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MULTIDIMENSIONAL FFT BASED POSITIVE DEFINITE GOLD DECONVOLUTION ALGORITHM

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The paper presents a multidimensional positive definite Gold deconvolution algorithm. A new version of the algorithm with optimization based on FFT convolution has been derived. It allows to decrease the computational complexity of its implementation and thus to make its realization possible for higher dimensions and resolutions.

K e y w o r d s: Gold deconvolution algorithm, multidimensional signal processing, FFT based convolutions, resolution improvement

1 INTRODUCTION

Recently, deconvolution algorithms have found many applications in various domains of digital signal processing and experimental science. From the numerical point of view, deconvolution belongs to one of the most critical problems. It is a so-called ill-posed problem, which means that many different functions solve the convolution equation within the allowed error bounds. The estimates of the solution are extremely sensitive to errors in the input data. Very frequently the noise present in the input data causes enormous oscillations in the result after deconvolution. Deconvolution methods can be classified from two aspects:

- quality of the deconvolved signal (smoothness, positive definite solution, oscillation, *etc*),
- computational complexity.

A method that gives very good results for positive definite input data is the Gold deconvolution algorithm [1, 2]. Starting with the positive definite initial solution the method always gives non- negative results. Thus it is suitable to be applied to process data being naturally positive definite (images, histograms, *etc*).

On the other hand, from the computational point of view the Gold deconvolution is a time- consuming operation. This problem is becoming relevant for big sizes of data and multidimensional data where the number of operations grows exponentially with sizes.

Hence the aim of the paper is to derive an efficient positive definite Gold deconvolution algorithm with a minimized number of numerical operations. Optimization is based on FFT.

2 PRINCIPLE OF THE GOLD DECONVOLUTION ALGORITHM

The relation between the input and output signals of a discrete linear time-invariant system can be described by convolution sums. For one-, two-, and n-dimensional systems one can write

$$y_1(i_1) = \sum_{k_1=0}^{N_1-1} h_1(i_1-k_1)x_1(k_1)\,;\; i_1 = 0,1,\ldots,2N_1-2\,, \tag{1}$$

$$y_2(i_1,i_2) = \sum_{k_1=0}^{N_1-1}\sum_{k_2=0}^{N_2-1} h_2(i_1-k_1,i_2-k_2)x_2(k_1,k_2)\,; \quad i_1 \in \langle 0,2N_1-2\rangle,\; i_2 \in \langle 0,2N_2-2\rangle\,, \tag{2}$$

$$\vdots$$

$$y_n(i_1,i_2,\ldots,i_n) = \sum_{k_1=0}^{N_1-1}\sum_{k_2=0}^{N_2-1}\cdots\sum_{k_n=0}^{N_n-1} h_n(i_1-k_1,\ldots,i_n-k_n)x_n(k_1,\ldots,k_n)\,; \quad i_j \in \langle 0,2N_j-2\rangle, j \in \langle 1,n\rangle\,. \tag{3}$$

We assume the knowledge of the impulse response function $h_n(k_1,\ldots,k_n)$ (resolution instrumental function) and the output data y_n. The impulse response function is supposed to have finite lengths in all dimensions. It implies that $h_j(i_1,\ldots,i_j) = 0$ for $i_k < 0$ and for $i_k \geq N_k$, $k \in \langle 1,j\rangle$. Without loss of generality we shall assume the same length of both impulse responses and the input data. During the deconvolution we are looking for a positive definite solution of the overdetermined systems of the linear equations (1), (2), and (3).

Using the matrix notation, one-dimensional system of linear equations (1) can be expressed as

$$\begin{bmatrix} y_1(0) & y_1(1) & \ldots & y_1(2N_1-2)\end{bmatrix}^\top = \begin{bmatrix} h_1(0) & 0 & 0 & \ldots \\ h_1(1) & h_1(0) & 0 & \ldots \\ h_1(2) & h_1(1) & h_1(0) & \ldots \\ \vdots & \vdots & \vdots & \\ h_1(N_1-1) & h_1(N_1-2) & h_1(N_1-3) & \ldots \\ 0 & h_1(N_1-1) & h_1(N_1-2) & \ldots \\ 0 & 0 & h_1(N_1-1) & \ldots \\ \vdots & \vdots & \vdots & \end{bmatrix} \begin{bmatrix} x_1(0) \\ x_1(1) \\ \\ \vdots \\ x_1(N_1-1) \end{bmatrix} \tag{4}$$

