

GATE Simulation study

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ROOT reference

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- There are three references for TSpectrum2.
 - For peak finding
 - “Identification of peaks in multidimensional coincidence γ -ray spectra”
 - For deconvolution
 - “EFFICIENT ONE AND TWO DIMENSIONAL GOLD DECONVOLUTION AND ITS APPLICATION TO γ -RAY SPECTRA DECOMPOSITION”
 - For eliminating background
 - “BACKGROUND ELIMINATION METHODS FOR MULTIDIMENSIONAL COINCIDENCE γ -RAY SPECTRA”
- These are published by Miroslav Morhac (Institute of Physics, Slovak Academy of Sciences)

Identification of peaks in multidimensional coincidence γ -ray spectra (for peak search)



- Study peak search algorithm for photon distribution
- This paper introduces the algorithm for multidimensional spectra measurement.

Introduction

- The progress in the nuclear structure understanding depends on the ability to analyze correctly multidimensional spectra.
- The positions of identified peaks can be fed as initial estimate into peak fitting.
- There are many well-known method of peak search for 1 dimensional spectra, but almost of them cannot be directly extended to search for peaks in multidimensional space.
- The algorithm introduced in this paper is used for especially 2 dimensional spectra. (2-fold coincidence γ -ray peaks)

Peak searching algorithm in 2-dimensional spectra

- Suppose that the number of counts in a 2-dimensional γ -ray spectrum in the channel x, y can be approximated by

$$N(x, y) = G_1(x, y) + G_2(x) + G_3(y) + B + Cx + Dy$$

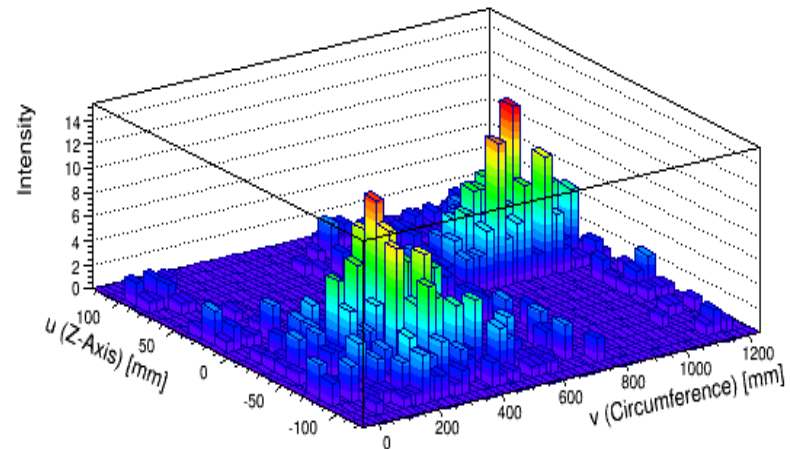
- G_1 is 2-dimensional gauss.

$$G_1(x, y) = A_1 \exp \left\{ -\frac{1}{2(1-\rho^2)} \left[\frac{(x-x_1)^2}{\sigma_{x_1}^2} - \frac{2\rho(x-x_1)(y-y_1)}{\sigma_{x_1}\sigma_{y_1}} + \frac{(y-y_1)^2}{\sigma_{y_1}^2} \right] \right\}$$

- G_2 and G_3 are 1-dimensional gauss.

$$G_{2,3}(\alpha) = A \exp \left\{ -\frac{(\alpha - \alpha_0)^2}{2\sigma_{\alpha_0}^2} \right\}$$

- $B+Cx+Dy$ is the assumed background



Peak searching algorithm in 2-dimensional spectra

- They shall replace the mixed partial second derivatives by the mixed partial second differences in both dimensions.

$$\begin{aligned}
 S(i, j) = & N(i+1, j+1) - 2N(i, j+1) + N(i-1, j+1) \\
 & - 2N(i+1, j) + 4N(i, j) - 2N(i-1, j) \\
 & + N(i+1, j-1) - 2N(i, j-1) + N(i-1, j-1)
 \end{aligned}$$

- In order to eliminate statistical fluctuations, they shall employ the smoothed mixed particle second differences in both dimensions. The smoothing is achieved by summing $S(i, j)$ in a given window

$$S_w(i, j) = \sum_{i_1=i-r}^{i+r} \sum_{j_1=j-r}^{j+r} S(i_1, j_1) \quad w = 2r + 1$$

- This is repeated z times to optimize the S_w . ($S_{z,w}$)

