

Package ‘iterClust’

October 18, 2022

Type Package

Title Iterative Clustering

Version 1.18.0

Author Hongxu Ding and Andrea Califano

Maintainer Hongxu Ding <hd2326@columbia.edu>

Description A framework for performing clustering analysis iteratively.

License file LICENSE

Depends R (>= 3.4.1)

LazyData TRUE

Imports Biobase, cluster, stats, methods

Suggests tsne, bcellViper

biocViews StatisticalMethod, Clustering

URL <https://github.com/hd2326/iterClust>

BugReports <https://github.com/hd2326/iterClust/issues>

RoxygenNote 6.0.1

git_url <https://git.bioconductor.org/packages/iterClust>

git_branch RELEASE_3_15

git_last_commit f0b4b11

git_last_commit_date 2022-04-26

Date/Publication 2022-10-18

R topics documented:

clustEval	2
clustHetero	3
coreClust	3
featureSelect	4
iterClust	5
obsEval	7
obsOutlier	8

clustEval	<i>Cluster-wise Clustering Robustness Evaluation</i>
-----------	--

Description

A sample cluster-wise clustering robustness evaluation framework (described in "Examples" section, used as default in iterClust framework). Customized frameworks can be defined following rules specified in "Usage", "Arguments" and "Value" sections.

Usage

```
clustEval(dset, iteration, clust)
```

Arguments

dset	(numeric matrix) features in rows and observations in columns
iteration	(positive integer) specifies current iteration
clust	return value of coreClust

Value

a numeric vector, specifies the clustering robustness (higher value means more robust) of each clustering scheme

Author(s)

DING, HONGXU (hd2326@columbia.edu)

Examples

```
clustEval <- function(dset, iteration, clust){  
  dist <- as.dist(1 - cor(dset))  
  clustEval <- vector("numeric", length(clust))  
  for (i in 1:length(clust)){  
    clustEval[i] <- mean(silhouette(clust[[i]], dist)[, "sil_width"])}  
  return(clustEval)}  
}
```

`clustHetero`*Cluster Heterogeneity Evaluation*

Description

A sample cluster heterogeneity evaluation framework (described in "Examples" section, used as default in iterClust framework). Customized frameworks can be defined following rules specified in "Usage", "Arguments" and "Value" sections.

Usage

```
clustHetero(clustEval, iteration)
```

Arguments

<code>clustEval</code> ,	return value of <code>clustEval</code>
<code>iteration</code>	(positive integer) specifies current iteration

Value

a boolean vector, specifies whether clusters are heterogenous

Author(s)

DING, HONGXU (hd2326@columbia.edu)

Examples

```
clustHetero <- function(clustEval, iteration){  
  return(clustEval > 0*iteration+0.15)}
```

`coreClust`*Clustering*

Description

A sample clustering framework (described in "Examples" section, used as default in iterClust framework). Customized frameworks can be defined following rules specified in "Usage", "Arguments" and "Value" sections.

Usage

```
coreClust(dset, iteration)
```

Arguments

dset (numeric matrix) features in rows and observations in columns
 iteration (positive integer) specifies current iteration

Value

a list, each element contains clustering vectors (named numeric vector with observation names as name and corresponding cluster number as element) under a specific clustering parameter

Author(s)

DING, HONGXU (hd2326@columbia.edu)

Examples

```
coreClust <- function(dset, iteration){
  dist <- as.dist(1 - cor(dset))
  range=seq(2, ncol(dset)-1, by = 1)
  clust <- vector("list", length(range))
  for (i in 1:length(range)) clust[[i]] <- pam(dist, range[i])$clustering
  return(clust)}
```

 featureSelect

Feature Selection

Description

A sample feature selection framework (described in "Examples" section, used as default in iter-Clust framework). Customized frameworks can be defined following rules specified in "Usage", "Arguments" and "Value" sections.

Usage

```
featureSelect(dset, iteration, feature)
```

Arguments

dset (numeric matrix) features in rows and observations in columns
 iteration (positive integer) specifies current iteration
 feature (character array) specifies user defined features, facilitating feature selection

Value

a character array, contains features selected

Author(s)

DING, HONGXU (hd2326@columbia.edu)

Examples

```
featureSelect <- function(dset, iteration, feature) return(rownames(dset))
```

iterClust	<i>Iterative Clustering</i>
-----------	-----------------------------

Description

A framework for performing clustering analysis iteratively

Usage

```
iterClust(dset, maxIter = 10, minFeatureSize = 100,
  featureSelect = iterClust::featureSelect, minClustSize = 10,
  coreClust = iterClust::coreClust, clustEval = iterClust::clustEval,
  clustHetero = iterClust::clustHetero, obsEval = iterClust::obsEval,
  obsOutlier = iterClust::obsOutlier)
```

Arguments

dset	(numeric matrix or data.frame) features in rows and observations in columns, or SummarizedExperiment0 and ExpressionSet object
maxIter	(positive integer) specifies maximum number iterations to be performed
minFeatureSize	(positive integer) specifies minimum number of features needed
featureSelect	(function) takes a dataset, depth(IV) and cluster\$feature(IV), returns a character array, containing features used for clustering analysis
minClustSize	(positive integer) specifies minimum cluster size
coreClust	(function) takes a dataset and depth(IV), returns a list, containing clustering vectors under different clustering parameters
clustEval	(function) takes a dataset, depth(IV) and coreClust result, returns a numeric vector, evaluating the robustness (higher value means more robust) of each clustering scheme
clustHetero	(function) takes depth(IV) and clustEval result, returns a boolean vector, deciding whether a cluster is considered as heterogenous
obsEval	(function) takes a dataset and optimal coreClust result determined by clustEval, returns a numeric vector, evaluating the clustering robustness of each observation
obsOutlier	(function) takes depth(IV) and obsEval result, returns a boolean vector, deciding whether an observation is outlier

Details

General Idea

In a scenario where populations A, B1, B2 exist, pronounce differences between A and B may mask subtle differences between B1 and B2. To solve this problem, so that heterogeneity can be better detected, clustering analysis needs to be performed iteratively, so that, for example, in iteration 1, A and B are separated and in iteration 2, B1 and B2 are separated.

