

# Package ‘clst’

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**Title** Classification by local similarity threshold

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**Imports** ROC, lattice

**Suggests** RUnit

**LazyLoad** yes

**LazyData** yes

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**Description** Package for modified nearest-neighbor classification based on calculation of a similarity threshold distinguishing within-group from between-group comparisons.

**License** GPL-3

**biocViews** Classification

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| clst-package | <i>Classification by local similarity threshold</i> |
|--------------|-----------------------------------------------------|

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**Description**

Package for modified nearest-neighbor classification based on calculation of a similarity threshold distinguishing within-group from between-group comparisons.

**Details**

Package:

Type:

License:

Author:

clst

Package

GPL-3

Noah Hoffman <ngh2@uw.edu>

Index:

Further information is available in the following vignettes:

clstDemo    clst (source, pdf)

TODO: write package overview.

**Author(s)**

Noah Hoffman

Maintainer: <ngh2@uw.edu>

**See Also**

[cmdscale](#)

**Examples**

```
library(clst)
packageDescription("clst")
data(iris)
dmat <- as.matrix(dist(iris[,1:4], method="euclidean"))
groups <- iris$Species
i <- 1
cc <- classify(dmat, groups, dvect=dmat[i,])
cat('query at i =',i,'is species',paste('I.', groups[i]),'\n')
printClst(cc)
i <- 125
cc <- classify(dmat, groups, dvect=dmat[i,])
cat('query at i =',i,'is species',paste('I.', groups[i]),'\n')
printClst(cc)
```

---

actino

*Actinomyces data set*


---

**Description**

Square matrices describing pairwise distances among 16S rRNA sequences.

**Usage**

```
data(actino)
```

**Format**

```
List of 5
 $ dmat1 : num [1:146, 1:146] 0 0.763 1.25 10.345 12.771 ...
  ..- attr(*, "dimnames")=List of 2
  .. ..$ : chr [1:146] "200" "201" "202" "203" ...
  .. ..$ : chr [1:146] "200" "201" "202" "203" ...
 $ dmat2 : num [1:146, 1:146] 0 0.574 1.044 5.669 8.409 ...
  ..- attr(*, "dimnames")=List of 2
  .. ..$ : chr [1:146] "200" "201" "202" "203" ...
  .. ..$ : chr [1:146] "200" "201" "202" "203" ...
 $ dmat3 : num [1:146, 1:146] 0 0.763 1.25 8.571 11.233 ...
  ..- attr(*, "dimnames")=List of 2
  .. ..$ : chr [1:146] "200" "201" "202" "203" ...
  .. ..$ : chr [1:146] "200" "201" "202" "203" ...
 $ taxa : Factor w/ 33 levels "Actinomyces bowdenii",...: 12 12 12 23 20 20 8 22 12 20 ...
 $ abbrev: Factor w/ 33 levels "A bowdenii","A canis",...: 12 12 12 23 20 20 8 22 12 20 ...
```

**Details**

The matrices \$dmat1, dmat2, and dmat3 contain percent nucleotide difference with indels penalized heavily, little, and somewhat, respectively.

\$taxa is a factor of species names; abbreviations of the same names are found in \$abbrev.

Examples

```
data(actino)
```

---

|        |                          |
|--------|--------------------------|
| bvseqs | <i>BV reference set.</i> |
|--------|--------------------------|

---

Description

Tree-derived pairwise distances and taxonomic assignments among 16S rRNA sequences representing bacteria represented in the vaginal mucosa.

Usage

```
data(bvseqs)
```

Format

```
The format is:
List of 3
$ dmat      : num [1:448, 1:448] 0 0.0494 0.0968 0.1002 0.1606 ...
..- attr(*, "dimnames")=List of 2
.. ..$ : chr [1:448] "S001098970" "S000859776" "S000539896" "S001352901" ...
.. ..$ : chr [1:448] "S001098970" "S000859776" "S000539896" "S001352901" ...
$ groupTab:'data.frame': 448 obs. of  12 variables:
..$ superkingdom   : chr [1:448] "2" "2" "2" "2" ...
..$ superphylum  : chr [1:448] NA NA NA NA ...
..$ phylum       : chr [1:448] "1224" "1224" "1224" "1224" ...
..$ class          : chr [1:448] "1236" "1236" "1236" "1236" ...
..$ subclass      : chr [1:448] NA NA NA NA ...
..$ order          : chr [1:448] "72274" "72274" "72274" "72274" ...
..$ suborder       : chr [1:448] NA NA NA NA ...
..$ family         : chr [1:448] "468" "468" "468" "468" ...
..$ genus          : chr [1:448] "469" "469" "469" "469" ...
..$ species_group  : chr [1:448] NA NA NA NA ...
..$ species_subgroup: chr [1:448] NA NA NA NA ...
..$ species        : chr [1:448] "470" "470" "471" "470" ...
$ taxNames: Named chr [1:212] "Actinomyces urogenitalis" "Lactobacillus jensenii" "Proteobacteria" "Ga
..- attr(*, "names")= chr [1:212] "103621" "109790" "1224" "1236" ...
```