Peak searching algorithm in 2-dimensional spectra

- The contents of the channel i, j of this difference spectrum can be expressed :

$$S_{z,w}(i, j) = \sum_{i_1=i-r}^{i+r} \sum_{j_1=j-r}^{j+r} C_{z,w}(i_1 - i, j_1 - j) N(i_1, j_1) \quad \begin{matrix} r=z \cdot m + 1 \\ m=(w-1)/2 \end{matrix}$$

- Elements of the filter matrix $C_{z,w}(i, j)$ can be factorized to products of vector elements

$$C_{z,w}(i, j) = C_{z,w}(i) \cdot C_{z,w}(j)$$

$$C_{z,w}(i) = \sum_{i_1=i-r}^{i+r} C_{z-1,w}(i_1)$$

- Standard deviation of $S_{z,w}$ is defined as :

$$F_{z,w}(i, j) = \sqrt{\sum_{i_1=i-r}^{i+r} \sum_{j_1=j-r}^{j+r} C_{z,w}^2(i_1 - i) C_{z,w}^2(j_1 - j) N(i_1, j_1)}$$

Peak searching algorithm in 2-dimensional spectra

- Another way to compute the coefficient of the filter vector C

$$C_{\sigma} = \frac{d^2}{dx^2} \exp\left(-\frac{x^2}{2\sigma^2}\right)$$

$$x = i$$

σ : standard deviation
of searched peak

- The choice of these calculations is optional and depends on application.
- In general independently of the way of calculation of the $S_{z,w}$ filter can be expressed :

$$S(i, j) = \sum_{i_1=i-r}^{i+r} \sum_{j_1=j-r}^{j+r} C(i_1 - i)C(j_1 - j)N(i_1, j_1)$$

$$F(i, j) = \sqrt{\sum_{i_1=i-r}^{i+r} \sum_{j_1=j-r}^{j+r} C^2(i_1 - i)C^2(j_1 - j)N(i_1, j_1)}$$

Peak searching algorithm in 2-dimensional spectra

- Example 1

- $G_{1A}(A_{1A}=100, x_{1A}=60, y_{1A}=8),$
 $G_{1B}(A_{1B}=50, x_{1B}=180, y_{1B}=200)$
- $G_{2A}(A_{2A}=200, x_{2A}=60),$
 $G_{2B}(A_{2B}=180, x_{2B}=180)$
- $G_{3A}(A_{3A}=200, x_{3A}=80),$
 $G_{3B}(A_{3B}=500, x_{3B}=200)$
- Background
 - $800 - 1.176x - 1.96y$
- σ was set to 6 and $\rho=0$

$$N(x, y) = G_1(x, y) + G_2(x) + G_3(y) + B + Cx + Dy$$

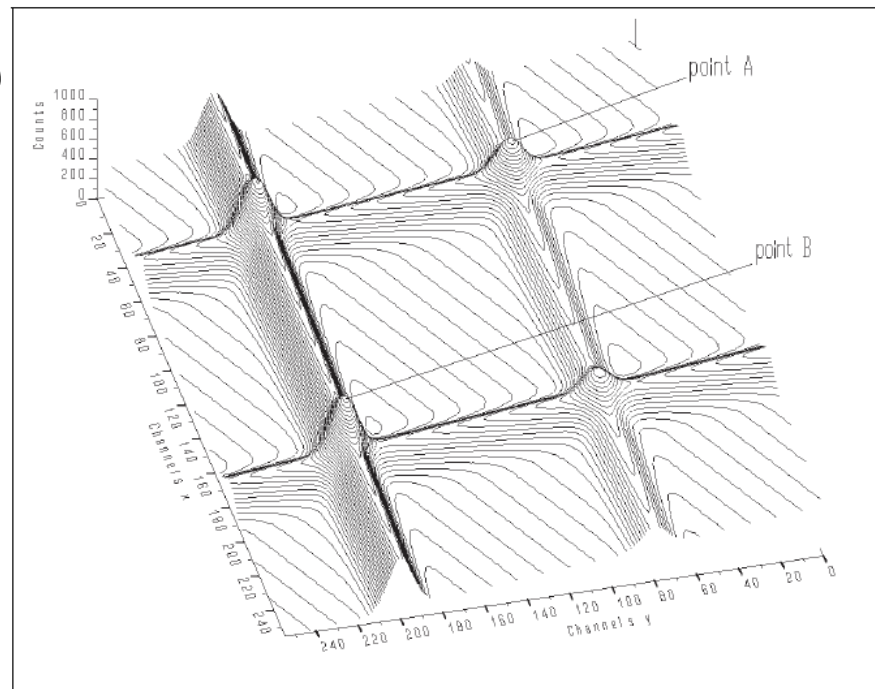


Figure 1: Synthetic spectrum with two two-dimensional Gaussians located at the points A, B

