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# **Processing and Visualization Functions**

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CONTENTS

## Chapter 1

# **BACKGROUND ELIMINATION**

### 1.1 1-DIMENSIONAL SPECTRA

This function calculates background spectrum from the source spectrum. The result is placed in the vector pointed by spectrum pointer. On successful completion it returns 0. On error it returns pointer to the string describing error.

char \*Background1(float \*spectrum,

int size, int number\_of\_iterations);

Function parameters:

- **spectrum**: pointer to the vector of the source spectrum
- **size**: length of spectrum
- number\_of\_iterations: or width of the clipping window

The function allows to separate useless spectrum information (continuous background) from peaks, based on Sensitive Nonlinear Iterative Peak Clipping Algorithm. In fact, it represents the second order difference filter (-1,2,-1). The basic algorithm is described in details in [1], [2].

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

where **p** can be changed as follows:

- a. from 1 up to a given parameter value  ${\tt w}$  by incrementing it in each iteration step by 1 INCREASING CLIPPING WINDOW
- b. from a given value w by decrementing it in each iteration step by 1 DECREASING CLIPPING WINDOW

An example of the original spectrum and estimated background (INCREASING CLIPPING WINDOW) is given in the Figure 1.1.

One can notice that on the edges of the peaks the estimated background goes under the peaks. An alternative approach is to decrease the clipping window from a given value to the value of one (DECREASING CLIPPING WINDOW). Then the result obtained is given in the Figure 1.2.

The estimated background is smoother. The method does not deform the shape of peaks.

However, sometimes the shape of the background is very complicated, and the second order filter is insufficient. Let us illustrate such a case in the Figure 1.3. The fourth order background estimation filter gives a better estimate of complicated background (the clipping window w=10).

4-th order algorithm ignores linear as well as cubic component of the background. In this case the filter is (1,-4,6,-4,1). In general, the allowed values for the order of the filter are 2, 4, 6, 8. An example of the same spectrum estimated with the clipping window w=40 and with filters of the orders 2, 4, 6, 8 is given in the Figure 1.4.

Sometimes it is necessary to also include the Compton edges into the estimate of the background. In Figure 1.5 we present the example of the synthetic spectrum with Compton edges. The background was estimated using the 8-th order filter



Figure 1.1: Example of the original spectrum and estimated background (INCREASING CLIPPING WINDOW)



Figure 1.2: An alternative approach is to decrease the clipping window from a given value to the value of one (DECREASING CLIPPING WINDOW)



Figure 1.3: The forth order background estimation filter gives better estimate of complicated background



Figure 1.4: The same spectrum estimated with the clipping window w=40 and with filters of the orders 2, 4, 6, 8

with the estimation of the Compton edges and decreasing clipping window. In the lower part of the Figure we present the background, which was added to the synthetic spectrum. One can observe good coincidence with the estimated background. The method of the estimation of Compton edge is described in details in [3].



Figure 1.5: Synthetic spectrum with Compton edges

The generalized form of the algorithm is implemented in the following function.

```
char *Background1General(float *spectrum,
```

```
int size,
int number_of_iterations,
int direction,
int filter_order,
bool compton);
```

The meaning of the parameters is as follows:

- **spectrum**: pointer to the vector of the source spectrum
- size: length of spectrum vector
- number\_of\_iterations: maximal width of clipping window
- direction: direction of change of clipping window. Possible values:
  - BACK1\_INCREASING\_WINDOW
  - BACK1\_DECREASING\_WINDOW
- filter\_order: order of clipping filter. Possible values:
  - BACK1\_ORDER2
  - BACK1\_ORDER4
  - BACK1\_ORDER6
  - BACK1 ORDER8
- compton: logical variable whether the estimation of Compton edge will be included. Possible values:
  - BACK1\_EXCLUDE\_COMPTON
  - BACK1\_INCLUDE\_COMPTON

## 1.2 2-DIMENSIONAL SPECTRA

This basic background estimation function allows to separate useless spectrum information (2D-continuous background and coincidences of peaks with background in both dimensions) from peaks. It calculates background spectrum from the source spectrum. The result is placed in the array pointed by spectrum pointer. On successful completion it returns 0. On error it returns a pointer to the string describing error.

Function parameters:

- **spectrum**: pointer to the array of the source spectrum
- **sizex**: x length of spectrum
- **sizey**: y length of spectrum
- number\_of\_iterations: width of the clipping window

In Figure 1.6 we present an example of a 2-dimensional spectrum before background elimination.



Figure 1.6: 2-dimensional spectrum before background elimination

Estimated background is shown in Figure 1.7. After subtraction we get pure 2-dimensional peaks.

Similarly to 1-dimensional case, we have generalized also the function for 2-dimensional background estimation. Sometimes the widths of peaks in both dimensions are different. As an example, we can introduce an n-gamma 2-dimensional spectra. Then it is necessary to set different widths of clipping window in both dimensions. In Figure 1.8 we give an example of such a spectrum.

Spectrum after background estimation (clipping window 10 for x-direction, 20 for y-direction) and subtraction is given in Figure 1.9.

Background estimation can be carried out using the algorithm of successive comparisons [1] or based on one-step filtering algorithm given by formula:

$$v_{p}(i) = min \left\{ v_{p-1}(i), \frac{\left[\begin{array}{c} -v_{p-1}(i+p,j+p) + 2 * v_{p-1}(i+p,j) - v_{p-1}(i+p,j-p) \\ +2 * v_{p-1}(i,j+p) + 2 * v_{p-1}(i,j-p) \\ -v_{p-1}(i-p,j+p) + 2 * v_{p-1}(i-p,j) - v_{p-1}(i-p,j-p) \end{array} \right] \\ 4 \right\}$$



Figure 1.7: Estimated background



Figure 1.8: It is necessary to set different widths of clipping window in both dimensions



Figure 1.9: Spectrum after background estimation (clipping window 10 for x-direction, 20 for y- direction) and subtraction

Illustrating example is given in the following 3 figures. In Figure 1.10 we present original (synthetic) 2-dimensional spectrum. In the Figure 1.11. we have spectrum after background elimination using successive comparisons algorithm and in Figure 1.12 after elimination using one-step filtering algorithm.

One can notice artificial ridges in the spectrum in Figure 1.11. In the estimation using filtration algorithm this effect disappears. The general function for estimation of 2-dimensional background with rectangular ridges has the form of

char \*Background2RectangularRidges(float \*\*spectrum,

```
int sizex,
int sizey,
int number_of_iterations_x,
int number_of_iterations_y,
int direction,
int filter_order,
int filter_type);
```

This function calculates background spectrum from source spectrum. The result is placed to the array pointed by spectrum pointer.

- **spectrum**: pointer to the array of the source spectrum
- **sizex**: x length of spectrum
- sizey: y length of spectrum
- number\_of\_iterations\_x\_maximal: x width of clipping window
- number\_of\_iterations\_y\_maximal: y width of clipping window
- direction: direction of change of clipping window. Possible values:
   BACK2\_INCREASING\_WINDOW
  - BACK2\_DECREASING\_WINDOW
- filter\_order: order of clipping filter. Possible values:
  - BACK2\_ORDER2 BACK2\_ORDER4
  - BACK2\_ORDER6 BACK2\_ORDER8
- filter\_type: determines the algorithm of the filtering. Possible values:



Figure 1.10: Original (synthetic) 2-dimensional spectrum



Figure 1.11: Spectrum after background elimination using successive comparisons algorithm



Figure 1.12: Spectrum after elimination using one-step filtering algorithm

- BACK2\_SUCCESSIVE\_FILTERING
- BACK2\_ONE\_STEP\_FILTERING

In what follows we describe a function to estimate a continuous 2-dimensional background together with rectangular and skew ridges. In Figure 1.13 we present a spectrum of this type.

The goal is to remove rectangular as well as skew ridges from the spectrum and to leave only 2-dimensional coincidence peaks. After applying background elimination function and subtraction we get the two-dimensional peaks presented in Figure 1.14

In Figures 1.15 and 1.16 we present an experimental spectrum with skew ridges and estimated background, respectively.

The function for the estimation of background together with skew ridges has the form of

```
char *Background2SkewRidges(float **spectrum,
```

```
int sizex,
int sizey,
int number_of_iterations_x,
int number_of_iterations_y,
int direction,
int filter_order);
```

The result is placed to the array pointed by spectrum pointer.

- **spectrum**: pointer to the array of the source spectrum
- **sizex**: x length of spectrum
- **sizey**: y length of spectrum
- number\_of\_iterations\_x: maximal x width of clipping window
- number\_of\_iterations\_y: maximal y width of clipping window
- direction: direction of change of clipping window. Possible values:
  - BACK2\_INCREASING\_WINDOW
  - BACK2\_DECREASING\_WINDOW



Figure 1.13: Function to estimate continuous 2-dimensional background together with rectangular and skew ridges



Figure 1.14: Two dimensional peaks obtained after applying background elimination function and subtraction



Figure 1.15: Experimental spectrum with skew ridges



Figure 1.16: Experimental spectrum with estimated background

- filter\_order: order of clipping filter. Possible values:
  - BACK2\_ORDER2
  - BACK2\_ORDER4
  - BACK2\_ORDER6
  - BACK2\_ORDER8

Next we present the function that estimates the continuous background together with rectangular and nonlinear ridges. To illustrate the data of such a form we present synthetic data shown in Figure 1.17. The estimated background is given in Figure 1.18. Pure Gaussian after subtracting the background from the original spectrum is shown in Figure 1.19.



Figure 1.17: Synthetic data

The function to estimate also the nonlinear ridges has the form of

```
char *Background2NonlinearRidges(float **spectrum,
```

```
int sizex,
int sizey,
int number_of_iterations_x,
int number_of_iterations_y,
int direction,
int filter_order);
```

The result is placed to the array pointed by spectrum pointer.