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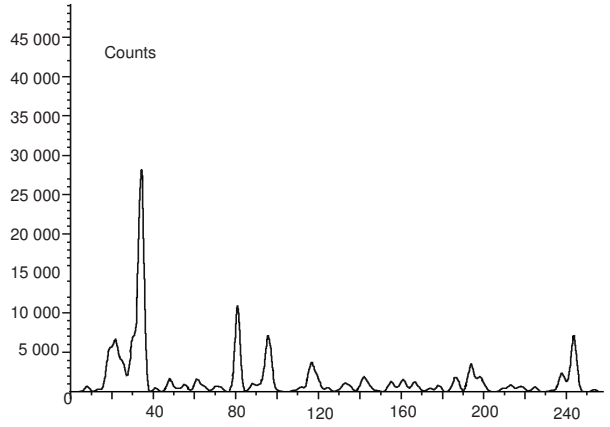

Fig. 1. The original one-dimensional γ-ray spectrum.

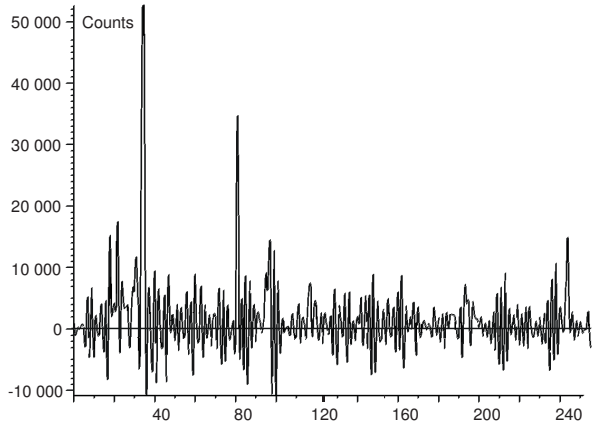

Fig. 2. The spectrum obtained after deconvolution by direct solving the Toeplitz system of linear equations.

or

$$\boldsymbol{y} = \mathbf{H}\boldsymbol{x}\,. \tag{5}$$

It means that the columns of $\mathbf{H}$ are represented by response vectors $\boldsymbol{h}$ mutually shifted by one position.

The positive definite solution of the overdetermined system of the linear equations (5), (6) can be obtained by employing of the Gold deconvolution algorithm that represents a specific form of the Van Cittert algorithm. As the Van Cittert algorithm is described in detail in [3, 4], we describe it only briefly. Its general form for a discrete system is

$$\boldsymbol{x}^{(k+1)} = \boldsymbol{x}^{(k)} + \mu\big(\boldsymbol{y} - \mathbf{T}\boldsymbol{x}^{(k)}\big)\,, \tag{6}$$

where k is the iteration number and μ is the relaxation factor. Multiplying both sides of (5) by $\mathbf{H}^\top$ we get

$$\mathbf{H}^\top\boldsymbol{y} = \mathbf{H}^\top\mathbf{H}\boldsymbol{x} \tag{7}$$

or

$$\boldsymbol{z} = \mathbf{T}\boldsymbol{x}\,. \tag{8}$$

Matrix $\mathbf{T} = \mathbf{H}^\top\mathbf{H}$ is a symmetrical Toeplitz matrix [4, 5]. The system of linear equations (8) is a discrete form of the Fredholm integral equation of the first kind that is often extremely ill-conditioned [6]. Vector $\boldsymbol{x}$ calculated by solving the system of linear equations (8) directly is an unconstrained least square estimate. For large systems, where the number of unknowns is of the order of hundreds or thousands (see examples of nuclear spectra in Section 5), this estimate is as a rule ill-conditioned, *ie* , it is extremely sensitive to the errors (noise) present in vector $\boldsymbol{y}$. Very small changes in vector $\boldsymbol{y}$ cause enormous oscillations in estimate $\boldsymbol{x}$. Direct inversion of $\mathbf{T}$ cannot lead to a stable solution. In what follows we replace the direct inversion of $\mathbf{T}$ by the approximate Gold deconvolution algorithm [1].

