrix composed of spectra after first level deconvolution for responses changing σ from 3 to 43

- successively according to the above-given algorithm from these data, we pick up the candidates for peaks, construct the appropriate response matrices and deconvolve again the spectrum from Figure 57.
- the evolution of the result for increasing σ is shown in next Figure.

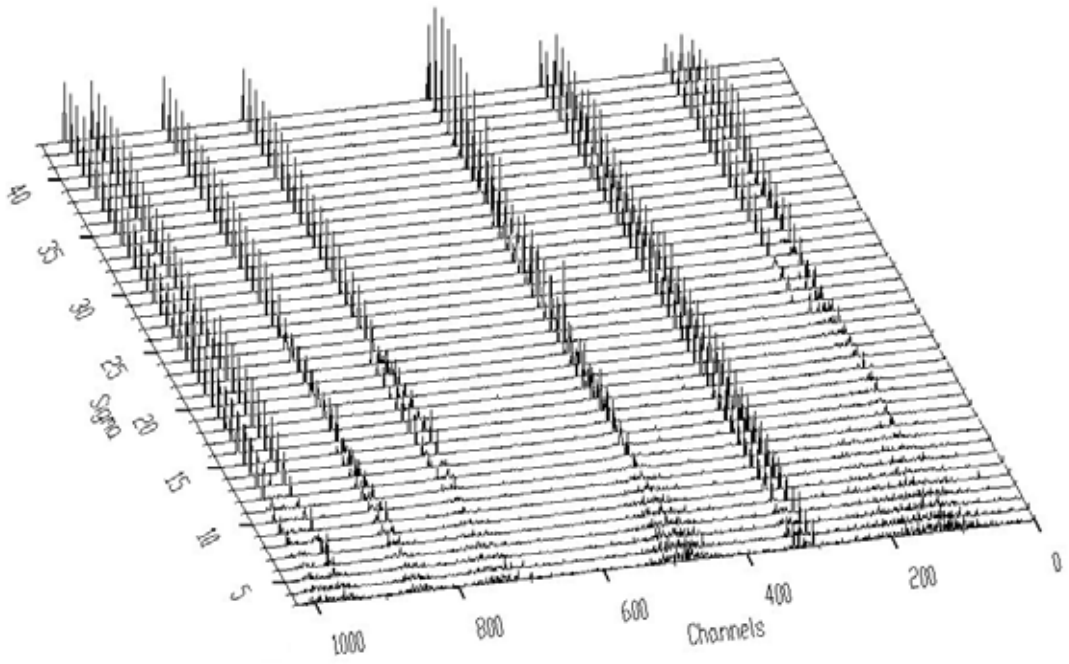


Figure 60 Matrix composed of spectra after second level deconvolutions

- from the last row of data, which are in fact spikes, we can identify (applying threshold parameter) the positions of peaks. The found peaks (denoted by markers with channel numbers) and the original spectrum are shown in next Figure.

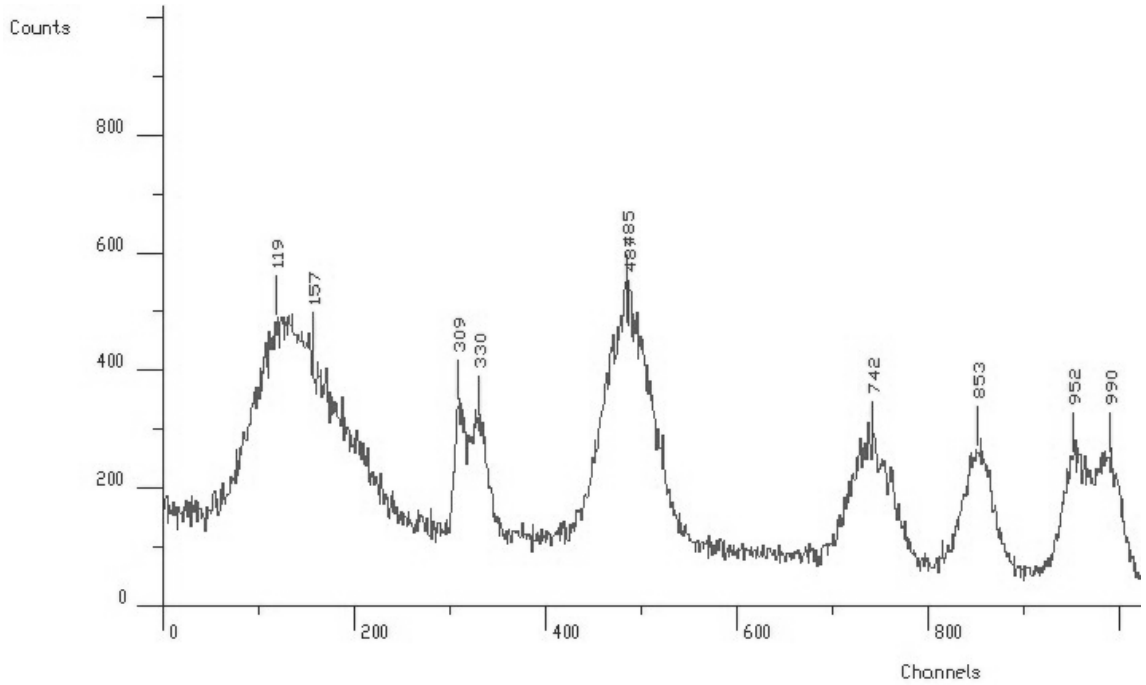


Figure 61 Original spectrum with found peaks denoted by markers

- in Table 5 we present the result of generated peaks and estimated parameters. In addition to the peak position the algorithm estimates even the σ of peaks. It is able to recognize also very closely positioned peaks.
- however, the estimate of the parameters is in some cases rather inaccurate mainly in poorly separated peaks of the spectrum. The problem is very complex and sometimes it is very difficult to decide whether a lobe represents two, eventually more, close positioned narrow peaks or one wide peak.

Peak #	Generated peaks (position/sigma)	Estimated peaks (position/sigma)
1	118/26	119/23
2	162/41	157/26
3	310/4	309/4
4	330/8	330/7
5	482/22	485/23
6	491/24	487/27
7	740/21	742/22
8	852/15	853/16
9	954/12	952/12
10	989/13	990/12

Table 5 Results of the estimation of peaks in spectrum shown in Figure 61

- we have verified the algorithm by its application to other spectra of this kind generated by especially proposed ROOT benchmark. The algorithm gives satisfactory results, though due to its complexity it is quite time consuming.

Conclusions

- the deconvolution methods represent an efficient tool to improve the resolution in the data.
- we have discussed and analyzed widely the existing deconvolution methods.
- we have developed modifications and extensions of iterative deconvolution algorithms, specific (new) regularization technique
- we proposed high-resolution peak searching algorithm based on Gold deconvolution for one-, and two-dimensional spectra. All these algorithms are derived only for given σ parameter.
- we have developed sophisticated algorithm of σ-range peak searching.
- the deconvolution and peak finder methods (and others) have been implemented in TSpectrum class of ROOT system.

Additional information:

http://www.fu.sav.sk/nph/projects/ProcFunc
http://www.fu.sav.sk/nph/projects/DaqProvis