- **spectrum**: pointer to the array of the source spectrum
- **sizex**: x length of spectrum
- **sizey**: y length of spectrum
- number\_of\_iterations\_x: maximal x width of clipping window
- number\_of\_iterations\_y: maximal y width of clipping window
- direction: direction of change of clipping window. Possible values:
  - BACK2\_INCREASING\_WINDOW
  - BACK2\_DECREASING\_WINDOW
- filter\_order: order of clipping filter. Possible values:
  - BACK2\_ORDER2



Figure 1.18: Estimated background



Figure 1.19: Pure Gaussian after subtracting the background from the original spectrum

- BACK2\_ORDER4
- BACK2\_ORDER6
- BACK2\_ORDER8

The information contained in the skew ridges and non-linear ridges can be interesting and one may wish to separate it from the rectangular ridges. Therefore we have also implemented two functions allowing to estimate ridges only in the direction rectangular to x-axis and y-axis. Let us have both rectangular and skew ridges from spectrum given in Figure 1.13 estimated using above described function Background2SkewRidges (Figure 1.20).



Figure 1.20: Background2SkewRidges9

Now let us estimate ridges rectangular to x-axis and y-axis (Figures 1.21, 1.22)

After subtraction these data from spectrum in Figure 1.20, we get separated skew ridge given in Figure 1.23.

The functions for estimation of 1-dimensional ridges in 2-dimensional spectra have the forms of

char \*Background2RectangularRidgesX(float \*\*spectrum,

```
int sizex,
int sizey,
int number_of_iterations,
int direction,
int filter_order);
```

- **spectrum**: pointer to the array of the source spectrum
- **sizex**: x length of spectrum
- **sizey**: y length of spectrum
- number\_of\_iterations: maximal x width of clipping window
- direction: direction of change of clipping window. Possible values:
  - BACK2\_INCREASING\_WINDOW
  - BACK2\_DECREASING\_WINDOW
- filter\_order: order of clipping filter. Possible values:
  - BACK2\_ORDER2
  - BACK2\_ORDER4



Figure 1.21: Ridges rectangular to x-axis



Figure 1.22: ridges rectangular to y-axis



Figure 1.23: Separated skew ridge

- BACK2\_ORDER6
- BACK2\_ORDER8

#### and

```
char *Background2RectangularRidgesY(float **spectrum,
```

int sizex, int sizey, int number\_of\_iterations, int direction, int filter\_order);

- **spectrum**: pointer to the array of source the spectrum
- **sizex**: x length of spectrum
- **sizey**: y length of spectrum
- number\_of\_iterations: maximal width of clipping window
- direction: direction of change of clipping window. Possible values:
  - BACK2\_INCREASING\_WINDOW
  - BACK2\_DECREASING\_WINDOW
- filter\_order: order of clipping filter. Possible values:
  - BACK2\_ORDER2
  - BACK2\_ORDER4
  - BACK2\_ORDER6
  - BACK2\_ORDER8

# Chapter 2

# SMOOTHING

## 2.1 1-DIMENSIONAL SPECTRA

The operation of the smoothing is based on the convolution of the original data with the filter of the type:

(1,2,1)/4 - three points smoothing

(-3,12,17,12,-3)/35 - five points smoothing

(-2,3,6,7,6,3,-2)/21 - seven points smoothing

(-21, 14, 39, 54, 59, 54, 39, 14, -21)/231 - nine points smoothing

(-36,9,44,69,84,89,84,69,44,9,-36)/429 - 11 points smoothing

(-11,0,9,16,21,24,25,24,21,16,9,0,-11)/143 - 13 points smoothing

(-78, -13, 42, 87, 122, 147, 162, 167, 162, 147, 122, 87, 42, -13, -78)/1105 -15 points smoothing. The function for one-dimensional smoothing has the form of

This function calculates smoothed spectrum from the source spectrum. The result is placed in the vector pointed by the spectrum pointer.

Function parameters:

- **spectrum**: pointer to the vector of the source spectrum
- size: length of spectrum
- points: width of smoothing window. Possible values:
  - SMOOTH1\_3POINTS
  - SMOOTH1\_5POINTS
  - SMOOTH1\_7POINTS
  - SMOOTH1\_9POINTS
  - SMOOTH1\_11POINTS
  - SMOOTH1 13POINTS
  - SMOOTH1 15POINTS

An example of 1-dimensional spectra smoothing and the influence of the filter width on the data is presented in Figure 2.1.

## 2.2 2-DIMENSIONAL SPECTRA

The smoothing of the two-dimensional data is similar to the one-dimensional case. The width of the filter can be chosen independently for each dimension. The form of the 2-D smoothing function is as follows:



Figure 2.1: 1-dimensional spectra smoothing and the influence of the filter width on the data

```
int sizey,
int pointsx,
int pointsy);
```

This function calculates smoothed spectrum from the source spectrum. The result is placed in the array pointed by the spectrum pointer.

Function parameters:

- **spectrum**: pointer to the array of the source spectrum
- ${\tt sizex:}\ x\ {\rm length}\ of\ {\rm spectrum}$
- **sizey**: y length of spectrum
- pointsx, pointsy: width of smoothing window. Possible values:
  - SMOOTH2\_3POINTS
  - SMOOTH2\_5POINTS
  - SMOOTH2\_7POINTS
  - SMOOTH2\_9POINTS
  - SMOOTH2\_11POINTS
  - SMOOTH2\_13POINTS
  - SMOOTH2\_15POINTS

An example of 2-D original data and data after smoothing is given in Figures 2.2, 2.3.



Figure 2.2: 2-D original data



Figure 2.3: Data after smoothing

# Chapter 3

# PEAK SEARCHING

## 3.1 1-DIMENSIONAL SPECTRA

The basic function of the 1-dimensional peak searching is described in details in [4], [5]. It allows to automatically identify the peaks in a spectrum with the presence of the continuous background and statistical fluctuations – noise. The algorithm is based on smoothed second differences that are compared to its standard deviations. Therefore it is necessary to pass a parameter of sigma to the peak searching function. The algorithm is selective to the peaks with a given sigma. The form of the basic peak searching function is

#### 

This function searches for peaks in the source spectrum. The number of found peaks and their positions are written into structure pointed by **one\_dim\_peak** structure pointer.

Function parameters:

- **source**: pointer to the vector of the source spectrum
- p: pointer to the one\_dim\_peak structure pointer
- size: length of the source spectrum
- sigma: sigma of searched peaks

The one\_dim\_peak structure has the form of

```
struct one_dim_peak{
    int number_of_peaks;
    double position[MAX_NUMBER_OF_PEAKS1];
};
```

An example of simple one-dimensional spectrum with identified peaks is given in Figure 3.1.

An example of 1-dimensional experimental spectrum with many identified peaks is given in Figure 3.2.

However, when we have noisy data, the number of peaks can be enormous. One such an example is given in Figure 3.3.

Therefore it can be useful to have a possibility to set a threshold value and to consider only the peaks higher than this threshold (see Figure 3.4, only three peaks were identified, threshold=50). The value in the center of the peak (value[i]) minus the average value in two symmetrically positioned channels (channels i-3\*sigma, i+3\*sigma) must be greater than threshold. Otherwise the peak is ignored.

An alternative approach was proposed in [6]. The algorithm generates new invariant spectrum based on discrete Markov chains. In this spectrum the noise is suppressed, the spectrum is smoother than the original one. On the other hand it emphasizes peaks (depending on the averaging window). The example of the part of original noisy spectrum and Markov spectrum for window=3 is given in Figure 3.5 Then the peaks can be found in Markov spectrum using standard above-presented algorithm.

The form of the generalized peak searching function is as follows:



Figure 3.1: Simple one-dimensional spectrum with identified peaks



Figure 3.2: 1-dimensional experimental spectrum with many identified peaks



Figure 3.3: With noisy data the number of peaks can be enormous



Figure 3.4: Iwth threshold=50, only three peaks were identified



Figure 3.5: Part of original noisy spectrum and Markov spectrum for window=3

```
Int_t Search1General(float *spectrum,
```

```
int size,
float sigma,
int threshold,
bool markov,
int aver_window);
```

This function searches for peaks in the source spectrum. The number of found peaks and their positions are written into the structure pointed by the one\_dim\_peak structure pointer.

Function parameters:

- **spectrum**: pointer to the vector of the source spectrum. This source spectrum is replaced by the new spectrum calculated using Markov chains method.
- size: length of the source spectrum
- **sigma**: sigma of searched peaks
- threshold: threshold value for peaks selection
- markov: logical variable. If it is set to true, then the source spectrum is first replaced by the new spectrum calculated using Markov chains method
- aver\_window: averaging window used in the calculation of Markov spectrum, applies only if the markov variable was set to true

The methods of peak searching are sensitive to the sigma. Usually the sigma value is known beforehand. It also changes only slightly with the energy. We have investigated as well the robustness of the proposed algorithms to the spectrum with the peaks with sigma changing from 1 to 10 (see Figure 3.6).

We applied peak searching algorithm based on Markov approach. We changed sigma in the interval from 1 to 10. The spectra for averaging windows 3, 5, 10 are shown in Figure 3.7.

When we applied peak searching function to the Markov spectrum averaged with the window=10, we obtained correct estimate of all 10 peak positions for sigma=2,3,4,5,6,7,8. It was not the case when we made the same experiment with the original spectrum. For all sigmas some peaks were not discovered.



Figure 3.6: Robustness of the proposed algorithms to the spectrum with the peaks with sigma changing from 1 to 10



Figure 3.7: Spectra for averaging windows 3, 5, 10

## 3.2 2-DIMENSIONAL SPECTRA

The basic function of the 2-dimensional peak searching is described in details in [4]. It automatically identifies the peaks in a spectrum with the presence of the continuous background, statistical fluctuations as well as coincidences of background in one dimension and peak in the other one-ridges. The form of the basic function of 2-dimensional peak searching is

This function searches for peaks in the source spectrum. The number of found peaks and their positions are written into the structure pointed by two\_dim\_peak structure pointer.

Function parameters:

- **source**: pointer to the vector of the source spectrum
- sizex: x length of the source spectrum
- sizey: y length of the source spectrum
- sigma: sigma of searched peaks

An example of the two-dimensional spectrum with the identified peaks is shown in Figure 3.8.