Details

(Describe creation of this data set)

Source

Sequences were assembled from both the RDP 16S rRNA database and from the laboratory of Dr. David Fredricks.

## References

RDP url here.

## Examples

```
data(bvseqs)
## maybe str(bvseqs) ; plot(bvseqs) ...
```

---

classify

*classify*

---

## Description

Functions to perform classification by local similarity threshold.

## Usage

```
classify(dmat, groups, dvect, method = "mutinfo", minScore = 0.45,
         doffset = 0.5, dStart = NA, maxDepth = 10, minGroupSize = 2,
         objNames = names(dvect), keep.data = TRUE, ..., verbose =
         FALSE)

classifyIter(dmat, groupTab, dvect, dStart = NA, multiple = FALSE,
            keep.data = TRUE, ..., verbose = FALSE)

classifier(dmat, groups, dvect, method = 'mutinfo', minScore = 0.45,
          doffset = 0.5, dStart = NA, minGroupSize = 2,
          objNames = names(dvect), keep.data = TRUE, ..., verbose = FALSE,
          depth = 1)

pull(dmat, groups, index)

pullTab(dmat, groupTab, index)
```

## Arguments

|          |                                                                                                                                                                                                                      |
|----------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| dmat     | Square matrix of pairwise distances.                                                                                                                                                                                 |
| groups   | Object coercible to a factor identifying group membership of objects corresponding to either edge of dmat.                                                                                                           |
| groupTab | a data.frame representing a taxonomy, with columns in increasing order of specificity from left to right (ie, Kingdom → Species). Column names are used to name taxonomic ranks. Rows correspond to margins of dmat. |
| dvect    | numeric vector of distance from query sequence to each reference corresponding to margins of dmat.                                                                                                                   |

|              |                                                                                                                                                 |
|--------------|-------------------------------------------------------------------------------------------------------------------------------------------------|
| method       | The method for calculating the threshold; only 'mutinfo' is currently implemented.                                                              |
| minScore     | Threshold value for the match score to define a match.                                                                                          |
| doffset      | Offset used in the denominator of the expression to calculate match score to penalize very small groups of reference objects.                   |
| dStart       | start with this value of D.                                                                                                                     |
| multiple     | if TRUE, stops at the rank that yields at least one match; if FALSE, continues to perform classification until exactly one match is identified. |
| maxDepth     | Maximum number of iterations that will be attempted to perform classification.                                                                  |
| minGroupSize | The minimal number of members comprising at least one group required to attempt classification.                                                 |
| objNames     | Optional character identifiers for objects corresponding to margin of dmat.                                                                     |
| keep.data    | Populates thresh\$distances (see <a href="#">findThreshold</a> ) if TRUE.                                                                       |
| verbose      | Terminal output is produced if TRUE.                                                                                                            |
| index        | an integer specifying an element in dmat                                                                                                        |
| ...          | see Details                                                                                                                                     |
| depth        | specifies iteration number (not meant to be user-defined)                                                                                       |

## Details

`classify` performs iterative classification. See the vignette vignette for package **clst** for a description of the classification algorithm.

`classifier` performs non-iterative classification, and is typically not called directly by the user.

The functions `pull` and `pullTab` are used to remove a single element of `dmatrix` for the purpose of performing classification against the remaining elements. The value of these two functions (a list) can be passed directly to `classify` or `classifyIter` directly (see examples).