General Work Flow

ith Iteration Start ==>

featureSelect (feature selection) ==>

minFeatureSize (confirm enough features are selected) ==>

clustHetero (confirm heterogeneity) ==>

coreClust (generate several clustering schemes to be evaluated) ==>

clustEval (pick optimal clustering scheme generated in previous step) ==>

minClustSize (remove clusters with few observations) ==>

obsEval (evaluate how each observations are clustered) ==>

obsOutlier (remove poorly clustered observations) ==>

results in Internal Variables (IV) ==>

ith Iteration End

Internal Variables (IV)

The following IVs are used in user-defined functions in each iteration:

cluster: (list) the return value, described in "Value" section

depth: (numeric) current round of iteration

Value

a list with the following structure containing iterClust result

-> \$cluster (list) \$Iter[i] (list) \$Cluster[j], (character array) names of observations belong to each cluster

-> \$feature (list) \$Iter[i] (list) \$Cluster[j]inIter[i-1], (character array) features used to split each cluster in the previous iteration thereby produce the current clusters

-> \$clusterScore (list) \$Iter[i] (list) \$Cluster[j]inIter[i-1], (numeric array) clustEval output for each clustering schemes

-> \$observationScore (list) \$Iter[i] (list) \$Cluster[j]inIter[i-1], (numeric array) obsEval output for each samples

Author(s)

DING, HONGXU (hd2326@columbia.edu)

Examples

```

library(tsne)
library(cluster)
library(bcellViper)

data(bcellViper)
exp <- exprs(dset)
pheno <- as.character(dset@phenoData@data$description)
exp <- exp[, pheno %in% names(table(pheno))[table(pheno) > 5]]
pheno <- pheno[pheno %in% names(table(pheno))[table(pheno) > 5]]
#load bcellViper expression and phenotype annotation

c <- iterClust(exp, maxIter=3, minClustSize=5)
#iterClust

dist <- as.dist(1 - cor(exp))
set.seed(1)
tsne <- tsne(dist, perplexity = 20, max_iter = 500) #'
for (j in 1:length(c$cluster)){
  COL <- structure(rep(1, ncol(exp)), names = colnames(exp))
  for (i in 1:length(c$cluster[[j]]) COL[c$cluster[[j]][[i]]] <- i+1
  plot(tsne[, 1], tsne[, 2], cex = 0, cex.lab = 1.5,
       xlab = "Dim1", ylab = "Dim2",
       main = paste("iterClust, iter=", j, sep = ""))
  text(tsne[, 1], tsne[, 2], labels = pheno, cex = 0.5, col = COL)
  legend("topleft", legend = "Outliers", fill = 1, bty = "n")}
#visualize results

```

obsEval

*Observation-wise Clustering Robustness Evaluation***Description**

A sample observation-wise clustering robustness evaluation framework (described in "Examples" section, used as default in iterClust framework). Customized frameworks can be defined following rules specified in "Usage", "Arguments" and "Value" sections.

Usage

```
obsEval(dset, clust, iteration)
```

Arguments

dset	(numeric matrix) features in rows and observations in columns
clust	optimal return value of coreClust
iteration	(positive integer) specifies current iteration

Value

a numeric vector, specifies the clustering robustness (higher value means more robust) of each observation under the optimal clustering scheme

Author(s)

DING, HONGXU (hd2326@columbia.edu)

Examples

```
obsEval <- function(dset, clust, iteration){  
  dist <- as.dist(1 - cor(dset))  
  obsEval <- vector("numeric", length(clust))  
  return(silhouette(clust, dist)[, "sil_width"])}  

```

obsOutlier

Outlier Observation Evaluation

Description

A sample outlier observation evaluation framework (described in "Examples" section, used as default in iterClust framework). Customized frameworks can be defined following rules specified in "Usage", "Arguments" and "Value" sections.

Usage

```
obsOutlier(obsEval, iteration)
```

Arguments

obsEval,	return value of obsEval
iteration	(positive integer) specifies current iteration

Value

a boolean vector, specifies whether an observation is outlier

Author(s)

DING, HONGXU (hd2326@columbia.edu)

Examples

```
obsOutlier <- function(obsEval, iteration) return(obsEval < 0*iteration-1)
```


Index

- * **clustEval**
 - clustEval, 2
 - * **clustHetero**
 - clustHetero, 3
 - * **coreClust**
 - coreClust, 3
 - * **featureSelect**
 - featureSelect, 4
 - * **iterClust**
 - iterClust, 5
 - * **obsEval**
 - obsEval, 7
 - * **obsOutlier**
 - obsOutlier, 8
- clustEval, 2
clustHetero, 3
coreClust, 3
- featureSelect, 4
- iterClust, 5
- obsEval, 7
obsOutlier, 8