Peak searching algorithm in 2-dimensional spectra

- two free parameters were set to $w=7$ and $z=7$.
- The different spectrum calculated with these are shown following :

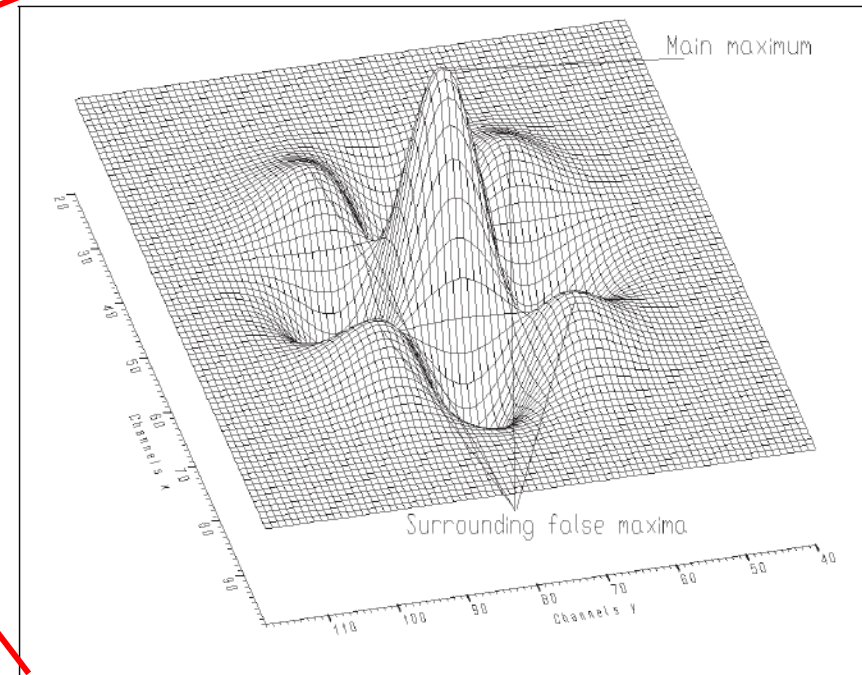
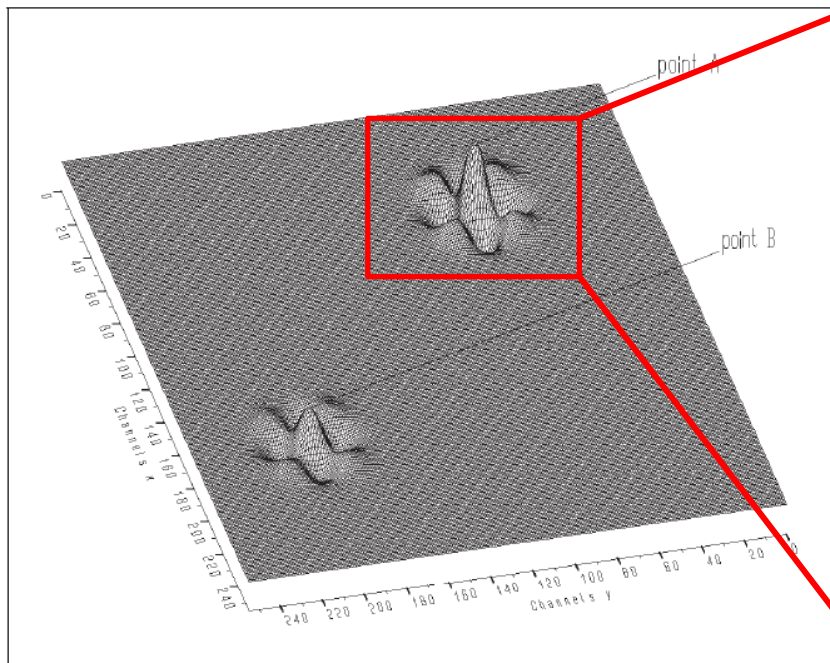