Figure 3.8: Two-dimensional spectrum with the identified peaks

We have also generalized the peak searching function similarly to one-dimensional data. The generalized peak searching function for two-dimensional spectra has the form of

#### 3.2. 2-DIMENSIONAL SPECTRA

This function searches for peaks in the source spectrum. The number of found peaks and their positions are written into the structure pointed by two\_dim\_peak structure pointer.

Function parameters:

- ${\tt source}:$  pointer to the vector of the source spectrum
- **sizex**: x length of the source spectrum
- sizey: y length of the source spectrum
- ${\tt sigma:}$  sigma of searched peaks
- threshold: threshold value for peaks selection
- **markov**: logical variable. If it is set to **true**, then the source spectrum is first replaced by the new spectrum calculated using Markov chains method
- aver\_window averaging window of searched peaks (applies only for the Markov method)

An example of experimental 2-dimensional spectrum is given in Figure 3.9. The number of peaks identified by the function now is 295.



Figure 3.9: Experimental 2-dimensional spectrum

The function works even for very noisy data. In Figure 3.10 we present synthetic 2-dimensional spectrum with 5 peaks. The method should recognize what is the real 2-dimensional peak and what is the crossing of two 1-dimensional ridges. The Markov spectrum with averaging window=3 is given in Figure 3.11. One can observe that this spectrum is smoother than the original one. After applying the general peak searching function to the Markov spectrum with sigma=2 and threshold=600, we get correctly identified peaks.



Figure 3.10: Synthetic 2-dimensional spectrum with 5 peaks



Figure 3.11: Markov spectrum with averaging window=3  $\,$ 

## Chapter 4

# **DECONVOLUTION - UNFOLDING**

### 4.1 1-DIMENSIONAL SPECTRA

Mathematical formulation of the convolution system is:

$$y(i) = \sum_{k=0}^{N-1} h(i-k)x(k), i = 0, 1, 2, ..., N-1$$

where h(i) is the impulse response function, x, y are input and output vectors, respectively, N is the length of x and h vectors. In matrix form we have:

$$\begin{bmatrix} y(0) \\ y(1) \\ \vdots \\ \vdots \\ \vdots \\ y(2N-2) \\ y(2N-1) \end{bmatrix} = \begin{bmatrix} h(0) & 0 & 0 & 0 & \dots & 0 \\ h(1) & h(0) & 0 & 0 & \dots & 0 \\ h(1) & h(0) & 0 & 0 & \dots & 0 \\ h(1) & h(0) & 0 & 0 & \dots & 0 \\ \vdots & h(1) & h(0) & 0 & \dots & 0 \\ h(N-1) & \vdots & h(1) & h(0) & \dots & 0 \\ 0 & h(N-1) & \vdots & h(1) & \dots & 0 \\ 0 & 0 & h(N-1) & \vdots & \dots & h(0) \\ 0 & 0 & 0 & h(N-1) & \dots & h(1) \\ \vdots & \vdots & \vdots & \vdots & \vdots & \dots & \vdots \\ 0 & 0 & 0 & 0 & \dots & h(N-1) \end{bmatrix} \begin{bmatrix} x(0) \\ x(1) \\ x(2) \\ \vdots \\ y(N-1) \end{bmatrix}$$

Let us assume that we know the response and the output vector (spectrum) of the above given system. The deconvolution represents solution of the overdetermined system of linear equations, i.e., the calculation of the vector  $\mathbf{x}$ .

The goal of the deconvolution methods is to improve the resolution in the spectrum and to decompose multiplets. From mathematical point of view the operation of deconvolution is extremely critical as well as time consuming. From all the studied methods, the Gold deconvolution (decomposition) proved to work best. It is suitable to process positive definite data (e.g., histograms). The method is described in details in [7], [8].

#### 4.2 Gold deconvolution algorithm

This algorithm proved to work best, other methods (Fourier, VanCittert etc.) oscillate.

$$\begin{split} y &= Hx \\ H^T &= H^T Hx \\ y^{'} &= H^{'}x \\ x^{(k+1)}_i &= \frac{y^{'}_i}{\sum_{m=0}^{N-1} H^{'}_{im} x^{(k)}_m} x^{(k)}_i, i=0,1,...,N-1, \end{split}$$

where:

$$k = 1, 2, 3, ..., I$$

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

The basic function has the form of

This function calculates deconvolution from the source spectrum according to the response spectrum.

Function parameters:

- source: pointer to the vector of the source spectrum
- **resp**: pointer to the vector of the response spectrum
- **size**: length of source and the response spectra
- number\_of\_iterations: for details see [8]

As an illustration of the method, let us introduce a small example. In Figure 4.1 we present original 1-dimensional spectrum. It contains multiplets that cannot be directly analyzed. The response function (one peak) is given in Figure 4.2. We assume the same response function (not changing the shape) along the entire energy scale. So the response matrix is composed of mutually shifted response functions by one channel, however of the same shape.



Figure 4.1: Original 1-dimensional spectrum

The result after deconvolution is given in Figure 4.3. It substantially improves the resolution in the spectrum.

We have developed a new high resolution deconvolution algorithm. We have observed that the Gold deconvolution converges to its stable state (solution). It is useless to increase the number of iterations, the result obtained does not change. To continue decreasing the width of peaks, we have found that when the solution reaches its stable state, it is necessary to stop iterations, then to change the vector in a way and repeat again the Gold deconvolution. We have found that in order to change the particular solution we need to apply a non-linear boosting function to it. The power function proved to give the best results. At the beginning the function calculates exact solution of the Toeplitz system of linear equations.

$$x^{(0)} = [x_e^2(0), x_e^2(1), ..., x_e^2(N-1), ]^T$$



Figure 4.2: Response function (one peak)



Figure 4.3: Result after deconvolution

where

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$$x_e = H^{'-1}y^{'}$$

Then it applies the Gold deconvolution algorithm to the solution and carries out preset number of iterations. Then the power function with the exponent equal to the boosting coefficient is applied to the deconvolved data. These data are then used as initial estimate of the solution of linear system of equations and again the Gold algorithm is employed. The whole procedure is repeated number\_of\_repetitions times.

The form of the high-resolution deconvolution function is

This function calculates deconvolution from the source spectrum according to the response spectrum.

The result is placed in the vector pointed by the source pointer.

Function parameters:

- source: pointer to the vector of the source spectrum
- **resp**: pointer to the vector of the response spectrum
- **size**: length of source and the response spectra
- **number\_of\_iterations**: for details we refer to manual
- number\_of\_repetitions: for details we refer to manual
- **boost**: boosting factor, for details we refer to manual

The result obtained using the data from Figures 4.1, 4.2 and applying the high resolution deconvolution is given in Figure 4.4. It decomposes the peaks even more (practically to 1, 2 channels).



Figure 4.4: Result obtained using the data from Figures 4.1, 4.2 and applying the high resolution deconvolution

Another example of synthetic data is given in Figure 4.5. We have positioned the two peaks very close to each other (2 channels). The method of high resolution deconvolution has decomposed these peaks practically to one channel. The
original data are shown as polyline, the data after deconvolution as bars. The numbers at the bars denote the heights of bars and the numbers in parenthesis the original area of peaks. The area of original peaks is concentrated into one channel.



Figure 4.5: Example of synthetic data

Up to now we assumed that the shape of the response is not changing. However, the method of Gold decomposition can be utilized also for the decomposition of input data (unfolding) with completely different responses. The form of the unfolding function is as follows:

This function unfolds the source spectrum according to response matrix columns. The result is placed in the vector pointed by the source pointer.

Function parameters:

- source: pointer to the vector of the source spectrum
- **resp**: pointer to the matrix of the response spectra
- **sizex**: length of source spectrum and # of rows of response matrix
- **sizey**: # of columns of response matrix
- number\_of\_iterations

Note that **sizex** must be equal to or greater than **sizey**. After decomposition, the resulting channels are written back to the first **sizey** channels of the source spectrum.

An example of the response matrix composed of the responses of different chemical elements is given in Figure 4.6.

The original spectrum before unfolding is given in Figure 4.7. The obtained coefficients after unfolding, i.e., the contents of the responses in the original spectrum, are presented in the Figure 4.8.

Another example where we have used the unfolding method is the decomposition of continuum of gamma-ray spectra. Using simulation and interpolation techniques, we have synthesized the response matrix (size 3400x3400 channels) of



Figure 4.6: Example of the response matrix composed of the responses of different chemical elements



Figure 4.7: Original spectrum before unfolding



Figure 4.8: Contents of the responses in the original spectrum

Gammasphere spectrometer (Figure 4.9). Its details are presented in Figure 4.10. The original spectrum of Co<sup>56</sup> before and after continuum decomposition are presented in Figures 4.11, 4.12, respectively.

### 4.3 2-DIMENSIONAL SPECTRA

We have extended the method of Gold deconvolution also for 2-dimensional data. Again, the goal of the deconvolution methods is to improve the resolution in the spectrum and to decompose multiplets. The method of optimized 2-dimensional deconvolution is described in details in [8].

Mathematical formulation of 2-dimensional convolution system is as follows:

$$y(i_1, i_2) = \sum_{k_1=0}^{N_1-1} \sum_{k_2=0}^{N_2-1} h(i_1 - k_1, i_2 - k_2) x(k_1, k_2), i_1 = 0, 1, 2, \dots, N_1 - 1, i_2 = 0, 1, 2, \dots, N_2 - 1$$

Assuming we know the output spectrum y and the response spectrum h, the task is to calculate the matrix x.

The basic function has the form of

This function calculates deconvolution from the source spectrum according to the response spectrum. The result is placed in the matrix pointed by the source pointer.

- **source**: pointer to the matrix of the source spectrum
- **resp**: pointer to the matrix of the response spectrum
- sizex: x length of source and the response spectra



Figure 4.9: Response matrix (size 3400x3400 channels) of Gammasphere spectrometer



Figure 4.10: Detail of Figure 4.9



Figure 4.11: Original spectrum of Co56 before continuum decomposition



Figure 4.12: Original spectrum of Co56 after continuum decomposition

- **sizey**: y length of source and the response spectra
- number\_of\_iterations: see [8] for details

The example of 2-dimensional spectrum before deconvolution is presented in Figure 4.13. In the process of deconvolution we have used the response matrix (one peak shifted to the beginning of the coordinate system) given in Figure 4.14. Employing the Gold deconvolution algorithm implemented in the decon2 function, we get the result shown in Figure 4.15. One can notice that the peaks became narrower, thus improving the resolution in the spectrum.



