

# Package ‘Peaks’

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**Title** Peaks

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**Depends** R (>= 2.5)

**Description** Spectrum manipulation: background estimation, Markov smoothing, deconvolution and peaks search functions. Ported from ROOT/TSpectrum class.

**License** LGPL

**Repository** CRAN

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SpectrumBackground     *Background estimation.*

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### Description

This function calculates background spectrum from source spectrum and separates useful information (peaks) from useless information (background).

### Usage

```
SpectrumBackground(y, iterations=100, decreasing=FALSE, order=c("2", "4", "6", "8"),
  smoothing=FALSE, window=c("3", "5", "7", "9", "11", "13", "15"), compton=FALSE)
```

### Arguments

y	the vector of source spectrum
iterations	maximal width of clipping window
decreasing	direction of change of clipping window. If TRUE the window is decreasing, otherwise the window is increasing.
order	order of clipping filter
smoothing	logical variable whether the smoothing operation in the estimation of background will be included
window	width of smoothing window
compton	logical variable whether the estimation of Compton edge (step-like feature at the peaks positions) will be included

### Details

Method is based on Sensitive Nonlinear Iterative Peak (SNIP) clipping algorithm.

New value in the channel  $i$  is calculated (in the case of second-order clipping filter) with formula:

$$v_p(i) = \min\{v_{p-1}(i), (v_{p-1}(i+p) + v_{p-1}(i-p))/2\}$$

### Value

Numeric vector with background profile.

### Author(s)

Miroslav Morhác

## References

- 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.
- M. Morhác, J. Kliman, V. Matoucek, M. Veselský, I. Turzo.: Background elimination methods for multidimensional gamma-ray spectra. NIM, A401 (1997) 113-132.
- D. D. Burgess, R. J. Tervo: Background estimation for gamma-ray spectroscopy. NIM 214 (1983), 431-434.

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SpectrumDeconvolution *Improvement of the resolution in spectra, decomposition of multiplets*

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## Description

This function is used to strip-off known instrumental function from source spectrum. It is achieved by deconvolution of source spectrum according to response spectrum using Gold or Richardson-Lucy algorithms. Both methods provides less oscillating solutions than Fourier or VanCittert algorithms.

## Usage

```
SpectrumDeconvolution(y,response,iterations=10,repetitions=1,
                      boost=1.0,method=c("Gold","RL"))
```

## Arguments

y	numeric vector of source spectrum
response	vector of response spectrum. Its length should be less or equal the length of y
iterations	number of iterations (parameter L in the Gold deconvolution algorithm) between boosting operations
repetitions	number of repetitions of boosting operations. It must be greater or equal to one. So the total number of iterations is repetitions*iterations
boost	boosting coefficient/exponent. Applies only if repetitions is greater than one. Recommended range [1..2].
method	method selected for deconvolution. Either Gold or Richardson-Lucy

## Details

Both methods search iteratively for solution of deconvolution problem

$$y(i) = \sum_{j=1}^n h(i-j)x(j) + e(i)$$

in the form

$$x^{(k)}(i) = M^{(k)}(i)x^{(k-1)}(i)$$

For Gold method:

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

For Richardson-Lucy:

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

Boosting is the exponentiation of iterated value with boosting coefficient/exponent. It is generally improve stability.

### Value

Numeric vector of the same length as y with deconvoluted spectrum.

### Author(s)

Miroslav Morhác

### References

- Abreu M.C. et al., A four-dimensional deconvolution method to correct NA38 experimental data, NIM A 405 (1998) 139.
- Lucy L.B., A.J. 79 (1974) 745.
- Richardson W.H., J. Opt. Soc. Am. 62 (1972) 55.
- Gold R., ANL-6984, Argonne National Laboratories, Argonne Ill, 1964.
- Coote G.E., Iterative smoothing and deconvolution of one- and two-dimensional elemental distribution data, NIM B 130 (1997) 118.
- M. Morhác, J. Kliman, V. Matousek, M. Veselský, I. Turzo.: Efficient one- and two-dimensional Gold deconvolution and its application to gamma-ray spectra decomposition. NIM, A401 (1997) 385-408.
- Morhác M., Matousek V., Kliman J., Efficient algorithm of multidimensional deconvolution and its application to nuclear data processing, Digital Signal Processing 13 (2003) 144.

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SpectrumSearch	<i>Automatical identification of the peaks in spectrum with the presence of the continuous background and statistical fluctuations - noise</i>
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### Description

This function searches for peaks in source spectrum. It is based on deconvolution method. First the background is removed (if desired), then Markov spectrum is calculated (if desired), then the response function is generated according to given sigma and deconvolution is carried out.

### Usage

```
SpectrumSearch(y, sigma=3.0, threshold=10.0, background=FALSE,  
               iterations=13, markov=FALSE, window=3)
```

### Arguments

y	numeric vector of source spectrum
sigma	sigma of searched peaks
threshold	threshold value in % for selected peaks, peaks with amplitude less than $\text{threshold} \cdot \text{highest\_peak} / 100$ are ignored
background	Remove background. Logical variable, set to TRUE if the removal of background before deconvolution is desired
iterations	number of iterations in deconvolution operation
markov	logical variable, if it is TRUE, first the source spectrum is replaced by new spectrum calculated using Markov chains method.
window	averaging window of searched peaks, applies only for Markov smoothing

### Details

Algorithm is straightforward. The function removes background and smooths (if requested) source vector y, then deconvolves it using Gaussian with sigma as response vector and after that searches for peaks in deconvoluted vector which are above threshold.

### Value

List with two vectors:

y	Deconvoluted source vector
pos	Indexes of found peaks in y spectrum

### Author(s)

Miroslav Morhác

**References**

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.

M. Morhác, J. Kliman, V. Matousek, M. Veselský, I. Turzo.:Identification of peaks in multidimensional coincidence gamma-ray spectra. NIM, A443 (2000) 108-125.

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

**See Also**

[SpectrumSmoothMarkov](#) , [SpectrumBackground](#) , [SpectrumDeconvolution](#)

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SpectrumSmoothMarkov *Suppression of statistical fluctuations with discrete Markov chain.*

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**Description**

This function calculates smoothed spectrum from source spectrum based on Markov chain method.

**Usage**

```
SpectrumSmoothMarkov(y,window=3)
```

**Arguments**

y	numeric vector of source spectrum
window	width of averaging smoothing window

**Details**

The algorithm is based on discrete Markov chain, which has very simple invariant distribution:

$$U_2 = \frac{p_{1,2}}{p_{2,1}} U_1$$

$$U_3 = \frac{p_{2,3}}{p_{3,2}} U_2 U_1$$

$$\dots$$

$$U_n = \frac{p_{n-1,n}}{p_{n,n-1}} U_{n-1} \dots U_2 U_1$$

and  $U_1$  being defined from the normalization condition:

$$\sum_{i=1}^n U_i = 1$$

$n$  is the length of the smoothed spectrum.

The probability of the change of the peak position from channel  $i$  to the channel  $i + 1$  is :

$$p_{i,i\pm 1} = A_i \sum_{k=1}^m \exp\left(\frac{y(i \pm k) - y(i)}{y(i \pm k) + y(i)}\right)$$

where  $A_i$  is the normalization constant so that:

$$p_{i,i-1} + p_{i,i+1} = 1$$

and  $m$  is a width of smoothing window.

**Value**

Numeric vector with smoothed spectrum.

**Author(s)**

Miroslav Morhác

**References**

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

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