## Value

`classify` and `classifyIter` return `x`, a list of lists, one for each iteration of the classifier. Each sub-list contains the following named elements:

|         |                                                                                                                                                                                                                                                                                                                                                                                         |
|---------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| depth   | An integer indicating the number of the iteration (where <code>x[[i]]\$depth == i</code> )                                                                                                                                                                                                                                                                                              |
| tally   | a data.frame with one row for each group or reference objects. Columns below and above contain counts of reference objects with distance values greater than or less than $D$ , respectively; score, containing match score $S$ ; match is 1 if $S \geq \text{minScore}$ , 0 otherwise; and the minimum, median, and maximum values of distances to all members of the indicated group. |
| details | a list of two matrices, named "below" and "above", itemizing each object with index $i$ in the reference set with distances below or above the distance threshold $D$ , respectively. Columns include index, the index $i$ ; dist, the distance between the object and the query; and group, indicating the classification of the object.                                               |
| matches | Character vector naming groups to which query object belongs.                                                                                                                                                                                                                                                                                                                           |
| thresh  | object returned by <a href="#">findThreshold</a>                                                                                                                                                                                                                                                                                                                                        |
| params  | a list of input arguments and their values                                                                                                                                                                                                                                                                                                                                              |
| input   | list containing copies of <code>dvector</code> and <code>groups</code>                                                                                                                                                                                                                                                                                                                  |

**Author(s)**

Noah Hoffman

**See Also**[findThreshold](#)**Examples**

```
## illustrate classification using the Iris data set
data(iris)
dmat <- as.matrix(dist(iris[,1:4], method="euclidean"))
groups <- iris$Species

## remove one element from the data set and perform classification using
## the remaining elements as the reference set
ind <- 1
cat(paste('class of "unknown" sample is Iris',groups[ind]),fill=TRUE)
cc <- classify(dmat[-ind,-ind], groups[-ind], dvect=dmat[ind, -ind])
printClst(cc)

## this operation can be performed conveniently using the `pull` function
ind <- 51
cat(paste('class of "unknown" sample is Iris',groups[ind]),fill=TRUE)
cc <- do.call(classify, pull(dmat, groups, ind))
printClst(cc)
str(cc)
```

findThreshold

*findThreshold***Description**

Identify a distance threshold predicting whether a pairwise distance represents a comparison between objects in the same class (within-group comparison) or different classes (between-group comparison) given a matrix providing distances between objects and the group membership of each object.

**Usage**

```
findThreshold(dmat, groups, distances, method = "mutinfo", prob = 0.5,
              na.rm = FALSE, keep.dists = TRUE, roundCuts = 2, minCuts =
              20, maxCuts = 300, targetCuts = 100, verbose = FALSE,
              depth = 1, ...)

partition(dmat, groups, include, verbose = FALSE)
```

**Arguments**

|                         |                                                                                                                                                                  |
|-------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <code>dmatrix</code>    | Square matrix of pairwise distances.                                                                                                                             |
| <code>groups</code>     | Object coercible to a factor identifying group membership of objects corresponding to either edge of <code>dmatrix</code> .                                      |
| <code>include</code>    | vector (numeric or boolean) indicating which elements to retain in the output; comparisons including an excluded element will have a value of NA                 |
| <code>distances</code>  | Optional output of <code>partition</code> provided in the place of <code>dmatrix</code> and <code>groups</code>                                                  |
| <code>method</code>     | The method for calculating the threshold; only 'mutinfo' is currently implemented.                                                                               |
| <code>prob</code>       | Sets the upper and lower bounds of $D$ as some quantile of the within class distances and between-class differences, respectively.                               |
| <code>na.rm</code>      | If TRUE, excludes NA elements in <code>groups</code> and corresponding rows and columns in <code>dmatrix</code> . Ignored if <code>distances</code> is provided. |
| <code>keep.dists</code> | If TRUE, the output will contain the <code>distances</code> element (output of <code>partition</code> ).                                                         |
| <code>roundCuts</code>  | Number of digits to round cutoff values (see Details)                                                                                                            |
| <code>minCuts</code>    | Minimal length of vector of cutoffs (see Details).                                                                                                               |
| <code>maxCuts</code>    | Maximal length of vector of cutoffs (see Details)                                                                                                                |
| <code>targetCuts</code> | Length of vector of cutoffs if conditions met by <code>minCuts</code> and <code>maxCuts</code> are not met (see Details).                                        |
| <code>verbose</code>    | Terminal output is produced if TRUE.                                                                                                                             |
| <code>depth</code>      | Private argument used to track level of recursion.                                                                                                               |
| <code>...</code>        | Extra arguments are ignored.                                                                                                                                     |

**Details**

`findThreshold` is used internally in `classify`, but may also be used to calculate a starting value of  $D$ .

`partition` is used to transform a square (or lower triangular) distance matrix into a `data.frame` containing a column of distances (`$vals`) along with a factor (`$comparison`) defining each distance as a within- or between-group comparison. Columns `$row` and `$col` provide indices of corresponding rows and columns of `dmatrix`.