Figure 2: The difference spectrum for the spectrum from Fig. 1

Figure 5: True and false local maxima for the two-dimensional peak

Peak searching algorithm in 2-dimensional spectra

- The position of one of the local maxima located in the middle of the surrounding ones corresponds to the position of two-dimensional peak.
 - true peak (middle peak)
 - false peak (other 4 peaks)
- False peak should be ignored by the searching algorithm

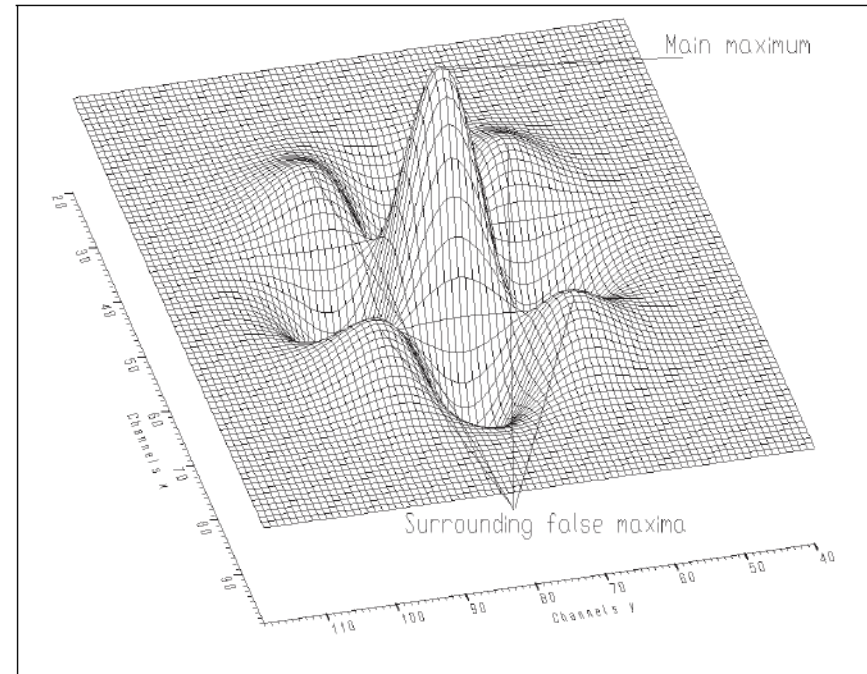


Figure 5: True and false local maxima for the two-dimensional peak

Peak searching algorithm in 2-dimensional spectra

- Example2
 - one peak from experiment of positron annihilation

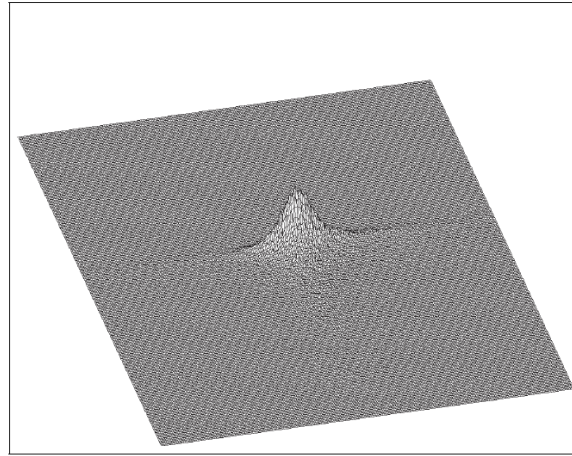


Figure 6: Spectrum with one peak from experiment of positron annihilation

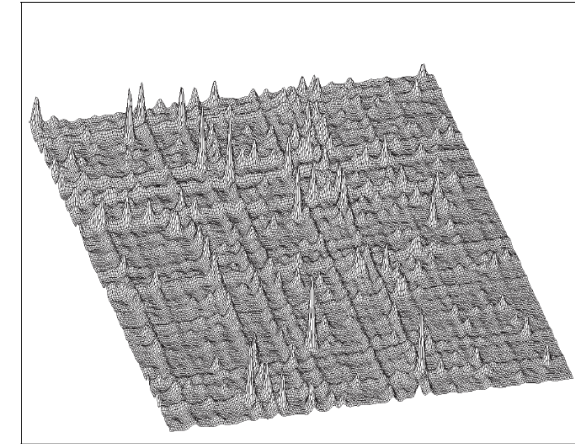


Figure 8: Two-dimensional γ -ray spectrum

- It is impossible to find five maxima in γ -ray spectrum.
- It is needed to suppress in a way the false maxima in the $S_{z,w}$