Substituting (8) into Van Cittert algorithm (6) gives

$$\boldsymbol{x}^{(k+1)} = \boldsymbol{x}^{(k)} + \mu\big(\boldsymbol{z} - \mathbf{T}\boldsymbol{x}^{(k)}\big)\,. \tag{9}$$

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

$$\mu_i = \frac{x^{(k)}(i)}{\sum_{m=0}^{N_1-1} T_{im}x^{(k)}(m)}\,. \tag{10}$$

Further let us define the vector

$$\boldsymbol{d} = \mathbf{T}\cdot\boldsymbol{x}^{(k)}\,. \tag{11}$$

Then substituting (11) into (10) one obtains the Gold deconvolution algorithm [1]:

$$\boldsymbol{x}^{(k+1)}(i) = \frac{z(i)\cdot x^{(k)}(i)}{d(i)}\,,\quad i \in \langle 0.N_1 - 1\rangle\,. \tag{12}$$

If we take the initial solution

$$\boldsymbol{x}^{(0)} = [1\,,\ 1\,,\ldots,\ 1]^\top\,, \tag{13}$$

then for all $k = 1, 2, 3, \ldots$ we always obtain positive definite solutions of the convolution system (4). It converges to the least square estimate in the constrained subspace of positive solutions. It is worth noticing that if all elements in vectors $\boldsymbol{h}$, $\boldsymbol{y}$ are positive and assuming the initial solution (13), estimates $\boldsymbol{x}^{(k+1)}$ are always positive.

3 ALGORITHM OF OPTIMIZED ONE–DIMENSIONAL GOLD DECONVOLUTION

Let us start with the Toeplitz system (7), (8). The elements of vector $\boldsymbol{z}$ can be expressed as:

$$z(i) = \sum_{j=0}^{N_i-1} y(i+j)h(j)\,,\quad i \in \langle 0, N_1 - 1\rangle\,.$$

Matrix $\mathbf{T}$ is the symmetrical Toeplitz matrix

$$\mathbf{T} = \begin{bmatrix} t(0) & t(1) & t(2) & \dots & t(N_1-1) \\ t(1) & t(0) & t(1) & \dots & t(N_1-2) \\ t(2) & t(1) & t(0) & \dots & t(N_1-3) \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ t(N_1-1) & t(N_1-2) & t(N_1-3) & \dots & t(0) \end{bmatrix}, \tag{14}$$

where

$$t(i) = \sum_{j=0}^{N_1-1-i} h(j)h(i+j)\,, \quad i \in \langle 0, N_1-1\rangle\,. \tag{15}$$

Let us extend matrix $\mathbf{T}$ to the $2N_1 \times 2N_1$ cyclic convolution matrix $\mathbf{C}$

$$\mathbf{C} = \begin{bmatrix} \mathbf{T} & \vdots & \mathbf{S} \\ \dots\dots\dots & & \\ \mathbf{S} & \vdots & \mathbf{T} \end{bmatrix}, \tag{16}$$

where

$$\mathbf{S} = \begin{bmatrix} 0 & t(N_1-1) & \dots & t(1) \\ t(N_1-1) & 0 & \dots & t(2) \\ t(N_1-2) & t(N_1-1) & \dots & t(3) \\ \vdots & \vdots & \vdots & \vdots \\ t(2) & t(3) & \dots & t(N_1-1) \\ t(1) & t(2) & \dots & 0 \end{bmatrix}. \tag{17}$$

Further, let us extend vector $\boldsymbol{x}$ by adding zeroes to vector $\boldsymbol{v}$ of length $2N_1$

$$\boldsymbol{v} = \big[\, x(0), x(1), \dots, x(N-1), \vdots\, 0, 0, \dots, 0 \,\big]^\top. \tag{18}$$

Obviously the multiplication of the cyclic convolution matrix $\mathbf{C}$ by vector $\boldsymbol{v}$ can be in the Fourier domain expressed by multiplication of the appropriate Fourier coefficients so that

$$d(i) = \mathrm{FFT}_i^{-1}\big(\mathrm{FFT}_j(\boldsymbol{c}) \cdot \mathrm{FFT}_j(\boldsymbol{v})\big)\,, \quad i \in \langle 0, N_1-1\rangle\,,\ j \in \langle 0, 2N_1-1\rangle\,, \tag{19}$$

where the cyclic symmetrical vector $\boldsymbol{c}$ is the first column of matrix $\mathbf{C}$

$$\boldsymbol{c} = \big[\, t(0), t(1), \dots, t(N-1), \vdots\, 0, t(N-1), t(N-2) \dots, t(2), t(1) \,\big]^\top \tag{20}$$

of the length $2N_1$. FFT( ) and FFT^{-1}( ) operators represent the direct and inverse discrete Fourier transform of the length $2N_1$, respectively. We assumed N_1 to be a power of 2.

