Package 'MassSpecWavelet'

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Description Processing Mass Spectrometry spectrum by using wavelet based algorithm

License LGPL (>= 2)

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R topics documented:

`MassSpecWavelet-package`

Peak detection of mass spectrum by Wavelet transform based methods

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Description

Process Mass Spectrum (MS) by Wavelet Transforms-based algorithms

Details

Package:	MassSpecWavelet
Type:	Package
Version:	1.0.4
Date:	2007-04-05
License:	GPL 2 or newer

MassSpecWavelet R package is aimed to process Mass Spectrometry (MS) data mainly based on Wavelet Transforms. The current version only supports the peak detection based on Continuous Wavelet Transform (CWT). Future versions will include more functions covering entire MS data processes.

Author(s)

Pan Du, Simon Lin

Maintainer: Pan Du <dupan@northwestern.edu>

References

Du, P., Kibbe, W.A. and Lin, S.M. (2006) Improved peak detection in mass spectrum by incorporating continuous wavelet transform-based pattern matching, Bioinformatics, 22, 2059-2065.

Examples

```
data(exampleMS)
SNR.Th <- 3
peakInfo <- peakDetectionCWT(exampleMS, SNR.Th=SNR.Th)
majorPeakInfo = peakInfo$majorPeakInfo
peakIndex <- majorPeakInfo$peakIndex
plotPeak(exampleMS, peakIndex, main=paste('Identified peaks with SNR >', SNR.Th))
```

cwt *Continuous Wavelet Transform (CWT)*

Description

CWT(Continuous Wavelet Transform) with Mexican Hat wavelet (by default) to match the peaks in Mass Spectrometry spectrum

Usage

```
cwt(ms, scales = 1, wavelet = "mexh")
```

Arguments

ms	Mass Spectrometry spectrum (a vector of MS intensities)
scales	a vector represents the scales at which to perform CWT.
wavelet	The wavelet base, Mexican Hat by default. User can provide wavelet Psi(x) as a form of two row matrix. The first row is the x value, and the second row is Psi(x) corresponding to x.

Value

The return is the 2-D CWT coefficient matrix, with column names as the scale. Each column is the CWT coefficients at that scale.

Author(s)

Pan Du, Simon Lin

Examples

```
data(exampleMS)
scales <- seq(1, 64, 3)
wCoefs <- cwt(exampleMS[5000:11000], scales=scales, wavelet='mexh')

## Plot the 2-D CWT coefficients as image (It may take a while!)
xTickInterval <- 1000
image(5000:11000, scales, wCoefs, col=terrain.colors(256), axes=FALSE, xlab='m/z index', ylab='CWT coefficien
axis(1, at=seq(5000, 11000, by=xTickInterval))
axis(2, at=c(1, seq(10, 64, by=10)))
box()
```

exampleMS *An example mass spectrum*

Description

An example mass spectrum from CAMDA 2006. All-in-1 Protein Standard II (Ciphergen Cat. \# C100-0007) were measured on Ciphergen NP20 chips. There are 7 polypeptides in the sample with m/z values of 7034, 12230, 16951, 29023, 46671, 66433, 147300.

Usage

```
data(exampleMS)
```

Format

A numeric vector represents the mass spectrum with equal sample intervals.

Source

CAMDA, CAMDA 2006 Competition Data Set. 2006, http://camda.duke.edu.

extendLength *Extend the length of a signal or matrix*

Description

Extend the length of a signal or matrix by row

Usage

```
extendLength(x, addLength = NULL, method = c("reflection", "open", "circular"), direction = c("right
```

Arguments

x	a vector or matrix with column with each column as a signal
addLength	the length to be extended
method	three methods available, c("reflection", "open", "circular"). By default, it is "reflection".
direction	three options available: c("right", "left", "both")

Value

return the extended vector or matrix.