Figure 4.13: 2-dimensional spectrum before deconvolution

Similarly to 1-dimensional case, we have developed high-resolution 2-dimensional deconvolution. From the beginning the exact solution of the cyclic convolution 2-dimensional system is calculated. Then we apply the repeated deconvolution with boosting in the same way like in 1-dimensional case. The form of the high-resolution 2-dimensional deconvolution function is:

#### char \*Deconvolution2HighResolution(float \*\*source,

const float \*\*resp, int sizex, int sizey, int number\_of\_iterations, int number\_of\_repetitions, double boost);

This function calculates deconvolution from source spectrum according to response spectrum. The result is placed in the matrix pointed by the source pointer.

- **source**: pointer to the matrix of the source spectrum
- **resp**: pointer to the matrix of the response spectrum
- sizex: x length of source and the response spectra
- sizey: y length of source and the response spectra
- number\_of\_iterations
- number\_of\_repetitions
- **boost**: boosting factor



Figure 4.14: Response matrix (one peak shifted to the beginning of the coordinate system)



Figure 4.15: Result obtained employing the Gold deconvolution algorithm implemented in the decon2 function

When we apply this function to the data from Figure 4.13 using the response matrix given in Figure 4.14, we get the result shown in Figure 4.16. It is obvious that the high-resolution deconvolution decomposes the input data even more than the original Gold deconvolution.



Figure 4.16: Result obtained applying Deconvolution2HighResolution to the data from Figure 4.13 using response matrix given in Figure 4.14

## Chapter 5

# FITTING

A lot of algorithms have been developed (Gauss-Newton, Levenber-Marquart conjugate gradients, etc.) and more or less successfully implemented into programs for analysis of complex spectra. They are based on matrix inversion that can impose appreciable convergence difficulties mainly for large number of fitted parameters. Peaks can be fitted separately, each peak (or multiplets) in a region or together all peaks in a spectrum. To fit separately each peak one needs to determine the fitted region. However it can happen that the regions of neighboring peaks are overlapping (mainly in 2-dimensional spectra). Then the results of fitting are very poor. On the other hand, when fitting together all the peaks found in a spectrum, one needs to have a method that is stable (i.e., converges) and fast enough to carry out the fitting in a reasonable time. The gradient methods based on the inversion of large matrices are not applicable because of two reasons:

- a. calculation of inverse matrix is extremely time consuming;
- b. due to accumulation of truncation and rounding-off errors, the result can become worthless.

We have implemented two kinds of fitting functions. The first approach is based on the algorithm without matrix inversion [9] - awmi algorithm. It allows to fit large blocks of data and large number of parameters.

The other one is based on a calculation of the system of linear equations using Stiefel-Hestens method [10]. It converges faster than the awmi algorithm, however, it is not suitable to fit large number of parameters.

#### 5.1 1-DIMENSIONAL SPECTRA

The quantity to be minimized in the fitting procedure for one-dimensional spectrum is defined as

$$\chi^{2} = \frac{1}{N - M} \sum_{i=1}^{N} \frac{[y_{i} - f(i, a)]^{2}}{y_{i}}$$

where i is the channel in the fitted spectrum, N is the number of channels in the fitting subregion, M is the number of free parameters, y\_i is the content of the i-th channel, a is a vector of the parameters being fitted and f(i,a) is a fitting or peak shape function.

Instead of the weighting coefficient  $y_i$  in the denominator of the formula given above, one can use also the value of f(i,a). It is suitable for data with poor statistics [11], [12].

The third statistic to be optimized, which is implemented in the fitting functions, is the Maximum Likelihood Method. It is up to the user to select a suitable statistic.

After differentiating chi<sup>2</sup> we obtain the following M simultaneous equations:

$$\sum_{i=1}^{N} \frac{y_i - f(i, a^{(t)})}{y_i} \frac{\partial f(i, a^t)}{\partial a_k} = \sum_{j=1}^{M} \sum_{i=1}^{N} \frac{\partial f(i, a^{(t)})}{\partial a_j} \frac{\partial f(i, a^{(t)})}{\partial a_k} \Delta a_j^{(t)}$$

- in gamma-ray spectra we have to fit together tens, hundreds of peaks simultaneously that sometimes represent thousands of parameters.
- the calculation of the inversion matrix of such a size is practically impossible.

• the awmi method is based on the assumption that the off-diagonal terms in the matrix A are equal to zero.

$$\Delta a_k^{(t+1)} = \alpha^{(t)} \frac{\sum_{i=1}^N \frac{e_i^{(t)}}{y_i} \frac{\partial f(i, a^{(t)})}{\partial a_k}}{\sum_{i=1}^N \left[\frac{\partial f(i, a^{(t)})}{\partial a_k}\right]^2 \frac{1}{y_i}}$$

where the error in the channel i is  $e_i^{(t)} = y_i - f(i, a^{(t)}); k = 1, 2, ..., M$  and  $\alpha^{(t)} = 1$  if the process is convergent or  $\alpha^{(t)} = 0.5\alpha^{(t-1)}$  if it is divergent. Another possibility is to optimize this coefficient.

The error of k-th parameter estimate is

$$\Delta a_k^{(e)} = \sqrt{\frac{\sum_{i=1}^N \frac{e_i^2}{y_i}}{\sum_{i=1}^N \left[\frac{\partial f(i, a^{(t)})}{\partial a_k}\right]^2 \frac{1}{y_i}}}$$

Algorithm with higher powers w=1,2,3...:

$$\Delta a_{k,w}^{(t+1)} = \alpha^{(t)} \frac{\sum_{i=1}^{N} \frac{e_i}{y_i} \left[\frac{\partial f(i,a^{(t)})}{\partial a_k}\right]^{2w-1}}{\sum_{i=1}^{N} \left[\frac{\partial f(i,a^{(t)})}{\partial a_k}\right]^{2w} \frac{1}{y_i}}$$

We have implemented the non-symmetrical semi-empirical peak shape function. It contains the symmetrical Gaussian as well as non-symmetrical terms:

$$f(i,a) = \sum_{i=1}^{M} A(j) \left\{ exp\left[\frac{-(i-p(j))^2}{2\sigma^2}\right] + \frac{1}{2}T.exp\left[\frac{(i-p(j))}{B\sigma}\right].erfc\left[\frac{(i-p(j))}{\sigma} + \frac{1}{2B}\right] + \frac{1}{2}S.erfc\left[\frac{(i-p(j))}{\sigma}\right] \right\}$$

where T, S are relative amplitudes and B is a slope.

Detailed description of the algorithm is given in [13].

The fitting function implementing the algorithm without matrix inversion has the form of

```
char* Fit1Awmi(float *source,
        TSpectrumOneDimFit *p,
        int size);
```

This function fits the source spectrum. The calling program should fill in the input parameters of the one\_dim\_fit structure. The fitted parameters are written into structure pointed by one\_dim\_fit structure pointer and fitted data are written into source spectrum.

Function parameters:

- source: pointer to the vector of the source spectrum
- p: pointer to the one\_dim\_fit structure pointer
- **size**: length of the source spectrum

The one\_dim\_fit structure has the form of

class TSpectrumOneDimFit{

public:

```
int number_of_peaks; // input parameter, should be >0
int number_of_iterations; // input parameter, should be >0
int xmin; // first fitted channel
int xmax; // last fitted channel
double alpha; // convergence coefficient, input parameter, it should be a positive number and
double chi; // here the function returns the resulting chi-square
int statistic_type; // type of statistics, possible values are:
```

};

```
// FIT1_OPTIM_CHI_COUNTS (chi square statistics with counts as weighting coeffic
                          // FIT1_OPTIM_CHI_FUNC_VALUES (chi square statistics with function values as wei
                          // FIT1 OPTIM MAX LIKELIHOOD
                          // optimization of convergence coefficients, possible values are:
int alpha_optim;
                          // FIT1_ALPHA_HALVING,
                          // FIT1_ALPHA_OPTIMAL
                          // possible values FIT1_FIT_POWER2,4,6,8,10,12
int power;
                          // order of Taylor expansion, possible values
int fit_taylor;
                          // FIT1_TAYLOR_ORDER_FIRST, FIT1_TAYLOR_ORDER_SECOND
double position_init[MAX_NUMBER_OF_PEAKS1]; // initial values of peaks positions, input parameters
double position_calc[MAX_NUMBER_OF_PEAKS1]; // calculated values of fitted positions, output parameters
double position_err[MAX_NUMBER_OF_PEAKS1]; // position errors
                                           // logical vector which allows to fix appropriate positions (m
bool fix_position[MAX_NUMBER_OF_PEAKS1];
double amp_init[MAX_NUMBER_OF_PEAKS1];
                                            // initial values of peaks amplitudes, input parameters
                                           // calculated values of fitted amplitudes, output parameters
double amp_calc[MAX_NUMBER_OF_PEAKS1];
double amp_err[MAX_NUMBER_OF_PEAKS1];
                                            // amplitude errors
                                            // logical vector, which allows to fix appropriate amplitudes
bool fix_amp[MAX_NUMBER_OF_PEAKS1];;
double area[MAX_NUMBER_OF_PEAKS1];
                                           // calculated areas of peaks
double area_err[MAX_NUMBER_OF_PEAKS1]; // errors of peak areas
double sigma_init; // sigma parameter, see peak shape function
double sigma_calc;
double sigma_err;
bool fix_sigma;
double t_init
                 // t parameter, see peak shape function
double t_calc;
double t_err;
bool fix_t;
                 // b parameter, see peak shape function
double b_init
double b_calc;
double b_err;
bool fix_b;
                 // s parameter, see peak shape function
double s_init;
double s_calc;
double s_err;
bool fix_s;
double a0 init;
                 // background is estimated as a0+a1*x+a2*x*x
double a0_calc;
double a0_err;
bool fix_a0;
double a1_init;
double a1_calc;
double a1_err;
bool fix_a1;
double a2_init;
double a2_calc;
double a2_err;
bool fix_a2;
```

As an example we present a simple 1-dimensional synthetic spectrum with 5 peaks. The fit (obtained using above-given awmi fitting function) is given in Figure 5.1. The chi-square achieved in this fit was 0.76873. The input value of the fit (positions of peaks and their amplitudes) were estimated using peak searching function.

