Package: clstutils (via r-universe)

November 2, 2026

Type Package

Title Tools for performing taxonomic assignment

Version 1.60.0

Depends R (>= 2.10), clst, rjson, ape

Imports lattice, RSQLite

Suggests RUnit

LazyLoad yes

LazyData yes

Author Noah Hoffman

Maintainer Noah Hoffman <ngh2@uw.edu>

Description Tools for performing taxonomic assignment based on phylogeny using pplacer and clst.

License GPL-3

biocViews Sequencing, Classification, Visualization, QualityControl

Repository Bioconductor 3.23

Date/Publication 2026-04-28 12:35:11 UTC

RemoteUrl https://github.com/bioc/clstutils

RemoteRef RELEASE_3_23

RemoteSha f02b6b9a57e5b33a6b0606f1414da79b4e15eaac

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`clstutils-package` *Sequence based classification and selection of reference sequences.*

Description

Tools for performing taxonomic assignment based on phylogeny using pplacer and clst.

Details

Package:	clstutils
Type:	Package
Author:	Noah Hoffman <ngh2@uw.edu>
License:	GPL3

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Author(s)

Noah Hoffman

Maintainer: <ngh2@uw.edu>

See Also

`clst`

Examples

```
library(clstutils)
packageDescription("clstutils")
```

classifyPlacements *Taxonomic classification by phylogenetic placement.*

Description

Given taxonomic information from a reference package and inter-node distances from a reference tree, perform classification of one or more placements provided by `pplacer`.

Usage

```
classifyPlacements(taxdata, treedists, placetab, ...,
    verbose = FALSE, debug = FALSE)
```

Arguments

taxdata	`data.frame`, output of `taxonomyFromRefpkg`
treedists	output of `treeDists`
placetab	a data.frame with columns `at`, `edge`, and `branch`
...	extra arguments passed to `classifyIter`
verbose	writes progress messages to terminal if TRUE
debug	be very verbose if TRUE

Value

The output is a `data.frame` describing the taxonomic assignment, along with a description of the confidence of the classification. See the man page for `classify` for details on the output.

Author(s)

Noah Hoffman

See Also

`treeDists`, `taxonomyFromRefpkg`

Examples

```
placefile <- system.file('extdata', 'merged.json', package='clstutils')
distfile <- system.file('extdata', 'merged.distmat.bz2', package='clstutils')
refpkgz <- system.file('extdata', 'vaginal_16s.refpkg.tar.gz', package='clstutils')

tmpdir <- tempdir()

orig.dir <- getwd()
setwd(tmpdir)
system(paste("tar --no-same-owner -xzf", refpkgz))
setwd(orig.dir)
```

```
refpkg <- file.path(tmpdir, "vaginal_16s.refpkg")

treedists <- treeDists(distfile=distfile, placefile=placefile)
taxdata <- taxonomyFromRefpkg(refpkg, seqnames=rownames(treedists$dmat), lowest_rank="species")
placetab <- data.frame(at=49, edge=5.14909e-07, branch=5.14909e-07)
result <- classifyPlacements(taxdata, treedists, placetab)
result
```

`findOutliers` *Identify outlier objects given a square distance matrix.*

Description

Outliers are defined as elements with edge length to the centermost element > cutoff. The distance threshold (cutoff) can be either specified, or calculated as a quantile of all pairwise distances in the matrix.

Usage

```
findOutliers(mat, quant, cutoff)
```

Arguments

`mat`	square matrix of distances
`quant`	given all pairwise distances x, calculate distance threshold as quantile(x, quant). Values closer to 0 are more stringent.
`cutoff`	an absolute cutoff overriding quant

Value

Returns a boolean vector corresponding to margin of mat; outliers have a value of TRUE.