Author(s)

Pan Du

See Also

extendNBase

Examples

```
# a = matrix(rnorm(9), 3)
# extendLength(a, 3, direction='right')  ## not exposed function
```

`extendNBase` *Extend the row number of a matrix as the exponential of base N*

Description

Extend the data as the exponential of base N by increasing row number.

Usage

```
extendNBase(x, nLevel=1, base=2, ...)
```

Arguments

`x`	data matrix
`nLevel`	the level of DWT decomposition. Basically, it is equivalent to changing the 'base' as base\^nLevel
`base`	the base, 2 by default
`...`	other parameters of used by `extendLength`

Details

The method 'open' is padding the the matrix with the last row.

Value

Return a extended matrix

Author(s)

Pan Du

See Also

extendLength

Examples

```
# a = matrix(rnorm(9), 3)
# extendNBase(a) ## not exposed function
```

`getLocalMaximumCWT` *Identify the local maximum of each column in 2-D CWT coefficients matrix*

Description

Identify the local maximum of each column in 2-D CWT coefficients matrix by using a slide window. The size of slide window linearly changes from the coarse scale (bigger window size) to detail scale. The scale of CWT increases with the column index.

Usage

```
getLocalMaximumCWT(wCoefs, minWinSize= 5, amp.Th = 0)
```

Arguments

`wCoefs`	2-D CWT coefficients, each column corresponding to CWT coefficient at one scale. The column name is the scale.
`minWinSize`	The minimum slide window size used.
`amp.Th`	The minimum peak amplitude.

Value

return a matrix with same dimension as CWT coefficient matrix, wCoefs. The local maxima are marked as 1, others are 0.

Author(s)

Pan Du

See Also

`localMaximum`

Examples

```
data(exampleMS)
scales <- seq(1, 64, 3)
wCoefs <- cwt(exampleMS[5000:11000], scales=scales, wavelet='mexh')

localMax <- getLocalMaximumCWT(wCoefs)
plotLocalMax(localMax)
```

getRidge *Identify ridges based on the local maximum matrix*

Description

Identify ridges by connecting the local maximum of 2-D CWT coefficients from the coarse scale to detail scale. The local maximum matrix is returned from getLocalMaximumCWT

Usage

```
getRidge(localMax, iInit = ncol(localMax), step = -1, iFinal = 1, minWinSize= 5, gapTh = 3, skip = NUL
```

Arguments

localMax	The local maximum matrix is returned from getLocalMaximumCWT with 1 represents maximum, others are 0.
iInit	The start column to search ridge. By default, it starts from the coarsest scale level.
step	Search step. -1 by default, which means searching from coarse scale to detail scale column by column.
iFinal	The final column index of search ridge.
minWinSize	The minimum slide window size used.
gapTh	The gap allowed during searching for ridge. 3 by default.
skip	The column to be skipped during search.

Value

Return a list of ridge. As some ridges may end at the scale larger than 1, in order to keep the uniqueness of the ridge names, we combined the smallest scale of the ridge and m/z index of the peak at that scale together to name the ridges. For example the ridge name "1_653" means the peak ridge ends at the CWT scale 1 with m/z index 653 at scale 1.

Author(s)

Pan Du, Simon Lin

References

Du, P., Kibbe, W.A. and Lin, S.M. (2006) Improved peak detection in mass spectrum by incorporating continuous wavelet transform-based pattern matching, Bioinformatics, 22, 2059-2065.

See Also

getLocalMaximumCWT, identifyMajorPeaks

Examples

```
data(exampleMS)
scales <- seq(1, 64, 3)
wCoefs <- cwt(exampleMS[5000:11000], scales=scales, wavelet='mexh')

localMax <- getLocalMaximumCWT(wCoefs)
ridgeList <- getRidge(localMax)
plotRidgeList(ridgeList)
```

`getRidgeLength` *Estimate the length of the ridge*

Description

Estimate the length of the ridge line, which is composed of local maxima at adjacent CWT scales. The ridge line is cut off at the end point, whose amplitude divided by the maximum ridge amplitude is larger than the cutoff amplitude ratio threshold (0.5 by default).

