Package 'flowPeaks'

October 9, 2013

Version 1.2.0
Date 1-12-2012
Title An R package for flow data clustering
Author Yongchao Ge <yongchao.ge@gmail.com></yongchao.ge@gmail.com>
Maintainer Yongchao Ge <yongchao.ge@gmail.com></yongchao.ge@gmail.com>
Depends R (>= 2.12.0)
Enhances flowCore
Description A fast and automatic clustering to classify the cells into subpopulations based on finding the peaks from the overall density function generated by K-means.
biocViews Flow cytometry, Clustering, Gating, Bioinformatics
License Artistic-1.0
R topics documented: adjust.flowPeaks assign.flowPeaks barcode concave evalCluster flowPeaks
plot.flowPeaks
Index 1

2 assign.flowPeaks

adjust.flowPeaks	Adjusting the smoothing and merging behavior of the flowPeaks results

Description

Adjusting the smoothing and merging behavior of the flowPeaks results by changing the multiplers of the covariance matrix and the tolerance level for joining two peaks

Usage

```
adjust.flowPeaks(object,tol,h0,h,...)
```

Arguments

object	The output from the function flowPeaks	
tol	See flowPeaks	

h0 See flowPeaks
h See flowPeaks

... Optional additional arguments. At present no additional arguments are used.

Value

It returns an updated object of class flowPeaks, the detail defintion of which can be seen in flowPeaks.

Author(s)

```
Yongchao Ge <yongchao.ge@gmail.com>
```

See Also

flowPeaks

assign.flowPeaks	Obtain the flowPeaks cluster lables with the option of identifying out-
	liers and applying to a new data set

Description

The function takes a flowPeaks output and a new data set (or could be the same dataset that generated the flowPeaks), and compute the cluster label assignment

```
assign.flowPeaks(fp,A,tol=0.01,fc=0.8)
```

barcode 3

Arguments

fp	an object of class flowPeaks, the output from the function flowPeaks or adjust.flowPeaks
Α	A data matrix with the same number of columns as the data that geneterated fp
tol	All points where the probability density is less than tol (default is 1%) of the peak denisty of that cluster are labled as outliers. If tol is set 0, no outliers according to this rule. The details can be seen in the first equation of Section 2.5 in the flowPeaks manuscript (Ge et al 2012)
fc	All points where the classified cluster contributes less than fc (default is 80%) of overall denstiy are labeled as outliers. if fc is set to 0%, no outliers can be found according to this rule. The details can be seen in the second equation of Section 2.5 in the flowPeaks manuscript (Ge et al 2012)

Value

It returns the class label assignment of each data point, where -1 indicates outliers. When A is the same data that generated fp, If tol is 1 and fc is 0, the returned labels are the same as fp\$peaks.cluster.

Author(s)

Yongchao Ge <yongchao.ge@gmail.com>

References

Ge Y. et al, flowPeaks: a fast unsupervised clustering for flow cytometry data via K-means and density peak finding, 2012, Bioinformatics, in press.

See Also

flowPeaks

barcode	The barcode dataset

Description

A flow cytometry data that is used barcode to measure many samples simultaneusly

Usage

data(barcode)

Format

An object (barcode) of data frame with 180912 rows and 3 columns and a vector (barcode.cid) for the cluster labels according to the manual gating.

4 evalCluster

Source

The data is a random subset of the full data set for Figure 3A of the paper (Sugar et al 2010), This subset was used to do all comparisons in the paper (Ge et al 2012) with other clustering algorithms.

References

Sugar I. P. and Sealfon S. C., Misty Mountain clustering: application to fast unsupervised flow cytometry gating, *BMC Bioinformatcs*, 2010, 11:502.

Ge Y. et al, flowPeaks: a fast unsupervised clustering for flow cytometry data via K-means and density peak finding, 2012, Bioinformatics, in press

concave

The concave dataset

Description

A simulated flowcytometry data with two concave shapes

Usage

data(concave)

Format

An object (concave) of data frame with rows and 3 columns and a vector (concave.cid) for the true cluster labels.