Now when looking back at the Gold deconvolution (11), (12), one can observe that the most time consuming operation that must be calculated in every iteration step is the matrix vector multiplication (11) with the number of arithmetic operations proportional to N_1^2. By using the above-described algorithm and by employing the fast Fourier transform it can be decreased to $4N_1 \log_2 2N_1 + 2N_1$. Then the algorithm of one-dimensional Gold deconvolution can be defined as follows.

Algorithm A

a. Calculate vector $\boldsymbol{z}$ of length N_1 using (13). In principle here one can employ also FFT. However, this calculation is to be done only once and thus it is not time critical.
b. Calculate vector $\boldsymbol{t}$ of length N_1 using (15).
c. Create vector $\boldsymbol{x}^{(0)}$ of length $2N_1$
$\boldsymbol{x}^{(0)} = \big[\, 1, 1, \dots, 1, \vdots\, 0, 0, \dots, 0 \,\big]$.
d. Create vector $\boldsymbol{c}$ of length $2N_1$ according to (20) and calculate its FFT. As $\boldsymbol{c}$ is a cyclic symmetrical vector, $\mathrm{FFT}(\boldsymbol{c})$ is a cyclic symmetrical vector of real coefficients.
e. Set $k = 0$.
f. Calculate FFT of vector $\boldsymbol{x}^{(k)}$ of length $2N_1$.
g. Calculate the elements of vector $\boldsymbol{d}$ (length $2N_1$) using (19).
h. Using (12) calculate new solution $\boldsymbol{x}^{(k+1)}$.
i. $k = k + 1$.
j. If k is less than the preset number of iterations, continue in step f.

4 FFT–BASED N–DIMENSIONAL GOLD DECONVOLUTION ALGORITHM

Let us continue with two-dimensional signals. Analogously to (12) one can write

$$x_2^{(k+1)}(i_1, i_2) = \frac{z(i_1, i_2) \cdot x_2^{(k)}(i_1, i_2)}{d(i_1, i_2)}\,. \tag{21}$$

Also relations (13), (15) turn now to be

$$z(i_1, i_2) = \sum_{j_1=0}^{N_1-1} \sum_{j_2=0}^{N_2-1} h_2(i_1, i_2) y_2(i_1+j_1, i_2+j_2)\,, \tag{22}$$

$$t(i_1, i_2) = \sum_{j_1=0}^{N_1-1-i_1} \sum_{j_2=0}^{N_2-1-i_2} h_2(j_1, j_2) h_2(i_1+j_1, i_2+j_2)\,, \tag{23}$$

where $i_1 \in \langle 0, N_1-1\rangle$, $i_2 \in \langle 0, N_2-1\rangle$. Then the symmetrical two-dimensional array $\boldsymbol{c}$ analogously to (20) is

$$\boldsymbol{c} = \begin{bmatrix} \mathbf{T}_{11} & \vdots & \mathbf{T}_{12} \\ \dots\dots\dots\dots & & \\ \mathbf{T}_{21} & \vdots & \mathbf{T}_{22} \end{bmatrix}, \tag{24}$$

where

$$\mathbf{T}_{11} = \begin{bmatrix} t(0,0) & t(0,1) & \dots & t(0,N_2-1) \\ t(1,0) & t(1,1) & \dots & t(1,N_2-1) \\ \vdots & \vdots & \ddots & \vdots \\ t(N_1-1,0) & t(N_1-1,1) & \dots & t(N_1-1,N_2-1) \end{bmatrix},$$

$$\mathbf{T}_{12} = \begin{bmatrix} 0 & t(0,N_2-1) & t(0,N_2-2) & \dots & t(0,1) \\ 0 & t(1,N_2-1) & t(1,N_2-2) & \dots & t(1,1) \\ \vdots & \vdots & \ddots & \vdots & \\ 0 & t(N_1-1,N_2-1) & t(N_1-1,N_2-2) & \dots & t(N_1-1,1) \end{bmatrix},$$