Usage

```
getRidgeLength(ridgeList, Th = 0.5)
```

Arguments

`ridgeList`	a list of identified ridges
`Th`	the cutoff amplitude ratio (the amplitude divided by the maximum amplitude of the ridge) threshold of the ridge line end.

Value

a vector of estimated ridge length

Author(s)

Pan Du

`getRidgeValue` *Get the CWT coefficient values corresponding to the peak ridge*

Description

Get the CWT coefficient values corresponding to the peak ridge

Usage

```
getRidgeValue(ridgeList, wCoefs, skip = 0)
```

Arguments

ridgeList	a list of ridge lines
wCoefs	2-D CWT coefficients
skip	the CWT scale level to be skipped, by default the 0 scale level (raw spectrum) is skipped.

Value

A list of ridge values corresponding to the input ridgeList.

Author(s)

Pan Du

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identifyMajorPeaks *Identify peaks based on the ridges in 2-D CWT coefficient matrix*

Description

Indentify the peaks based on the ridge list (returned by getRidge) in 2-D CWT coefficient matrix and estimated Signal to Noise Ratio (SNR)

Usage

```
identifyMajorPeaks(ms, ridgeList, wCoefs, scales = as.numeric(colnames(wCoefs)), SNR.Th = 3, peakSc
```

Arguments

ms	the mass spectrometry spectrum
ridgeList	returned by getRidge
wCoefs	2-D CWT coefficients
scales	scales of CWT, by default it is the colnames of wCoefs
SNR.Th	threshold of SNR
peakScaleRange	the CWT scale range of the peak.
ridgeLength	the maximum ridge scale of the major peaks.
nearbyPeak	determine whether to include the small peaks close to large major peaks
nearbyWinSize	the window size to determine the nearby peaks. Only effective when nearbyPeak is true.
winSize.noise	the local window size to estimate the noise level.
SNR.method	method to estimate noise level. Currently, only 95 percentage quantile is supported.
minNoiseLevel	the minimum noise level used in calculating SNR, i.e., if the estimated noise level is less than "minNoiseLevel", it will use "minNoiseLevel" instead. If the noise level is less than 0.5, it will be treated as the ratio to the maximum amplitude of the spectrum.

Details

The determination of the peaks is based on three rules: Rule 1: The maximum ridge scale of the peak should larger than a certain threshold Rule 2: Based on the scale of the peak (corresponding to the maximum value of the peak ridge) should be within certain range Rule 3: Based on the peak SNR

Value

Return a list with following elements:

`peakIndex` the m/z indexes of the identified peaks

`peakCenterIndex`
the m/z indexes of peak centers, which correspond to the maximum on the ridge. peakCenterIndex includes all the peaks, not just the identified major peaks.

`peakCenterValue`
the CWT coefficients (the maximum on the ridge) corresponding to peakCenterIndex

`peakSNR` the SNR of the peak, which is the ratio of peakCenterValue and noise level

`peakScale` the estimated scale of the peak, which corresponds to the peakCenerIndex

`potentialPeakIndex`
the m/z indexes of all potential peaks, which satisfy all requirements of a peak without considering its SNR. Useful, if you want to change to a lower SNR threshold later.

`allPeakIndex` the m/z indexes of all the peaks, whose order is the same as peakCenterIndex, peakCenterValue, peakSNR and peakScale.

All of these return elements have peak names, which are the same as the corresponding peak ridges. see `getRidge` for details.

Author(s)

Pan Du, Simon Lin

References

Du, P., Kibbe, W.A. and Lin, S.M. (2006) Improved peak detection in mass spectrum by incorporating continuous wavelet transform-based pattern matching, Bioinformatics, 22, 2059-2065.