Author(s)

Noah Hoffman

Examples

```
library(ape)
data(seqs)
data(seqdat)
dmat <- ape::dist.dna(seqs[seqdat$tax_name == 'Enterococcus faecium',],
        pairwise.deletion=TRUE, as.matrix=TRUE, model='raw')
summary(dmat[lower.tri(dmat)])
outliers <- findOutliers(dmat, cutoff=0.015)
table(outliers)
```

maxDists *Select a maximally diverse set of items given a distance matrix.*

Description

Given a square matrix of pairwise distances, return indices of N objects with a maximal sum of pairwise distances.

Usage

```
maxDists(mat, idx = NA, N = 1,
         exclude = rep(FALSE, nrow(mat)),
         include.center = TRUE)
```

Arguments

mat	square distance matrix
idx	starting indices; if missing, starts with the object with the maximum median distance to all other objects.
N	total number of selections; length of idx is subtracted.
exclude	boolean vector indicating elements to exclude from the calculation.
include.center	includes the "most central" element (ie, the one with the smallest median of pairwise distances to all other elements) if TRUE

Value

A vector of indices corresponding to the margin of mat.

Note

Note that it is important to evaluate if the candidate sequences contain outliers (for example, mislabeled sequences), because these will assuredly be included in a maximally diverse set of elements!

Author(s)

Noah Hoffman

See Also

findOutliers

Examples

```
library(ape)
library(clstutils)
data(seqs)
data(seqdat)
efaecium <- seqdat$tax_name == 'Enterococcus faecium'
seqdat <- subset(seqdat, efaecium)
seqs <- seqs[efaecium,]
dmat <- ape::dist.dna(seqs, pairwise.deletion=TRUE, as.matrix=TRUE, model='raw')

## find a maximally diverse set without first identifying outliers
picked <- maxDists(dmat, N=10)
picked
prettyTree(nj(dmat), groups=ifelse(1:nrow(dmat) %in% picked,'picked','not picked'))

## restrict selected elements to non-outliers
outliers <- findOutliers(dmat, cutoff=0.015)
picked <- maxDists(dmat, N=10, exclude=outliers)
picked
prettyTree(nj(dmat), groups=ifelse(1:nrow(dmat) %in% picked,'picked','not picked'),
X = outliers)
```

`prettyTree` *Draw an annotated phylogenetic tree.*

Description

Extends `plot.phylo` to draw a phylogenetic tree with additional annotation.

Usage

```
prettyTree(x, groups, fill,
           X, O, indices, labels,
           show = rep(TRUE, length(x)),
           largs = list(cex = 0.75, bty = "n", yjust = 0.5),
           parargs = list(mar = c(bottom = 5, left = 2, top = 2,
                                  right = ifelse(is.null(largs), 2, 8)),
               xpd = NA),
           pointargs = list(), glyphs,
           shuffleGlyphs = NA, ...)
```

Arguments

`x`	an object of class phylo, eg `x <- nj(ddist)`
`groups`	a factor (or object coercible) to a factor assigning group identity to leaf nodes in x

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)
labels	character vector of tip labels in the same order as x$tip.label
show	boolean vector of points to show
largs	arguments controlling appearance of the legend or NULL for no legend
parargs	arguments to pass par()
pointargs	arguments to pass points() (other than pch, col, bg)
glyphs	a data.frame with columns named 'col' and 'pch' corresponding to elements of unique(groups)
shuffleGlyphs	NA or an integer (argument to set.seed)
...	passed to plot.phylo

Details

prettyTree adds to a plot drawn by plot.phylo

Vectors specifying annotation should be in the order of row or column labels of the distance matrix used to generate x.

Value

Plots to the active device; no return value.

Note

See package vignette for additional examples.

Author(s)

Noah Hoffman

See Also

plot.phylo

Examples

```
library(ape)
data(seqs)
data(seqdat)
prettyTree(nj(dist.dna(seqs)), groups=seqdat$tax_name)
```

refpkgContents *Read the contents of a collection of reference sequences ("refpkg").*

Description

Read the manifest file from a refpackage and return a list containing the package contents.

Usage

```
refpkgContents(path, manifest = "CONTENTS.json")
```

Arguments

path	path to a refpkg directory
manifest	name of the manifest file

Value

Returns a list of lists. Run `example(refpkgContents)` for details.