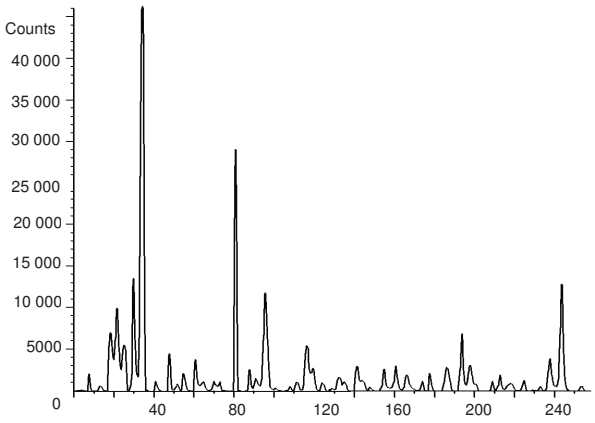

Fig. 3. The spectrum obtained after Gold deconvolution (1000 iterations).

$$\mathbf{T}_{21} = \begin{bmatrix} 0 & 0 & \dots & 0 \\ t(N_1-1,0) & t(N_1-1,1) & \dots & t(N_1-1,N_2-1) \\ t(N_1-2,0) & t(N_1-2,1) & \dots & t(N_1-2,N_2-1) \\ \vdots & \vdots & \ddots & \vdots \\ t(1,0) & t(1,1) & \dots & t(1,N_2-1) \end{bmatrix},$$

$$\mathbf{T}_{22} = \begin{bmatrix} 0 & 0 & 0 & \dots & 0 \\ 0 & t(N_1-1,N_2-1) & t(N_1-1,N_2-2) & \dots & t(N_1-1,1) \\ 0 & t(N_1-2,N_2-1) & t(N_1-2,N_2-2) & \dots & t(N_1-2,1) \\ \vdots & \vdots & \ddots & \vdots & \\ 0 & t(1,N_2-1) & t(1,N_2-2) & \dots & t(1,1) \end{bmatrix}.$$

Then obviously the two-dimensional array can be initialized according to the following algorithm, which is expressed in C language commands.

Algorithm B

```
for(i1=0;i1< 2*N1;i1++){
    for(i2=0;i2< 2*N2;i2++){
        j1=i1, j2=i2;
        if (i1>N1)
        j1=2*N1-i1;
        if (i2>N2)
        j2=2*N2-i2;
        if (i1= =N1 || i2= =N2)
        c [i1][i2]=0;
        else
        c[i1][i2]=t[j1][j2];
    }
}
```

Generalization of the above given relations to an n-dimensional case is straightforward:

$$x_n^{(k+1)}(i_1,i_2,\dots,i_n) = \frac{z(i_1,i_2,\dots,i_n)\cdot x_n^{(k)}(i_1,i_2,\dots,i_n)}{d(i_1,i_2,\dots,i_n)}, \quad (25)$$

$$z(i_1,i_2,\dots,i_n) = \sum_{j_1=0}^{N_1-1}\sum_{j_2=0}^{N_2-1}\cdots\sum_{j_n=0}^{N_n-1} h_n(j_1,j_2,\dots,j_n)y(i_1+j_1,i_2+j_2,\dots,i_n+j_n), \quad (26)$$

$$t(i_1,i_2,\dots,i_n) = \sum_{j_1=0}^{N_1-1-j_1}\sum_{j_2=0}^{N_2-1-j_2}\cdots\sum_{j_n=0}^{N_n-1-j_n} h_n(j_1,j_2,\dots,j_n)h_n(i_1+j_1,i_2+j_2,\dots,i_n+j_n), \quad (27)$$

where $i_m \in \langle 0, n_m\rangle$ and $m = 1,2,\dots,N$. Generalization of algorithm B for initialization of an n-dimensional array $\boldsymbol{c}$ is also straightforward. Then the algorithm of n-dimensional positive definite Gold deconvolution is:

Algorithm C

a. Calculate the n-dimensional array $\boldsymbol{z}$ according to (26).

b. Calculate the n-dimensional array $\boldsymbol{t}$ according to (27).

c. Initialize the n-dimensional array $\boldsymbol{x}^{(0)}$ of the length $2N_1 * 2N_2 * \dots * 2N_n$
$x^{(0)}(i_1,i_2,\dots,i_n)$
$$= \begin{cases} 1 & \text{if } i_1 < N_1 \,\&\, i_2 < N_2 \,\&\, \dots \,\&\, i_n < N_n, \\ 0 & \text{else.} \end{cases}$$

d. Initialize the n-dimensional array $\boldsymbol{c}$ employing the n-dimensional version of the algorithm B and calculate its n-dimensional FFT.

e. Set $k = 0$.

f. Calculate FFT of the array $\boldsymbol{x}$ (length $2N_1 * \dots * 2N_n$).