See Also

`peakDetectionCWT`, `tuneInPeakInfo`

Examples

```
data(exampleMS)
scales <- seq(1, 64, 3)
wCoefs <- cwt(exampleMS, scales=scales, wavelet='mexh')

localMax <- getLocalMaximumCWT(wCoefs)
ridgeList <- getRidge(localMax)

SNR.Th <- 3
majorPeakInfo <- identifyMajorPeaks(exampleMS, ridgeList, wCoefs, SNR.Th=SNR.Th)
```

```
## Plot the identified peaks
peakIndex <- majorPeakInfo$peakIndex
plotPeak(exampleMS, peakIndex, main=paste('Identified peaks with SNR >', SNR.Th))
```

`localMaximum` *Identify local maximum within a slide window.*

Description

Find local maximum by transform the vector as matrix, then get the the maximum of each column. This operation is performed twice with vecctor shifted half of the winSize.

Usage

```
localMaximum(x, winSize = 5)
```

Arguments

`x`	a vector represents a signal profile
`winSize`	the slide window size, 5 by default.

Details

Instead of find the local maximum by a slide window, which slide all possible positions, we find local maximum by transform the vector as matrix, then get the the maximum of each column. This operation is performed twice with vecctor shifted half of the winSize. The main purpose of this is to increase the efficiency of the algorithm.

Value

Return a vector with the same length of the input x. The position of local maximum is set as 1, 0 else where.

Author(s)

Pan Du

See Also

`getLocalMaximumCWT`

Examples

```
x <- rnorm(200)
lmax <- localMaximum(x, 5)
maxInd <- which(lmax > 0)
plot(x, type='l')
points(maxInd, x[maxInd], col='red')
```

mzInd2vRange — *Match m/z index to m/z value with a certain error range*

Description

Match m/z index to m/z value with a certain error range

Usage

```
mzInd2vRange(mzInd, error = 0.003)
```

Arguments

mzInd	a vector of m/z index
error	error range

Value

return a vector of sorted m/z values

Author(s)

Pan Du

See Also

mzV2indRange

mzV2indRange — *Match m/z value to m/z index with a certain error range*

Description

Match m/z value to m/z index with a certain error range

Usage

```
mzV2indRange(mzV, error = 0.003)
```

Arguments

mzV	a vector of m/z value
error	error range

Value

return a vector of sorted m/z indexes

Author(s)

Pan Du

See Also

mzInd2vRange

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peakDetectionCWT *The main function of peak detection by CWT based pattern matching*

Description

This function is a wrapper of cwt, getLocalMaximumCWT, getRidge, identifyMajorPeaks

Usage

```
peakDetectionCWT(ms, scales = c(1, seq(2, 30, 2), seq(32, 64, 4)), SNR.Th = 3, nearbyPeak = TRUE, pea
```

Arguments

ms	the mass spectrometry spectrum
scales	scales of CWT
SNR.Th	SNR (Signal to Noise Ratio) threshold
nearbyPeak	Determine whether to include the nearby small peaks of major peaks. TRUE by default
peakScaleRange	the scale range of the peak. larger than 5 by default.
amp.Th	the minimum required relative amplitude of the peak (ratio to the maximum of CWT coefficients)
minNoiseLevel	the minimum noise level used in computing the SNR
ridgeLength	the minimum highest scale of the peak in 2-D CWT coefficient matrix
peakThr	Minimal absolute intensity (above the baseline) of peaks to be picked. If this value is provided, then the smoothing function sav.gol will be called to estimate the local intensity.(added based on the suggestion and code of Steffen Neumann)
tuneIn	determine whether to tune in the parameter estimation of the detected peaks
...	other parameters used by identifyMajorPeaks and smoothing function sav.gol

Value

majorPeakInfo	return of identifyMajorPeaks
ridgeList	return of getRidge
localMax	return of getLocalMaximumCWT
wCoefs	2-D CWT coefficient matrix, see cwt for details.