Let us go to a more complicated fit with a lot of overlapping peaks as in Figure 5.2. The initial positions of peaks were determined from original data, using peak searching function. The fit is not very good, as there are some peaks missing.

However, in order to analyze the spectrum, we can proceed in a completely different way employing the sophisticated functions of background elimination and deconvolution. First, let us remove background from the original raw data. We get spectrum given in Figure 5.3.



Figure 5.1: Fit obtained using above given awmi fitting function



Figure 5.2: More complicated fit with lot of overlapping peaks



Figure 5.3: Removed background from the original raw data

Then we can apply the Gold deconvolution function to these data. We obtain the result presented in Figure 5.4.

Using peaks searching method, looking just for local maxima, (sigma=0) with appropriate threshold (threshold=50), we can estimate initial positions of peaks for the fitting function. After the fit of the original experimental spectrum (with background), we obtain the result shown in Figure 5.5. Now the fitted function corresponds much better to the experimental values.

We have also implemented the fitting function with matrix inversion based on Stiefel-Hestens method of the solution of the system of linear equations. The form of the function is as follows:

This function fits the source spectrum. The calling program should fill in the input parameters of the one\_dim\_fit structure. The fitted parameters are written into structure pointed by one\_dim\_fit structure pointer and fitted data are written into source spectrum.

Function parameters:

- source: pointer to the vector of the source spectrum
- p: pointer to the one\_dim\_fit structure pointer
- size: length of the source spectrum

The structure one\_dim\_fit is the same as in awmi function. The parameters power, fit\_taylor, are not applicable for this function.

The results for small number of fitted parameters are the same as with awmi function. However, it converges faster. The example for data given in Figure 5.1 is given in the following table:

# of iterations	Chi awmi	Chi-Stiefel
1	924	89.042
5	773.15	0.96242
10	38.13	0.77041

Chi awmi	Chi-Stiefel
0.90293	0.76873
0.76886	0.76873
0.76873	0.76873
	Chi awmi 0.90293 0.76886 0.76873

### 5.2 2-DIMENSIONAL SPECTRA

It is straightforward that for two-dimensional spectra one can write

$$\Delta a_k^{(t+1)} = \alpha^{(t)} \frac{\sum_{i_1=1}^{N_1} \sum_{i_2=1}^{N_2} \frac{e_{i_1,i_2}^{(t)}}{y_{i_1,i_2}} \frac{\partial f(i_1,i_2,a^{(t)})}{\partial a_k}}{\sum_{i_1=1}^{N_1} \sum_{i_2=1}^{N_2} \left[\frac{\partial f(i_1,i_2,a^{(t)})}{\partial a_k}\right]^2 \frac{1}{y_{i_1,i_2}}}$$

In a similar way, for two-dimensional peaks we have chosen the peak shape function of the following form:

$$f(i_1, i_2, a) = \sum_{j=1}^M \left\{ \begin{array}{l} A_{xy}(j)exp\left\{ -\frac{1}{2(1-\rho^2)} \left[ \frac{(i_1-p_x(j))^2}{\sigma_x^2} - \frac{2\rho(i_1-p_x(j))(i_2-p_y(j))}{\sigma_x\sigma_y} + \frac{(i_2-p_y(j))^2}{\sigma_y^2} \right] \right\} \\ +A_x(j)exp\left[ -\frac{(i_1-p_{x_1}(j))^2}{2\sigma_x^2} \right] + A_y(j)exp\left[ -\frac{(i_2-p_{y_1}(j))^2}{2\sigma_y^2} \right] \end{array} \right\} \\ + b_0 + b_1i_1 + b_2i_2 + b_0 + b_0 + b_1i_1 + b_2i_2 + b_0 + b$$

The meaning of the parameters is similar to 1-dimensional case. Again, all the details can be found in [13].

The fitting function implementing the algorithm without matrix inversion for 2-dimensional data has the form of

```
char* Fit2Awmi(float **source,
        TSpectrumTwoDimFit* p,
        int sizex,
        int sizey);
```

This function fits the source spectrum. The calling program should fill in the input parameters of the two\_dim\_fit structure. The fitted parameters are written into the structure pointed by two\_dim\_fit structure pointer and fitted data are written back into the source spectrum.

Function parameters:

- **source**: pointer to the matrix of the source spectrum
- p: pointer to the two\_dim\_fit structure pointer, see manual
- **sizex**: length x of the source spectrum
- sizey: length y of the source spectrum

The two\_dim\_fit structure has the form of

```
class TSpectrumTwoDimFit{
```

```
public:
```

<pre>int number_of_peaks;</pre>	// input parameter, should be>0
<pre>int number_of_iterations;</pre>	// input parameter, should be >0
<pre>int xmin;</pre>	// first fitted channel in x direction
<pre>int xmax;</pre>	// last fitted channel in x direction
<pre>int ymin;</pre>	// first fitted channel in y direction
<pre>int ymax;</pre>	// last fitted channel in y direction
double alpha;	// convergence coefficient, input parameter, it should be a positive number and
double chi;	// here the function returns resulting chi square
<pre>int statistic_type;</pre>	<pre>// type of statistics, possible values are:</pre>
	// FIT2_OPTIM_CHI_COUNTS (chi square statistics with counts as weighting coefficients)
	// FIT2_OPTIM_CHI_FUNC_VALUES (chi square statistics with function values as we
	// FIT2_OPTIM_MAX_LIKELIHOOD
<pre>int alpha_optim;</pre>	<pre>// optimization of convergence coefficients, possible values are:</pre>
	// FIT2 ALPHA HALVING, FIT2 ALPHA OPTIMAL



Figure 5.4: Gold deconvolution function applied to the data



Figure 5.5: Fit of the original experimental spectrum (with background)

CHAPTER 5. FITTING

```
// possible values are: FIT21_FIT_POWER2,4,6,8,10,12
int power;
int fit_taylor;
                          // order of Taylor expansion, possible values are:
                          // FIT2 TAYLOR ORDER FIRST,
                          // FIT2 TAYLOR ORDER SECOND
double position_init_x[MAX_NUMBER_OF_PEAKS2]; // initial values of x positions of 2D peaks, input paramet
double position_calc_x[MAX_NUMBER_OF_PEAKS2]; // calculated values of fitted x positions of 2D peaks, or
                                               // x position errors of 2D peaks
double position_err_x[MAX_NUMBER_OF_PEAKS2];
bool fix_position_x[MAX_NUMBER_OF_PEAKS2];
                                               // logical vector which allows to fix the appropriate x pos
double position_init_y[MAX_NUMBER_OF_PEAKS2]; // initial values of y positions of 2D peaks, input paramet
double position_calc_y[MAX_NUMBER_OF_PEAKS2]; // calculated values of fitted y positions of 2D peaks, out
double position_err_y[MAX_NUMBER_OF_PEAKS2];
                                               // y position errors of 2D peaks
bool fix_position_y[MAX_NUMBER_OF_PEAKS2];
                                               // logical vector which allows to fix the appropriate y pos
double position_init_x1[MAX_NUMBER_OF_PEAKS2]; // initial values of x positions of 1D ridges, input param
double position_calc_x1[MAX_NUMBER_OF_PEAKS2]; // calculated values of fitted x positions of 1D ridges, or
                                              // x position errors of 1D ridges
double position_err_x1[MAX_NUMBER_OF_PEAKS2];
                                               // logical vector which allows to fix appropriate x position
bool fix_position_x1[MAX_NUMBER_OF_PEAKS2];
double position_init_y1[MAX_NUMBER_OF_PEAKS2]; // initial values of y positions of 1D ridges, input parameters
double position_calc_y1[MAX_NUMBER_OF_PEAKS2]; // calculated values of fitted y positions of 1D ridges, or
double position_err_y1[MAX_NUMBER_OF_PEAKS2]; // y position errors of 1D ridges
bool fix position y1[MAX NUMBER OF PEAKS2];
                                               // logical vector which allows to fix the appropriate y pos
double amp_init[MAX_NUMBER_OF_PEAKS2];
                                               // initial values of 2D peaks amplitudes, input parameters
                                               // calculated values of fitted amplitudes of 2D peaks, outp
double amp_calc[MAX_NUMBER_OF_PEAKS2];
double amp_err[MAX_NUMBER_OF_PEAKS2];
                                               // amplitude errors of 2D peaks
bool fix_amp[MAX_NUMBER_OF_PEAKS2];
                                               // logical vector which allows to fix appropriate amplitude
                                               // initial values of 1D ridges amplitudes, input parameters
double amp_init_x1[MAX_NUMBER_OF_PEAKS2];
double amp_calc_x1[MAX_NUMBER_OF_PEAKS2];
                                               // calculated values of fitted amplitudes of 1D ridges, out
double amp_err_x1[MAX_NUMBER_OF_PEAKS2];
                                               // amplitude errors of 1D ridges
bool fix_amp_x1[MAX_NUMBER_OF_PEAKS2];
                                               // logical vector which allows to fix the appropriate ampli
                                               // initial values of 1D ridges amplitudes, input parameters
double amp_init_y1[MAX_NUMBER_OF_PEAKS2];
double amp_calc_y1[MAX_NUMBER_OF_PEAKS2];
                                               // calculated values of fitted amplitudes of 1D ridges, out
double amp_err_y1[MAX_NUMBER_OF_PEAKS2];
                                               // amplitude errors of 1D ridges
bool fix_amp_y1[MAX_NUMBER_OF_PEAKS2];
                                               // logical vector which allows to fix the appropriate ampli
double volume[MAX_NUMBER_OF_PEAKS1];
                                               // calculated volumes of peaks
double volume_err[MAX_NUMBER_OF_PEAKS1];
                                               // errors of peak volumes
                                               // sigma x parameter
double sigma_init_x;
double sigma_calc_x;
double sigma_err_x;
bool fix_sigma_x;
double sigma_init_y;
                                               // sigma y parameter
double sigma_calc_y;
double sigma_err_y;
bool fix_sigma_y;
                                               // correlation coefficient
double ro_init;
double ro_calc;
double ro_err;
bool fix_ro;
double txy_init;
                                               // t parameter for 2D peaks
double txy_calc;
double txy_err;
bool fix_txy;
double sxy_init;
                                               // s parameter for 2D peaks
double sxy_calc;
double sxy_err;
bool fix sxy;
                                               // t parameter for 1D ridges (x direction)
double tx_init;
double tx_calc;
double tx_err;
bool fix_tx;
double ty_init;
                                               // t parameter for 1D ridges (y direction)
```

```
double ty_calc;
   double ty_err;
   bool fix ty;
   double sx_init;
                                                   // s parameter for 1D ridges (x direction)
   double sx_calc;
   double sx_err;
   bool fix_sx;
                                                   // s parameter for 1D ridges (y direction)
   double sy_init;
   double sy_calc;
   double sy_err;
   bool fix_sy;
                                                   // b parameter for 1D ridges (x direction)
   double bx_init;
   double bx_calc;
   double bx_err;
   bool fix_bx;
                                                   // b parameter for 1D ridges (y direction)
   double by_init;
   double by_calc;
   double by_err;
   bool fix_by;
   double a0 init;
                                                   // background is estimated as a0+ax*x+ay*y
   double a0_calc;
   double a0_err;
   bool fix_a0;
   double ax_init;
   double ax_calc;
   double ax_err;
   bool fix_ax;
   double ay_init;
   double ay_calc;
   double ay_err;
   bool fix_ay;
}:
```