References

Ge Y. et al, flowPeaks: a fast unsupervised clustering for flow cytometry data via K-means and density peak finding, 2012, Bioinformatics, in press.

evalCluster

evaulate the result of a clustering algorihm by comparing it with the gold standard

Description

This function takes the cluster labels of the two clusterings, one is based on the gold standard, the other is a candidate clusterign, and compute one of the three metrics to assess the candidate clustering performance.

flowPeaks 5

Usage

Arguments

gs A integer-valued vector of length n for the cluster labels of the gold standard

clustering, where negative numbers such as -1 is for the outerliers

cand A integer-valued vector of length n for the cluster label of a candidate clustering,

where -1 is for the outliers

rm.gs.outliers Determining whether the outliers of the gold standard clustering should be re-

moved in the comparison

method A single character to indicate which one of three metrics should be used to

evaluate the clustering. The details are described in Ge (2012) and references

mentioned in that paper

Rand.index The adjusted Rand.index

Fmeasure F-measure **Vmeasure** V-measure

Author(s)

Yongchao Ge <yongchao.ge@gmail.com>

References

Ge Y. et al, flowPeaks: a fast unsupervised clustering for flow cytometry data via K-means and density peak finding, 2012, Bioinformatics, in press.

See Also

flowPeaks

flowPeaks Doing the flowPeaks analysis

Description

This is the core function in the flowPeaks package. It generates the output of the cluster and information associated with each cluster, which can be used by the function plot for visualization

```
flowPeaks(x, tol=0.1, h0=1, h=1.5)
```

6 flowPeaks

Arguments

X	a data matrix for the flow cytometry data, it needs to have at least two rows, and the names for each column should be unique. For a flowFrame data, its expression matrix slot should be used as x, where only channles of interest are selected (see the example below).
tol	The tolerance (between 0 and 1) when neighboring clusters should be considered to be merged
h0	The multiplier of the vaiarance matrix S0
h	The multiplier of the variance matrix S

Value

It returns an object of class flowPeaks, which is a list of the following variables:

 $peaks.cluster \quad \text{An integer shows the cluster labels (between 1 and K for K clusters) for each K of K clusters are shown in the cluster labels (between 1 and K for K clusters) for each K of K clusters are shown in the cluster labels (between 1 and K for K clusters) for each K of K clusters are shown in the cluster labels (between 1 and K for K clusters) for each K of K clusters are shown in the cluster labels (between 1 and K for K clusters) for each K of K clusters are shown in the cluster labels (between 1 and K for K clusters) for each K of K clusters are shown in the cluster labels (between 1 and K for K clusters) for each K of K clusters are shown in the cluster labels (between 1 and K for K clusters) for each K of K of K clusters are shown in the cluster labels (between 1 and K for K clusters). }$

cell. The clustering is based on the flowPeaks algorithm

peaks A summary of the cluster information. It is a list with the following three vari-

ables:

• cid: cluster labels, should always be 1:K;

• w: the weights of the K clusters;

• mu: The mean of all cells in the K clusters;

• S: The variance matrix of the K clusters. Note that each variance matrix for

each cluster has been stacked as a column vector

kmeans.cluster An integer shows the cluster labels for the initial kmeans clustering

A summary of the initial kmeans clustering. The meaning of the variables can

be seens in the description of peaks above

info The information that can be used for plot, and how the initial kmeans clustering

and the final flowPeaks clustering are connected

x The input data x

Author(s)

kmeans

Yongchao Ge <yongchao.ge@gmail.com>

References

Ge Y. et al, flowPeaks: a fast unsupervised clustering for flow cytometry data via K-means and density peak finding, 2012, Bioinformatics, in press.

