Package 'iterClust'

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Type Package

Title Iterative Clustering

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Author Hongxu Ding and Andrea Califano

Maintainer Hongxu Ding <hd2326@columbia.edu>

Description A framework for performing clustering analysis iteratively.

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Imports Biobase, cluster, stats, methods

Suggests tsne, bcellViper

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

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`clustEval` *Cluster-wise Clustering Robustness Evaluation*

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

clustEval,	return value of clustEval
iteration	(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 iterClust 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` *Iterative Clustering*

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 seperated and in iteration 2, B1 and B2 are seperated.

#################### 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