The example of the original spectrum and the fitted spectrum is given in Figures 5.6 and 5.7, respectively. We have fitted 5 peaks. Each peak was represented by 7 parameters, which together with sigmax, sigmay and b0 resulted in 38 parameters. The chi-square after 1000 iterations was 0.6571.

The awmi algorithm can also be applied to large blocks of data and large number of peaks. In the next example we present spectrum with identified 295 peaks. Each peak is represented by 7 parameters, which together with sigmax, y and b0 resulted in 2068 fitted parameters. The original spectrum and fitted function are given in Figures 5.8 and 5.9, respectively. The obtained chi-square was 0.76732.

We have implemented the fitting function with matrix inversion based on Stiefel-Hestens method of the solution of the system of linear equations also for 2-dimensional data. The form of the function is as follows

```
char* Fit2Stiefel(float **source,
        TSpectrumTwoDimFit* p,
        int sizex,
        int sizey);
```

This function fits the source spectrum. The calling program should fill in the input parameters of the two\_dim\_fit structure. The fitted parameters are written into structure pointed by two\_dim\_fit structure pointer and fitted data are written back into the source spectrum.

Function parameters:

- **source**: pointer to the matrix of the source spectrum
- p: pointer to the two\_dim\_fit structure pointer, see manual
- **sizex**: length x of the source spectrum
- **sizey**: length y of the source spectrum

The structure  $two_dim_fit$  is the same as in the awmi function. The parameters power,  $fit_taylor$  are not applicable for this function



Figure 5.6: 2-dimensional Cosine transform



Figure 5.7: Fitted spectrum



Figure 5.8: Original spectrum



Figure 5.9: Fitted function

# of iterations	Chi awmi	Chi-Stiefel
1	24.989	10.415
5	20.546	1.0553
10	6.256	0.84383
50	1.0985	0.64297
100	0.6571	0.64297
500	0.65194	0.64297

The results for small number of fitted parameters are the same as with awmi function. However, it converges faster. The example for data given in Figure 5.6 (38 parameters) is presented in the following table:

Again, Stiefel-Hestens method converges faster. However, its calculation is for this number of parameters takes approximately 3 times longer. For larger number of parameters the time needed to calculate the inversion grows with the cube of the number of fitted parameters. For example, the fit of large number of parameters (2068) for data in Figure 5.8 using awmi algorithm took about 12 hours (using 450 MHz PC). The calculation using matrix inversion method is not realizable in any reasonable time.

## Chapter 6

## TRANSFORMS

### 6.1 1-DIMENSIONAL SPECTRA

Orthogonal transforms can be successfully used for the processing of nuclear spectra. They can be used to remove high frequency noise, to increase signal-to-background ratio as well as to enhance low intensity components [14]. We have implemented also the function for the calculation of the commonly used orthogonal transforms:

- Haar
- Walsh
- Cos
- Sin
- Fourier
- Hartley

Between these transform one can define so called generalized mixed transforms that are also implemented in the transform function:

- Fourier-Haar
- Fourier-Walsh
- Walsh-Haar
- Cos-Walsh
- Cos-Haar
- Sin-Walsh
- Sin-Haar

The suitability of the application of appropriate transform depends on the character of the data, i.e., on the shape of dominant components contained in the data. The form of the transform function is as follows:

```
char *Transform1(const float *source,
        float *dest,
        int size,
        int type,
        int direction,
        int degree);
```

This function transforms the source spectrum. The calling program should fill in the input parameters. Transformed data are written into the dest spectrum.

- **source**: pointer to the vector of the source spectrum, its length should be equal to the **size** parameter except for inverse FOURIER, FOUR-WALSH, FOUR-HAAR transform. These need 2\*size length to supply real and imaginary coefficients
- **dest**: pointer to the vector of the dest data, its length should be equal to the size parameter except for direct FOURIER, FOUR-WALSh, FOUR-HAAR. These need 2\*size length to store real and imaginary coefficients
- size: basic length of the source and dest spectra
- type: type of transform

- TRANSFORM1\_HAAR
- TRANSFORM1\_WALSH
- TRANSFORM1\_COS
- TRANSFORM1\_SIN
- TRANSFORM1\_FOURIER
- TRANSFORM1\_HARTLEY
- TRANSFORM1\_FOURIER\_WALSH
- TRANSFORM1\_FOURIER\_HAAR
- TRANSFORM1\_WALSH\_HAAR
- TRANSFORM1\_COS\_WALSH
- TRANSFORM1\_COS\_HAAR
- TRANSFORM1\_SIN\_WALSH
- TRANSFORM1\_SIN\_HAAR
- direction: transform direction (forward, inverse)
  - TRANSFORM1\_FORWARD
  - TRANSFORM1\_INVERSE
- degree: applies only for mixed transforms

Let us illustrate the applications of the transform using an example. In Figure 6.1 we have spectrum with many peaks, complicated background and high level of noise.



Figure 6.1: Spectrum with many peaks

In Figures 6.2, 6.3, 6.4 we present this spectrum transformed using Haar, Walsh and Cosine transforms, respectively.

Haar transforms (Figure 6.2) creates clusters of data. These coefficients can be analyzed and then filtered, enhanced, etc. On the other hand, the Walsh transform (Figure 6.3) concentrates the dominant components near zero of the coordinate system. It is more suitable to process data of a rectangular shape (e.g., in the field of digital signal processing). Finally, Cosine transform concentrates in the best way the transform coefficients to the beginning of the coordinate system. From the point of view of the variance distribution, it is sometimes called suboptimal. One can notice that approximately one half of the coefficients are negligible. This fact can be used to the compression purposes (in two- or more dimensional data), filtering (smoothing), etc.

We have implemented several application functions exploiting the properties of the orthogonal transforms. Let us start with zonal filtration function. It has the following form:



Figure 6.2: Spectrum transformed using Haar transform



Figure 6.3: Spectrum transformed using Walsh transform



Figure 6.4: Spectrum transformed using Cosine transform

```
char *Filter1Zonal(const float *source,
```

```
float *dest,
int size,
int type,
int degree,
int xmin,
int xmax,
float filter_coeff);
```

This function transforms the source spectrum. The calling program should fill in the input parameters. Then it sets transformed coefficients in the given region (xmin, xmax) to the given filter\_coeff and transforms it back. Filtered data are written into the dest spectrum.

- source: pointer to the vector of the source spectrum, its length should be equal to size
- dest: pointer to the vector of dest data, its length should be equal to size
- size: basic length of the source and dest spectra
- type: type of transform
  - TRANSFORM1\_HAAR
  - TRANSFORM1\_WALSH
  - TRANSFORM1\_COS
  - TRANSFORM1\_SIN
  - TRANSFORM1\_FOURIER
  - TRANSFORM1\_HARTLEY
  - TRANSFORM1\_FOURIER\_WALSH
  - TRANSFORM1\_FOURIER\_HAAR
  - TRANSFORM1\_WALSH\_HAAR
  - TRANSFORM1\_COS\_WALSH
  - TRANSFORM1\_COS\_HAAR
  - TRANSFORM1\_SIN\_WALSH
  - TRANSFORM1\_SIN\_HAAR

- degree: applied only for mixed transforms
- **xmin**: low limit of filtered region
- **xmax**: high limit of filtered region
- filter\_coeff: value which is set in filtered region

An example of the filtration using Cosine transform is given in the Figure 6.5. It illustrates a part of the spectrum from Figure 6.1 and two spectra after filtration preserving 2048 coefficients and 1536 coefficients. One can observe a very good fidelity of the overall shape of both spectra with the original data. However, some distortion can be observed in details of the second spectrum after filtration preserving only 1536 coefficients. The useful information in the transform domain can be compressed into one half of the original space.



Figure 6.5: Filtration using Cosine transform

In the transform domain one can also enhance (multiply with the constant > 1) some regions. This way, one can change peak-to-background ratio. This function has a form of

```
char *Enhance1(const float *source,
    float *dest,
    int size,
    int type,
    int degree,
    int xmin,
    int xmax,
    float enhance_coeff);
```

This function transforms the source spectrum. The calling program should fill in the input parameters. Then it multiplies transformed coefficients in the given region (xmin, xmax) by the given enhance\_coeff and transforms it back. Processed data are written into the dest spectrum.