Author(s)

Pan Du, Simon Lin

References

Du, P., Kibbe, W.A. and Lin, S.M. (2006) Improved peak detection in mass spectrum by incorporating continuous wavelet transform-based pattern matching, Bioinformatics, 22, 2059-2065.

See Also

cwt, getLocalMaximumCWT, getRidge, identifyMajorPeaks

Examples

```
data(exampleMS)
SNR.Th <- 3
peakInfo <- peakDetectionCWT(exampleMS, SNR.Th=SNR.Th)
majorPeakInfo = peakInfo$majorPeakInfo
peakIndex <- majorPeakInfo$peakIndex
plotPeak(exampleMS, peakIndex, main=paste('Identified peaks with SNR >', SNR.Th))

## In some cases, users may want to add peak filtering based on the absolute peak amplitude
peakInfo <- peakDetectionCWT(exampleMS, SNR.Th=SNR.Th, peakThr=500)
majorPeakInfo = peakInfo$majorPeakInfo
peakIndex <- majorPeakInfo$peakIndex
plotPeak(exampleMS, peakIndex, main=paste('Identified peaks with SNR >', SNR.Th))
```

---

plotLocalMax *Plot the local maximum matrix*

Description

Plot the local maximum matrix of 2-D CWT coefficients returned by getLocalMaximumCWT

Usage

```
plotLocalMax(localMax, wCoefs = NULL, range = c(1, nrow(localMax)), colorMap = "RYB", main = NULL, ce
```

Arguments

localMax	local maximum matrix of 2-D CWT coefficients returned by getLocalMaximumCWT
wCoefs	2-D CWT coefficients
range	plot range of m/z index
colorMap	the colormap used in plotting the points
main	parameter of plot
cex	parameter of plot
pch	parameter of plot
...	other parameters of points

Author(s)

Pan Du

See Also

getLocalMaximumCWT

Examples

```
data(exampleMS)
scales <- seq(1, 64, 3)
wCoefs <- cwt(exampleMS[5000:11000], scales=scales, wavelet='mexh')

localMax <- getLocalMaximumCWT(wCoefs)
plotLocalMax(localMax)
```

---

plotPeak *Plot the identified peaks over the spectrum*

Description

Plot the identified peaks over the spectrum. The identified peaks are returned by peakDetectionCWT or identifyMajorPeaks

Usage

```
plotPeak(ms, peakIndex = NULL, mz = 1:length(ms), range = c(min(mz), max(mz)), method = c("p", "l"),
```

Arguments

ms	the MS spectrum
peakIndex	m/z indexes of the identified peaks
mz	m/z value correspond to m/z index
range	the plot range of m/z value
method	plot method of the identified peaks. method 'p' plot circles on the peaks; method 'l' add vertical lines over the peaks.
main	parameter of plot
log	parameter of plot
...	other parameters of points

Author(s)

Pan Du

See Also

peakDetectionCWT, identifyMajorPeaks

Examples

```
data(exampleMS)
SNR.Th <- 3
peakInfo <- peakDetectionCWT(exampleMS, SNR.Th=SNR.Th)
majorPeakInfo = peakInfo$majorPeakInfo
peakIndex <- majorPeakInfo$peakIndex
plotPeak(exampleMS, peakIndex, main=paste('Identified peaks with SNR >', SNR.Th))
```

plotRidgeList *Plot the ridge list*

Description

Plot the ridge list returned by getRidge

Usage

```
plotRidgeList(ridgeList, wCoefs = NULL, range = NULL, colorMap = "RYB", main = NULL, pch = ".", cex =
```

Arguments

ridgeList	returned by getRidge
wCoefs	2-D CWT coefficients
range	plot range of m/z index
colorMap	colorMap to plot the points of local maximum
main	parameter of plot
pch	parameter of plot
cex	parameter of plot
...	other parameters of points

Author(s)

