binspec

May 23, 2016

`binary_peaks` *Find binary peaks*

Description

Find peaks in window of size 2*neighbors + 1 and label m/z integers within the error as peaks. Returns vector of peak m/z integers.

Usage

```
binary_peaks(df, neighbors, error = 0)
```

Arguments

`df`	Data frame of m/z and intensities
`neighbors`	Number of neighboring m/z values to compare on right and left
`error`	m/z Decimal error value

`classifier_accuracies`
Classifier Accuracies

Description

Find the best classifier using leave-one-out cross validation (svm) and out-of-bag error (random forests). Returns a vector of classification accuracies

Usage

```
classifier_accuracies(peaks, labels, minpeaks)
```

Arguments

`peaks`	Boolean matrix of mass spectra rows with m/z columns, indicating if an m/z value corresponds to a peak.
`labels`	The correct classifications of the peaks.
`minpeaks`	How many "true" values must show up for a given m/z value for it to be considered a feature.

combine_peaks *Combine peak vectors*

Description

Create a binary matrix, each column represents an m/z value, and each row represents a mass spectra. The value indicates whether or not the m/z of this spectra is a peak.

Usage

```
combine_peaks(list_mz_peaks)
```

Arguments

list_mz_peaks	List of m/z peak vectors

round_df *Round data frame*

Description

Round all m/z and intensity values to integers.

Usage

```
round_df(df)
```

Arguments

df	Data frame

Index