- source: pointer to the vector of the source spectrum, its length should be equal to size
- dest: pointer to the vector of the dest data, its length should be equal to size
- **size**: basic length of the source and dest spectra
- type: type of transform
  - TRANSFORM1\_HAAR

- TRANSFORM1\_WALSH
- TRANSFORM1\_COS
- TRANSFORM1\_SIN
- TRANSFORM1\_FOURIER
- TRANSFORM1\_HARTLEY
- TRANSFORM1\_FOURIER\_WALSH
- TRANSFORM1\_FOURIER\_HAAR
- TRANSFORM1\_WALSH\_HAAR
- TRANSFORM1\_COS\_WALSH
- TRANSFORM1\_COS\_HAAR
- TRANSFORM1\_SIN\_WALSH
- TRANSFORM1\_SIN\_HAAR
- degree: applied only for mixed transforms
- **xmin**: low limit of filtered region
- **xmax**: high limit of filtered region
- enhance\_coeff: value by which the filtered region is multiplied

An example of enhancement of the coefficients from region 380-800 by the constant 2 in the Cosine transform domain is given in the Figure 6.6. The determination of the region is a matter of analysis in the appropriate transform domain. We assumed that low frequency components are placed in the low coefficients. As it can be observed, the enhancement changes the peak-to-background ratio.



Figure 6.6: Enhancement of the coefficients from region 380-800 by the constant 2 in the Cosine transform domain

### 6.2 2-DIMENSIONAL SPECTRA

Similarly to 1-dimensional data, we have implemented the transforms also for 2-dimensional data. Besides the classic orthogonal transforms like

- Haar
- Walsh
- Cos
- Sin

- Fourier
- Hartley
- Fourier-Haar
- Fourier-Walsh
- Walsh-Haar
- Cos-Walsh
- Cos-Haar
- Sin-Walsh
- Sin-Haar

```
char *Transform2(const float **source,
```

```
float **dest,
int sizex,
int sizey,
int type,
int direction,
int degree);
```

This function transforms the source spectrum. The calling program should fill in the input parameters. Transformed data are written into the dest spectrum.

Function parameters:

- source: pointer to the matrix of the source spectrum, its size should be sizex\*sizey except for inverse FOURIER, FOUR-WALSH, FOUR-HAAR transform. These need sizex\*2\*sizey length to supply real and imaginary coefficients.
- dest: pointer to the matrix of destination data, its size should be sizex\*sizey except for direct FOURIER, FOUR-WALSh, FOUR-HAAR. These need sizex\*2\*sizey length to store real and imaginary coefficients
- **sizex, sizey**: basic dimensions of the source and dest spectra
- **type**: type of transform
  - TRANSFORM2\_HAAR
  - TRANSFORM2\_WALSH
  - TRANSFORM2\_COS
  - TRANSFORM2\_SIN
  - TRANSFORM2\_FOURIER
  - TRANSFORM2\_HARTLEY
  - TRANSFORM2\_FOURIER\_WALSH
  - TRANSFORM2\_FOURIER\_HAAR
  - TRANSFORM2\_WALSH\_HAAR
  - TRANSFORM2\_COS\_WALSH
  - TRANSFORM2\_COS\_HAAR
  - TRANSFORM2\_SIN\_WALSH
  - TRANSFORM2\_SIN\_HAAR
- direction: transform direction (forward, inverse)
- degree: applies only for mixed transforms

An example of the 2-dimensional Cosine transform of data from Figure 5.6 is given in Figure 6.7. One can notice that the data are concentrated again around the beginning of the coordinate system. This allows to apply filtration, enhancement and compression techniques in the transform domain.

In some cases, when the spectrum is smooth, the cosine transforms are very efficient. In Figures 6.8, 6.9 we show original spectrum and transformed coefficients using Cosine transform, respectively.

Similarly to 1-dimensional case we have also implemented the functions for zonal filtration, Gauss filtration and enhancement. The zonal filtration function using classic transforms has the form of



Figure 6.7: 2-dimensional Cosine transform of data from Figure 5.6



Figure 6.8: Original spectrum



Figure 6.9: Transformed coefficients using Cosine transform

int ymin, int ymax, float filter\_coeff);

This function transforms the source spectrum. The calling program should fill in the input parameters. Then it sets transformed coefficients in the given region to the given filter\_coeff and transforms it back. Filtered data are written into the dest spectrum.

- source: pointer to the matrix of source spectrum, its size should be sizex\*sizey
- dest: pointer to the matrix of destination data, its size should be sizex\*sizey
- sizex, sizey: basic dimensions of source and dest spectra
- **type**: type of transform:
  - TRANSFORM2\_HAAR
  - TRANSFORM2\_WALSH
  - TRANSFORM2\_COS
  - TRANSFORM2\_SIN
  - TRANSFORM2 FOURIER
  - TRANSFORM2\_HARTLEY
  - TRANSFORM2\_FOURIER\_WALSH
  - TRANSFORM2\_FOURIER\_HAAR
  - TRANSFORM2\_WALSH\_HAAR
  - TRANSFORM2\_COS\_WALSH
  - TRANSFORM2\_COS\_HAAR
  - TRANSFORM2\_SIN\_WALSH
  - TRANSFORM2\_SIN\_HAAR
- degree: applies only for mixed transforms
- **xmin**: low limit x of filtered region
- **xmax**: high limit x of filtered region
- ymin: low limit y of filtered region
- ymax: high limit y of filtered region

• filter\_coeff: value which is set in filtered region

The enhancement function using transforms has a form of

```
char *Enhance2(const float **source,
    float **dest,
    int sizex,
    int sizey,
    int type,
    int degree,
    int xmin,
    int xmax,
    int ymin,
    int ymax,
    float enhance_coeff);
```

This function transforms the source spectrum. The calling program should fill in the input parameters. Then it multiplies transformed coefficients in the given region by the given enhance\_coeff and transforms it back.

- source: pointer to the matrix of the source spectrum, its size should be sizex\*sizey
- dest: pointer to the matrix of the destination data, its size should be sizex\*sizey
- **sizex, sizey**: basic dimensions of the source and dest spectra
- **type**: type of transform
  - TRANSFORM2\_HAAR
  - TRANSFORM2\_WALSH
  - TRANSFORM2\_COS
  - TRANSFORM2\_SIN
  - TRANSFORM2\_FOURIER
  - TRANSFORM2\_HARTLEY
  - TRANSFORM2\_FOURIER\_WALSH
  - TRANSFORM2\_FOURIER\_HAAR
  - TRANSFORM2\_WALSH\_HAAR
  - TRANSFORM2\_COS\_WALSH
  - TRANSFORM2\_COS\_HAAR
  - TRANSFORM2\_SIN\_WALSH
  - TRANSFORM2\_SIN\_HAAR
- degree: applies only for mixed transforms
- **xmin**: low limit x of filtered region
- **xmax**: high limit x of filtered region
- ymin: low limit y of filtered region
- ymax: high limit y of filtered region
- enhance\_coeff: value which is set in filtered region

### Chapter 7

struct one\_dim\_pic {

## VISUALIZATION

#### 7.1 1-DIMENSIONAL SPECTRA

The 1-dimensional visualization function displays spectrum (or its part) on the Canvas of a form. Before calling the function, one has to fill in the one\_dim\_pic structure containing all parameters of the display. The function has a form of

```
char *display1(struct one_dim_pic* p);
```

This function displays the source spectrum on Canvas. All parameters are grouped in one\_dim\_pic structure. Before calling the display1 function, the structure should be filled in and the address of one\_dim\_pic should be passed as a parameter to display1 function. The meaning of the appropriate parameters is apparent from description of one\_dim\_pic structure. The constants, which can be used for appropriate parameters, are defined in procfunc.h header file.

```
float *source; // spectrum to be displayed
TCanvas *Canvas; // Canvas where the spectrum will be displayed
int size; // size of source spectrum
int xmin; // x-starting channel of spectrum
int xmax; // x-end channel of spectrum
int ymin; // base counts
int ymax; // count full scale
int bx1; // position of picture on Canvas, min x
int bx2; // position of picture on Canvas, max x
int by1; // position of picture on Canvas, min y
int by2; // position of picture on Canvas, max y
                    // spectrum display mode (points, polyline, bars, rainbow, steps, bezier)
int display_mode;
int y scale;
                     // y scale (linear, log, sqrt)
int levels;
                     // # of color levels for rainbow display mode, it does not apply
                     // for other display modes
float rainbow1_step; // determines the first color component step for neighboring
                     // color levels, applies only for rainbow display mode
float rainbow2 step; // determines the second component color step for
                     // neighboring color levels, applies only for rainbow display mode
float rainbow3_step; // determines the third component color step for
                     // neighboring color levels, applies only for rainbow display mode
int color_alg; // applies only for rainbow display mode (rqb smooth algorithm, rqb
               // modulo color component, cmy smooth algorithm, cmy modulo color
               // component, cie smooth algorithm, cie modulo color component, yig
               // smooth algorithm, yig modulo color component, hsv smooth
```

// algorithm, hsv modulo color component [15]

```
int bar thickness;
                            // applies only for bar display mode
int bar empty flag;
                            // (empty bars, full bars) applies only for bar display mode
int border_color;
                            // color of background of the picture
int full_border;
                            // decides whether background is painted
                            // decides whether the axes and rasters are shown
int raster_en_dis;
int raster_long;
                            // decides whether the rasters are drawn as long lines
                            // color of the rasters
int raster_color;
char *raster_description_x; // x axis description
char *raster_description_y; // y axis description
int pen_color; // color of spectrum
int pen_dash; // style of pen
int pen width; // width of line
int chanmark_style; // style of channel marks
int chanmark_width; // width of channel marks
int chanmark_height; // height of channel marks
int chanmark en dis; // decides whether the channel marks are shown
int chanmark color; // color of channel marks
// auxiliary variables, transform coefficients, for internal use only
double mx;
double my;
double px;
double py;
// auxiliary internal variables, working place
double gbezx,gbezy;
TPoint bz[4];
```

The examples using different display parameters are shown in the next few Figures.