See Also

plot.flowPeaks

plot.flowPeaks 7

Examples

```
##demonstrate how to use a flowFrame
## Not run:
require(flowCore)
samp <- read.FCS(system.file("extdata","0877408774.B08",</pre>
package="flowCore"))
##do the clustering based on the asinh transforamtion of
##the first two FL channels
fp<-flowPeaks(asinh(samp@exprs[,3:4]))</pre>
plot(fp)
## End(Not run)
data(barcode)
fp<-flowPeaks(barcode[,c(1,3)])</pre>
plot(fp)
##to compare it with the gold standard
evalCluster(barcode.cid,fp$peaks.cluster,method="Vmeasure")
#to remove the outliers
fpc<-assign.flowPeaks(fp,fp$x)</pre>
plot(fp,classlab=fpc,drawboundary=FALSE,
  drawvor=FALSE,drawkmeans=FALSE,drawlab=TRUE)
#to adjust the cluster by increasing the tol,h0, h, which results
#in a smaller number of clusters
fp2<-adjust.flowPeaks(fp,tol=0.5,h0=2,h=2)</pre>
summary(fp2)
print(fp) #an alternative of using summary(fp)
```

plot.flowPeaks

Plot the results generated by flowPeaks

Description

This function takes the results generated from flowPeaks as an input, and plot the data in 2D. These plots display the clustering structure

8 print.flowPeaks

Arguments

x	An object of class flow Peaks, e.g., t the output from the functions flow Peaks or adjust. flow Peaks
idx	The index of the columns will be used to plot the clustering. idx needs to be at least legnth 2, and have no duplicate elements, and the values can only take from 1 to d, where d is the number of columns for the input matrix x that is used as an input of the function flowPeaks
drawlab	The option to decide whether we should draw the cluster labels
cols	The color specification for plotting the points in each cluster. Please note, "white" and "black" are not allowed, which are reserved for other purpse
drawvor	Deciding whether the voronoi diagram should be drawn, only good for 2D data
drawlocalpeaks	Decding whether the local peaks with a triangle symbol should be drawn
drawkmeans	Deciding whether the kmeans center with a filled circle should be drawn
drawboundary	Deciding whether the boudary between clusters should be drawn, only good for 2D data
classlab	Use this to replace the default class labels from x\$peak.cluster, for example, the classlab may come from assign.flowPeaks
negcol	Deciding the color of the negative, which are outliers
negpch	Deciing the symbols for the outliers
	Optional additional arguments. At present no additional arguments are used.

Author(s)

Yongchao Ge <yongchao.ge@gmail.com>

See Also

flowPeaks

print.flowPeaks The display of the flowPeaks results

Description

The display of the flowPeaks results

```
## S3 method for class 'flowPeaks' print(x,...)
```

summary.flowPeaks 9

Arguments

x The output from the function flowPeaks

... Optional additional arguments. At present no additional arguments are used.

Author(s)

Yongchao Ge <yongchao.ge@gmail.com>

See Also

flowPeaks

summary.flowPeaks

The summary of the flowPeaks results

Description

The summary of the flowPeaks results

Usage

```
## S3 method for class 'flowPeaks'
summary(object,...)
```

Arguments

object The output from the function flowPeaks

... Optional additional arguments. At present no additional arguments are used.

Author(s)

Yongchao Ge <yongchao.ge@gmail.com>

See Also

flowPeaks

Index

```
*Topic adjust
    adjust.flowPeaks, 2
*Topic cluster, multivariate, smooth
    flowPeaks, 5
*Topic cluster,multivarite
    assign.flowPeaks, 2
*Topic cluster,utiliteis
    evalCluster, 4
*Topic datasets
    barcode, 3
    concave, 4
*Topic plot, multivariate, smooth
    plot.flowPeaks, 7
*Topic print
    print.flowPeaks,8
*Topic summary
    summary.flowPeaks, 9
adjust.flowPeaks, 2, 3, 8
assign.flowPeaks, 2, 8
barcode, 3
concave, 4
evalCluster, 4
flowPeaks, 2, 3, 5, 5, 8, 9
plot.flowPeaks, 6, 7
print.flowPeaks, 8
summary.flowPeaks,9
```