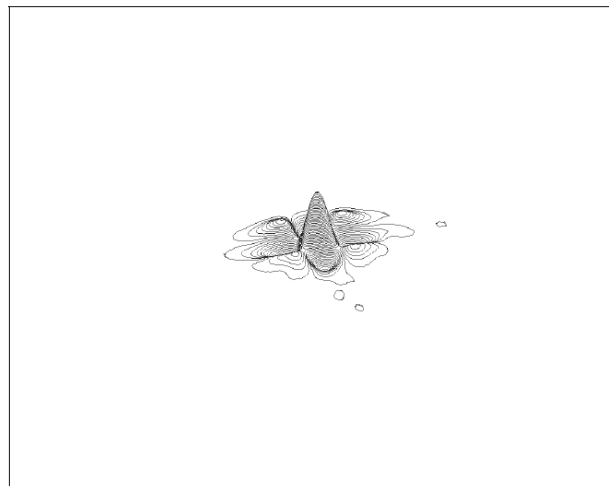


Figure 7: Two-parameter SSD spectrum from Fig. 6

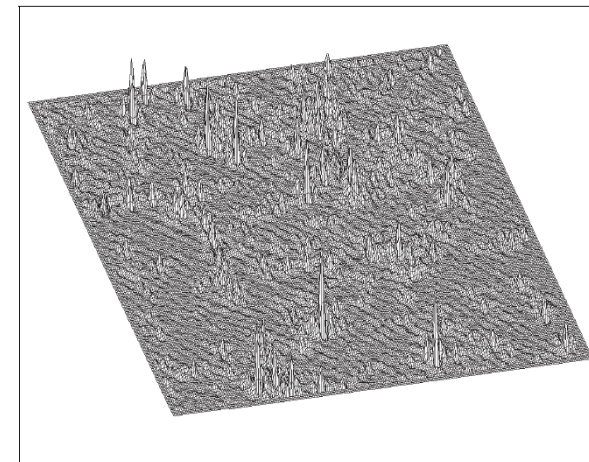


Figure 9: Two-parameter SSD spectrum from Fig. 8

Peak searching algorithm in 2-dimensional spectra

- Define spectra of the one-parameter smoothed $S_{z,w}$ in both x and y independent variables

$$X(i, j) = \sum_{i_1=i-r}^{i+r} C(i_1 - i)N(i_1, j)$$

$$Y(i, j) = \sum_{j_1=j-r}^{j+r} C(j_1 - j)N(i, j_1)$$

- Example
 - $z=w=0$
- From the filters defined in this way we can observe that in the expected position of two-dimensional peak

	$C_s(i, j)$			$C_x(i, j)$			$C_y(i, j)$			
j_1	i_1	$i-1$	i	$i+1$	$i-1$	i	$i+1$	$i-1$	i	$i+1$
$j-1$		1	-2	1	1	-2	1	1	1	1
j		-2	4	-2	1	-2	1	-2	-2	-2
$j+1$		1	-2	1	1	-2	1	1	1	1

Table 1: Examples of the filters $C_s(i, j)$ for $z = w = 0$ according to (10) for two-parameter SSD and $C_x(i), C_y(j)$ for one-parameter SSDs in two-dimensional space.

Peak searching algorithm in 2-dimensional spectra



- In the position of true local maximum of $S(i_p, j_t)$ the following conditions satisfied (S is different from $S_{z,w}$)

$$\underline{S(i_p, j_t) > 0 \text{ and } X(i_p, j_t) < 0 \text{ and } Y(i_p, j_t) < 0}$$

- Along with this condition also the following conditions, saying that in the point X, Y in both dimensions have local minima, must be satisfied

$$\underline{X(i_{t-1}, j_t) \geq X(i_p, j_t) \leq X(i_{t+1}, j_t) < 0}$$

$$\underline{Y(i_p, j_{t-1}) \geq Y(i_p, j_t) \leq Y(i_p, j_{t+1}) < 0}$$

- The above condition is not satisfied in the point of false local maxima

$$\underline{S(i_f, j_f) > 0 \text{ and } (X(i_f, j_f) \geq 0 \text{ or } Y(i_f, j_f) \geq 0)}$$