### 7.2 2-DIMENSIONAL SPECTRA

The 2-dimensional visualization function displays spectrum (or its part) on the Canvas of a form. Before calling the function, one has to fill in the two\_dim\_pic structure containing all parameters of the display. The function has a form of

```
char *display2(struct two_dim_pic* p);
```

This function displays the source two-dimensional spectrum on Canvas. All parameters are grouped in the two\_dim\_pic structure. Before calling the display2 function, the structure should be filled in and the address of two\_dim\_pic should be passed as a parameter to display2 function. The meaning of corresponding parameters is apparent from the description of one\_dim\_pic structure. The constants, which can be used for appropriate parameters, are defined in the procfunc.h header file.

```
struct two_dim_pic {
```

<pre>float **source;</pre>	// source spectrum to be displayed
TCanvas *Canvas;	// Canvas where the spectrum will be displayed
<pre>int sizex;</pre>	// x-size of source spectrum
<pre>int sizey;</pre>	// y-size of source spectrum
<pre>int xmin;</pre>	// x-starting channel of spectrum
<pre>int xmax;</pre>	// x-end channel of spectrum
<pre>int ymin;</pre>	// y-starting channel of spectrum
<pre>int ymax;</pre>	// y-end channel of spectrum

}:



Figure 7.1: Display mode -polyline, width of pen=3



Figure 7.2: Display mode- bars, shown channel marks



Figure 7.3: Display mode- steps, log scale, shown channel marks



Figure 7.4: Display mode -Bezier curve interpolation, shown channel marks



Figure 7.5: Display mode- rainbow bars, color algorithm (model) RGB, number of color levels=1024, pen width=3



Figure 7.6: Display mode-empty bars, color algorithm YIQ, number of color levels 2048

<pre>int zmin;</pre>	// base counts
int zmax;	// counts full scale
<pre>int bx1;</pre>	// position of picture on Canvas, min x
<pre>int bx2;</pre>	// position of picture on Canvas, max x
<pre>int by1;</pre>	// position of picture on Canvas, min y
<pre>int by2;</pre>	// position of picture on Canvas, max y
<pre>int mode_group;</pre>	// display mode algorithm group (simple modes-
	// PICTURE2_MUDE_GRUUP_SIMPLE, modes with shading
	// accoraing to light-PICIOREZ_MUDE_GRUUP_LIGHI, modes with
	// Shauing according to channels counts-
	// shading according to light and to channels counts-
	// PICTURE2 MODE GROUP LIGHT HEIGHT)
int displav mode:	// spectrum display mode (points. grid. contours. bars. x lines.
,,,,,	// y lines, bars x, bars y, needles, surface, triangles)
<pre>int z_scale;</pre>	// z scale (linear, log, sqrt)
int nodesx;	// number of nodes in x dimension of grid
<pre>int nodesy;</pre>	// number of nodes in y dimension of grid
<pre>int count_reg;</pre>	// width between contours, applies only for contours display mode
<pre>int alfa;</pre>	// angles of display,alfa+beta must be less or equal to 90, alpha- angle
	// between base line of Canvas and left lower edge of picture picture
	// base plane
int beta;	// angle between base line of Canvas and right lower edge of picture base plane
int view_angle;	// rotation angle of the view, it can be 0, 90, 180, 270 degrees
int levels;	// # of color levels for rainbowed display modes, it does not apply for
floot mainhaul story	// simple aisplay modes algorithm group
<pre>iloat fainbowi_step;</pre>	// determines the just component step for neighbouring color
	// for simple display modes algorithm aroun
<pre>float rainbow2 step:</pre>	// determines the second component step for neighboring
11000 101100 #2_000p;	// color levels. applies only for rainbowed display modes. it does not
	// apply for simple display modes algorithm group
<pre>float rainbow3_step;</pre>	// determines the third component step for neighboring
	// color levels, applies only for rainbowed display modes, it does not
	// apply for simple display modes algorithm group
<pre>int color_alg;</pre>	// applies only for rainbowed display modes (rgb smooth algorithm,
	// rgb modulo color component, cmy smooth algorithm, cmy modulo
	// color component, cie smooth algorithm, cie modulo color component,
	// yiq smooth algorithm, yiq modulo color component, hsv smooth
	// algorithm, hsv modulo color component, it does not apply for simple
float 1 h woight.	// aisplay modes algoriling group [15]
110at 1_11_weight,	// according to channels counts annlies only for
	// PICTURE2 MODE GROUP LIGHT HEIGHT modes aroun
int xlight:	// x position of fictive light source. applies only for rainbowed display
,	<pre>// modes with shading according to light</pre>
<pre>int ylight;</pre>	// y position of fictive light source, applies only for rainbowed display
	// modes with shading according to light
<pre>int zlight;</pre>	// z position of fictive light source, applies only for rainbowed display
	// modes with shading according to light
<pre>int shadow;</pre>	// determines whether shadow will be drawn (no shadow, shadow),
	// for rainbowed display modes with shading according to light
<pre>int shading;</pre>	// determines whether the picture will shaded, smoothed (no shading,
	// shading), for rainbowed display modes only
<pre>int bezier;</pre>	// determines Bezier interpolation (applies only for simple display
int hander erler	// moaes group for gria, x_lines, y_lines display modes)
int full border:	// color of oackground of the picture
int raster on dis:	// decides whether the resters are shown
THO TABUEL_EH_UID,	// WEELWES WIEELIEL LIE INSTELS WIE SILUMI
```
// decides whether the rasters are drawn as long lines
 int raster_long;
                                        // color of the rasters
int raster_color;
char *raster description x; // x axis description
char *raster_description_y; // y axis description
char *raster_description_z; // z axis description
char *raster_description_z; // z axis description
int pen_color; // color of spectrum
int pen_dash; // style of pen
int pen_width; // width of line
int chanmark_en_dis; // decides whether the channel marks are shown
int chanmark_style; // style of channel marks
int chanmark_width; // width of channel marks
int chanmark_height; // height of channel marks
int chanmark_color; // color of channel marks
int chanline_en_dis; // decides whether the channel lines (grid) are shown
// auxiliary variables, transformation coefficients for internal use only
double kx;
double ky;
double mxx;
double mxy;
double myx;
double myy;
double txx;
double txy;
double tyx;
double tyy;
double tyz;
double vx;
double vy;
double nu_sli;
// auxiliary internal variables, working place
double z,zeq,gbezx,gbezy,dxspline,dyspline;
 int xt,yt,xs,ys,xe,ye,priamka,z_preset_value;
unsigned short obal[MAXIMUM_XSCREEN_RESOLUTION];
unsigned short obal_cont[MAXIMUM_XSCREEN_RESOLUTION];
TPoint bz[4];
```

## };

The examples using different display parameters are shown in the next few Figures.



Figure 7.7: Display mode-bars, pen width=2



Figure 7.8: Display mode-triangles, log scale



Figure 7.9: Display mode-contours



Figure 7.10: Display mode surface shading according to height



Figure 7.11: Display mode-surface shading according to light point



Figure 7.12: Display mode-surface shading according to height+light position with ratio 50:50, CMY color model



Figure 7.13: Display mode bars shaded according to height



Figure 7.14: Display mode- surface shading according to light position with shadows



Figure 7.15: Display mode- surface shading according to height with 10 levels of contours



Figure 7.16: Display mode- surface shading according to height, sqrt scale, channel marks and lines shown



Figure 7.17: Display mode- surface shading according to height-contours, rasters allowing to localize interesting parts are shown.

## Chapter 8

## References

[1] M. Morháč, J. Kliman, V. Matoušek, M. Veselský, I. Turzo.: Background elimination methods for multidimensional gamma-ray spectra. NIM, A401 (1997) 113-132.

[2] C. G Ryan et al.: SNIP, a statistics-sensitive background treatment for the quantitative analysis of PIXE spectra in geoscience applications. NIM, B34 (1988), 396-402.

[3] D. D. Burgess, R. J. Tervo: Background estimation for gamma-ray spectroscopy. NIM 214 (1983), 431-434.

[4] M. Morháč, J. Kliman, V. Matoušek, M. Veselský, I. Turzo.:Identification of peaks in multidimensional coincidence gamma-ray spectra. NIM, A443 (2000) 108-125.

[5] M.A. Mariscotti: A method for identification of peaks in the presence of background and its application to spectrum analysis. NIM 50 (1967), 309-320.

[6] Z.K. Silagadze, A new algorithm for automatic photopeak searches. NIM A 376 (1996), 451.

[7] P. Bandžuch, M. Morháč, J. Krištiak: Study of the VanCitter and Gold iterative methods of deconvolution and their application in the deconvolution of experimental spectra of positron annihilation, NIM A 384 (1997) 506-515.

[8] M. Morháč, J. Kliman, V. Matoušek, M. Veselský, I. Turzo.: Efficient one- and two-dimensional Gold deconvolution and its application to gamma-ray spectra decomposition. NIM, A401 (1997) 385-408.

[9] I. A. Slavic: Nonlinear least-squares fitting without matrix inversion applied to complex Gaussian spectra analysis. NIM 134 (1976) 285-289.

[10] B. Mihaila: Analysis of complex gamma spectra, Rom. Jorn. Phys., Vol. 39, No. 2, (1994), 139-148.

[11] T. Awaya: A new method for curve fitting to the data with low statistics not using chi-square method. NIM 165 (1979) 317-323.

[12] T. Hauschild, M. Jentschel: Comparison of maximum likelihood estimation and chi-square statistics applied to counting experiments. NIM A 457 (2001) 384-401.

[13] M. Morháč, J. Kliman, M. Jandel, E. Krupa, V. Matoušek: Study of fitting algorithms applied to simultaneous analysis of large number of peaks in γ-ray spectra. Applied Spectroscopy, Vol. 57, No. 7 (2003) 753-760.

[14] C.V. Hampton, B. Lian, Wm. C. McHarris: Fast-Fourier-transform spectral enhancement techniques for gamma-ray spectroscopy. NIM A353 (1994) 280-284.

[15] D. Hearn, M. P. Baker: Computer Graphics, Prentice-Hall International, Inc., 1994.