**Value**

In the case of `findThreshold`, output is a list with elements described below. In the case of `partition`, output is the `data.frame` returned as the element named `$distances` in the output of `findThreshold`.

|                       |                                                                                                               |
|-----------------------|---------------------------------------------------------------------------------------------------------------|
| <code>D</code>        | The distance threshold (distance cutoff corresponding to the PMMI).                                           |
| <code>pmmi</code>     | Value of the point of maximal mutual information (PMMI)                                                       |
| <code>interval</code> | A vector of length 2 indicating the upper and lower bounds over which values for the threshold are evaluated. |

|           |                                                                                                                              |
|-----------|------------------------------------------------------------------------------------------------------------------------------|
| breaks    | A data.frame with columns x and y providing candidate breakpoints and corresponding mutual information values, respectively. |
| distances | If keep.distances is TRUE, a data.frame containing pairwise distances identified as within- or between classes.              |
| method    | Character corresponding to input argument method.                                                                            |
| params    | Additional input parameters.                                                                                                 |

**Author(s)**

Noah Hoffman

**See Also**

[plotDistances](#), [plotMutinfo](#)

**Examples**

```
data(iris)
dmat <- as.matrix(dist(iris[,1:4], method="euclidean"))
groups <- iris$Species
thresh <- findThreshold(dmat, groups, type="mutinfo")
str(thresh)
```

---

|               |                                                              |
|---------------|--------------------------------------------------------------|
| plotDistances | <i>Visualize results of <code>link{findThreshold}</code></i> |
|---------------|--------------------------------------------------------------|

---

**Description**

The functions `plotDistances` and `plotMutinfo` are used to visualize the distance threshold calculated by [findThreshold](#) in the context of pairwise distances among objects in the reference set.

**Usage**

```
plotDistances(distances, D = NA, interval = NA,
              ylab = "distances", ...)

plotMutinfo(breaks, D = NA, interval = NA,
            xlab = "distance", ylab = "mutual information", ...)
```

**Arguments**

|           |                                                                              |
|-----------|------------------------------------------------------------------------------|
| distances | The \$distances element of the output value of <a href="#">findThreshold</a> |
| breaks    | The \$breaks element of the output value of <a href="#">findThreshold</a>    |
| D         | The distance threshold                                                       |
| interval  | The range of values over which candidate values of PMMI are evaluated.       |
| xlab      | Label the x axis of the plot.                                                |

ylab                Label the y axis of the plot.  
 ...                Additional arguments are passed to [bwplot](#) (plotDistances) or [xyplot](#)  
 (plotMutinfo)

### Details

plotDistances produces a box-and-whisker plot contrasting within- and between-group distances.  
 plotMutinfo produces a plot of cutpoints vs mutual information scores.

### Value

Returns a lattice grid object.

### Author(s)

Noah Hoffman

### See Also

[findThreshold](#)

### Examples

```
data(iris)
dmat <- as.matrix(dist(iris[,1:4], method="euclidean"))
groups <- iris$Species
thresh <- findThreshold(dmat, groups)
do.call(plotDistances, thresh)
do.call(plotMutinfo, thresh)
```

---

|           |                                                  |
|-----------|--------------------------------------------------|
| printClst | <i>Print a summary of the classifier output.</i> |
|-----------|--------------------------------------------------|

---

### Description

Prints a description of the output of classify.

### Usage

```
printClst(cc, rows = 8, nameWidth = 30, groupNames)
```

### Arguments

|            |                                                                                                                                                                 |
|------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------|
| cc         | Output of <a href="#">classify</a>                                                                                                                              |
| rows       | Number of rows corresponding to groups of reference objects to show.                                                                                            |
| nameWidth  | Character width of group names.                                                                                                                                 |
| groupNames | a named vector containing replacement names for groups keyed by categories in groups ( <a href="#">classify</a> ) or groupTab ( <a href="#">classifyIter</a> ). |

**Value**

Output value is NULL; output is to stdout.

**Author(s)**

Noah Hoffman

**See Also**

[classify](#), [classifyIter](#)

**Examples**

```
data(iris)
dmat <- as.matrix(dist(iris[,1:4], method="euclidean"))
groups <- iris$Species
```

---

|               |                                                  |
|---------------|--------------------------------------------------|
| scaleDistPlot | <i>Annotated multidimensional scaling plots.</i> |
|---------------|--------------------------------------------------|

---

**Description**

Produces annotated representations of two-dimensional multidimensional scaling plots using [cmdscale](#).