Pan Du

See Also

getRidge

Examples

```
data(exampleMS)
scales <- seq(1, 64, 3)
wCoefs <- cwt(exampleMS[5000:11000], scales=scales, wavelet='mexh')

localMax <- getLocalMaximumCWT(wCoefs)
ridgeList <- getRidge(localMax)
plotRidgeList(ridgeList)
```

sav.gol *Estimate the baseline by using Savitzky-Golay Algorithm*

Description

Estimate the baseline by using Savitzky-Golay Algorithm

Usage

```
sav.gol(T, fl, forder = 4, dorder = 0)
```

Arguments

T	vector of signals to be filtered
fl	filter length (for instance fl = 51..151)
forder	filter order (2 = quadratic filter, 4= quartic)
dorder	derivative order (0 = smoothing, 1 = first derivative, etc.)

Value

The return is a smoothed vector (baseline).

Note

This function was added by Steffen Neumann. We appreciated his help to make the package better.

Author(s)

Steffen Neumann <sneumann@ipb-halle.de>

smoothDWT *smooth (denoise) the spectrum by DWT (Discrete Wavelet Transform)*

Description

Smooth (denoise) the spectrum by DWT (Discrete Wavelet Transform)

Usage

```
smoothDWT(ms, nLevel = 6, wf = "la8", localNoiseTh = seq(1, 0, by = -0.2), localWinSize = 500, globalN
```

Arguments

ms	a vector representing the mass spectrum
nLevel	the level of DWT decomposition
wf	the name of wavelet for DWT
localNoiseTh	local noise level threshold
localWinSize	local window size for estimate local noise threshold
globalNoiseTh	global noise level threshold
smoothMethod	the method used for denoising. 'hard' means keeping the dwt coefficients higher than the threshold unchanged; "soft" means the dwt coefficients higher than the threshold were subtracted by the threshold.
method	'dwt' or 'modwt' used for decomposition

Value

return the smoothed mass spectrum with the 'detail' component of DWT as an attribute 'detail'.

Author(s)

Pan Du

---

tuneInPeakInfo *Tune in the peak information: peak position and peak scale*

Description

Based on the identified peak position, more precise estimation of the peak information, i.e., peak position and peak scale, can be got by this function. The basic idea is to cut the segment of spectrum near the identified peaks, and then do similar procedures as peakDetectionCWT, but with more detailed scales around the estimated peak scale.

Usage

```
tuneInPeakInfo(ms, majorPeakInfo = NULL, peakIndex = NULL, peakScale = NULL, maxScale = 128, ...)
```

Arguments

ms	the mass spectrometry spectrum
majorPeakInfo	return of identifyMajorPeaks
peakIndex	the m/z index of the identified peaks
peakScale	the scales of the identified peaks
maxScale	the maximum scale allowed for the peak
...	other parameters of used by getLocalMaximumCWT, getRidge, identifyMajorPeaks

Details

The majorPeakInfo or peakIndex and peakScale must be provided.

Value

`peakCenterIndex` the updated peak center m/z index

`peakScale` the updated peak scale

`peakValue` the corresponding peak value

Author(s)

Pan Du

References

Du, P., Kibbe, W.A. and Lin, S.M. (2006) Improved peak detection in mass spectrum by incorporating continuous wavelet transform-based pattern matching, Bioinformatics, 22, 2059-2065.

See Also

`peakDetectionCWT`

Examples

```
data(exampleMS)
SNR.Th <- 3
peakInfo <- peakDetectionCWT(exampleMS, SNR.Th=SNR.Th)
majorPeakInfo <- peakInfo$majorPeakInfo
betterPeakInfo <- tuneInPeakInfo(exampleMS, majorPeakInfo)
plot(500:length(exampleMS), exampleMS[500:length(exampleMS)], type='l', log='x')
abline(v=betterPeakInfo$peakCenterIndex, col='red')
```

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