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.

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R topics documented:

`SpectrumBackground` *Background estimation.*

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.

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

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 osccillating 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 shold 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.

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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.

SpectrumSearch — *Automatical identification of the peaks in spectrum with the presence of the continuous background and statistical fluctuations - noise*

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 `threshold*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`	averanging 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 responce 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`

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

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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