**Usage**

```
scaleDistPlot(dmat, groups, fill, X, O, indices = "no",
              include, display, labels,
              shuffleGlyphs = NA, key = "top",
              keyCols = 4, glyphs,
              xflip = FALSE, yflip = FALSE, ...)
```

**Arguments**

|         |                                                                                                            |
|---------|------------------------------------------------------------------------------------------------------------|
| dmat    | Square matrix of pairwise distances.                                                                       |
| groups  | Object coercible to a factor identifying group membership of objects corresponding to either edge of dmat. |
| fill    | vector (logical or indices) of points to fill                                                              |
| X       | vector of points to mark with an X                                                                         |
| O       | vector of points to mark with a circle                                                                     |
| indices | label points with indices (all points if 'yes', or a subset indicated by a vector)                         |
| include | boolean or numeric vector of elements to include in call to cmdscale                                       |
| display | boolean or numeric vector of elements to include in call to display                                        |

|               |                                                                                                      |
|---------------|------------------------------------------------------------------------------------------------------|
| labels        | list or data frame with parameters $\$i$ indicating indices and $\$text$ containing labels.          |
| shuffleGlyphs | modify permutation of shapes and colors given an integer to serve as a random seed.                  |
| key           | 'right' (single column), 'top' (variable number of columns), or NULL for no key                      |
| keyCols       | number of columns in key                                                                             |
| glyphs        | a data.frame with columns named col and pch corresponding to elements of <code>unique(groups)</code> |
| xflip         | if TRUE, flip orientation of x-axis                                                                  |
| yflip         | if TRUE, flip orientation of y-axis                                                                  |
| ...           | additional arguments are passed to <a href="#">xyplot</a>                                            |

**Value**

Returns a lattice grid object.

**Author(s)**

Noah Hoffman

**See Also**

[cmdscale](#), [xyplot](#)

**Examples**

```
data(iris)
dmat <- as.matrix(dist(iris[,1:4], method="euclidean"))
groups <- iris$Species

## visualize pairwise euclidean distances among items in the Iris data set
fig <- scaleDistPlot(dmat, groups)
plot(fig)

## leave-one-out analysis of the classifier
loo <- lapply(seq_along(groups), function(i){
  do.call(classify, pull(dmat, groups, i))
})
matches <- lapply(loo, function(x) rev(x)[[1]]$matches)
result <- sapply(matches, paste, collapse='-')
confusion <- sapply(matches, length) > 1
no_match <- sapply(matches, length) < 1
plot(scaleDistPlot(dmat, groups, fill=confusion, 0=confusion, X=no_match))
```

---

|       |                                |
|-------|--------------------------------|
| strep | <i>Streptococcus data set.</i> |
|-------|--------------------------------|

---

## Description

Square matrices describing pairwise distances among 16s rRNA sequences.

## Usage

```
data(strep)
```

## Format

```
List of 5
 $ dmat1 : num [1:150, 1:150] 0 5.81 8.38 10.28 10.64 ...
   ..- attr(*, "dimnames")=List of 2
   .. ..$ : chr [1:150] "197" "199" "207" "208" ...
   .. ..$ : chr [1:150] "197" "199" "207" "208" ...
 $ dmat2 : num [1:150, 1:150] 0 5.09 3.82 7.21 7.59 ...
   ..- attr(*, "dimnames")=List of 2
   .. ..$ : chr [1:150] "197" "199" "207" "208" ...
   .. ..$ : chr [1:150] "197" "199" "207" "208" ...
 $ dmat3 : num [1:150, 1:150] 0 5.63 5.81 8.77 9.14 ...
   ..- attr(*, "dimnames")=List of 2
   .. ..$ : chr [1:150] "197" "199" "207" "208" ...
   .. ..$ : chr [1:150] "197" "199" "207" "208" ...
 $ taxa  : Factor w/ 50 levels "Streptococcus acidominimus",...: 31 44 26 4 4 31 32 39 42 31 ...
 $ abbrev: Factor w/ 50 levels "S acidominimus",...: 31 44 26 4 4 31 32 39 42 31 ...
```

## Details

The matrices \$dmat1, dmat2, and dmat3 contain percent nucleotide difference with indels penalized heavily, little, and somewhat, respectively.

\$taxa is a factor of species names; abbreviations of the same names are found in \$abbrev.

## Examples

```
data(strep)
```

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