g. Calculate the elements of the n-dimensional array $\boldsymbol{d}$
$d(i_1,i_2,\dots,i_n) =$
$$\mathrm{FFT}^{-1}_{i_1,i_2,\dots,i_n}\big(\mathrm{FFT}_{i_1,i_2,\dots,i_n}(\boldsymbol{c})\cdot\mathrm{FFT}_{i_1,i_2,\dots,i_n}(\boldsymbol{x})\big)$$
where $i_m \in \langle 0, N_m - 1\rangle$ and $j_m \in \langle 0, 2N_m - 1\rangle$, $m = 1,2,\dots,n$.

h. Using (25) calculate new solution $\boldsymbol{x}^{(k+1)}$.

i. $k = k + 1$.

j. If k is less than the preset number of iterations, continue in step f.

5 ILLUSTRATIVE EXAMPLES

The algorithms of optimized positive definite Gold deconvolution described so far have been used to process γ-ray nuclear spectra. The γ-ray spectra are very complex due to the enormous number of isotopes produced in spontaneous fission. Peaks in the spectra are frequently positioned very close to each other. They are overlapping. The resolution in the spectra can be improved by employing the Gold deconvolution algorithm. Figure 1 presents the original one-dimensional γ-ray spectrum.

When we solve directly the Toeplitz system of linear equations, we obtain the unconstrained solution shown in Fig. 2.

The spectrum (histogram) contains unrealistic negative values. It oscillates and such a result is practically

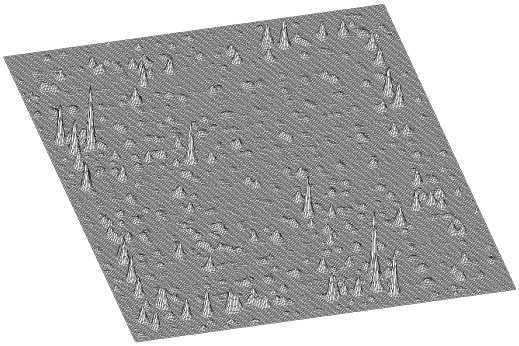

Fig. 4. Two-dimensional γ-ray spectrum (256×256 points).

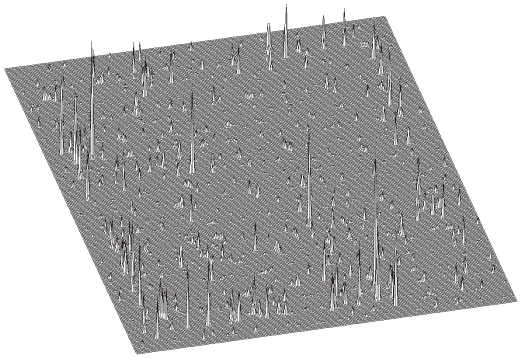

Fig. 5. The same spectrum after the Gold deconvolution (200 iterations).

worthless. Due to relations (7), (8), (11), (12) if all elements of the input (initial estimate), the output and the response vectors are positive, the estimated vectors are always non-negative. Therefore, when we employ the above-described Gold deconvolution (1000 iterations) we obtain the result constrained to the subspace of non-negative values (Fig. 3). The method unfolds multiplets. It preserves the peak positions and the peak areas. It even discovers peaks whose existence in the original spectrum is indistinct.

The above-presented optimization of the deconvolution algorithm permitted its implementation for two and three dimensional coincidence nuclear spectra. Figure 4 shows two-dimensional γ-ray spectrum (256×256 points). The result after the Gold deconvolution (200 iterations) is shown in Fig. 5. Apparently the method improves the resolution. It unfolds spatial doublets and multiplets.

6 CONCLUSIONS

The paper presents a multidimensional Gold deconvolution algorithm with numerical optimization based on an FFT convolution algorithm. In principle the operation of convolution in the denominators of relations (12), (21) can be carried out by employing any fast convolution algorithm (see *eg* [7]). In a multidimensional case the method proposed in the paper decreases the number of operations (multiplications and additions) to calculate the matrix vector product from $\left(\prod_{i=1}^{N} N_i\right)^2$ to $\prod_{i=1}^{n}(4N_i \log_2 2N_i + 2N_i$. Starting from a positive definite initial solution the Gold deconvolution method always gives a non-negative result. However, its calculation is time- consuming. Hundreds and sometimes thousands of iterations are needed to achieve the required result. Therefore, without optimization the realization of some calculations would be practically impossible.

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