Peak searching algorithm in 2-dimensional spectra

- Applied the conditions to
figure7

and

figure9

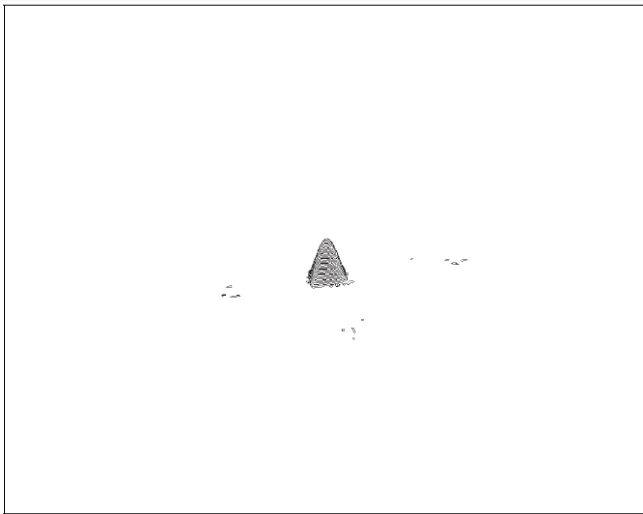


Figure 10: Two-parameter SSD spectrum from Fig. 7 after application of the condition (20)

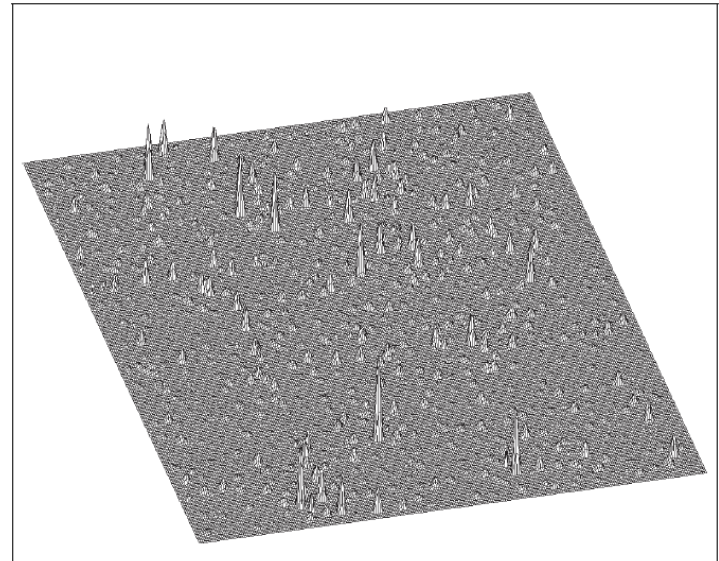


Figure 11: Two-parameter SSD spectrum from Fig. 9 after application of the condition (20)

the algorithm to search for peaks in two-dimensional spectrum is as follows:

Peak searching algorithm in 2-dimensional spectra

- Algorithm

- 1. using $S(i, j) = \sum_{i_1=i-r}^{i+r} \sum_{j_1=j-r}^{j+r} C(i_1-i)C(j_1-j)N(i_1, j_1)$ it calculates spectrum of the smoothed second differences in both dimensions
- 2. using $F(i, j) = \sqrt{\sum_{i_1=i-r}^{i+r} \sum_{j_1=j-r}^{j+r} C^2(i_1-i)C^2(j_1-j)N(i_1, j_1)}$ it calculates spectrum of standard deviation of the smoothed second differences
- 3. for $i \in \langle 0, n_1-1 \rangle, j \in \langle 0, n_2-1 \rangle$, where n_1, n_2 are sizes of the spectrum, we search for local maxima in the spectrum of S
- 4. once it has found a local maximum in the position i_l, j_l then using $X(i, j) = \sum_{i_1=i-r}^{i+r} C(i_1-i)N(i_1, j)$ $Y(i, j) = \sum_{j_1=j-r}^{j+r} C(j_1-j)N(i, j_1)$ it calculates spectra of X, Y respectively. Then applying condition $S(i_l, j_l) > 0$ and $X(i_l, j_l) < 0$ and $Y(i_l, j_l) < 0$ it decides whether the found local maximum is true or false.
- 5. It tests $S(i, j_l), F(i, j_l), i \in \langle 0, n_1-1 \rangle$ for the shape of the peak in x dimension. Likewise it tests y dimension.
- 6. If the shape of the peak in both dimensions satisfied these criteria we have found two-dimensional peak in the position i_l, j_l .
- 7. It repeats the whole procedure for another local maximum from the point 3 on.