Author(s)

Noah Hoffman

References

The decsription and specification for a reference package can be found in the project repository in github: https://github.com/fhcrc/taxtastic

Scripts and tools for creating reference packages are provided in the python package `taxonomy`, also available from the taxtastic project site.

See Also

taxonomyFromRefpkg

Examples

```
archive <- 'vaginal_16s.refpkg.tar.gz'
destdir <- tempdir()
system(gettextf('tar -xzf %s --directory="%s"',
                system.file('extdata',archive,package='clstutils'),
                destdir))
refpkg <- file.path(destdir, sub('.tar.gz','',archive))
contents <- refpkgContents(refpkg)
str(refpkg)
```

seqdat *Annotation for the Enterococcus sequence data set.*

Description

Provides annotation for `link{seqs}`, an aligned 16S rRNA sequences representing three Enterococcus species.

Usage

```
data(seqdat)
```

Format

A data frame with 200 observations on the following 5 variables.

`seqname` a character vector

`accession` a character vector containing GenBank accession numbers.

`tax_id` a character vector

`tax_name` a character vector

`isType` a logical vector indicating if the sequence is from a type strain.

Source

These sequences were downloaded from the Ribosomal Database Project website http://rdp.cme.msu.edu/

Examples

```
data(seqdat)
with(seqdat,{
table(tax_name, isType)
})
```

seqs *Enterococcus sequence data set.*

Description

Aligned 16S rRNA sequences representing three Enterococcus species.

Usage

```
data(seqs)
```

Format

The format is: 'DNAbin' raw [1:200, 1:1848] - - - - ... - attr(*, "dimnames")=List of 2 ..$: chr [1:200] "S000001976" "S000008133" "S000013428" "S000127028" ... ..$: NULL

Source

These sequences were downloaded from the Ribosomal Database Project website http://rdp.cme.msu.edu/

Examples

```
data(seqs)
seqs
```

---

taxonomyFromRefpkg *Extract taxonomic information from a refpkg.*

Description

Construct a data.frame providing the lineage of each sequence represented in the reference package.

Usage

```
taxonomyFromRefpkg(path, seqnames, lowest_rank = NA)
```

Arguments

path	path to a refpkg directory
seqnames	optional character vector of sequence names. If provided, determines the order of rows in $taxTab
lowest_rank	name of the most specific (ie, rightmost) rank to include. Default is the name of the rightmost column in refpkg_contents$taxonomy

Value

A list with the following elements:

taxNames	a named character vector of taxonomic names (names are tax_ids)
taxTab	a data.frame in which each row corresponds to a reference sequence and contains a tax_id followed by the corresponding lineage (columns are "root"...lowest_rank)

Author(s)

Noah Hoffman

References

The decsription and specification for a reference package can be found in the project repository in github: https://github.com/fhcrc/taxtastic

Scripts and tools for creating reference packages are provided in the python package `taxonomy`, also available from the taxtastic project site.

See Also

refpkgContents

Examples

```
archive <- 'vaginal_16s.refpkg.tar.gz'
destdir <- tempdir()
system(gettextf('tar -xzf %s --directory="%s"',
                system.file('extdata',archive,package='clstutils'),
                destdir))
refpkg <- file.path(destdir, sub('.tar.gz','',archive))
reftax <- taxonomyFromRefpkg(refpkg)
str(reftax)
```

`treeDists` *Provide objects for determining distances among nodes of a reference tree.*

Description

Provides objects (dists, paths) that can be used to calculate vectors of distances between an internal node and each leaf node. Also returns a square matrix of distances between leaf nodes.

Usage

```
treeDists(placefile, distfile)
```

Arguments

`placefile`	path to `pplacer` output
`distfile`	path to output of guppy `distmat`

Details

A placement on an edge looks like this:

```
proximal
  |
  |   d_p
  |
```

```
  |---- x
  |
  |   d_d
  |
  |
distal
```

d_p is the distance from the placement x to the proximal side of the edge, and d_d the distance to the distal side.

If the distance from x to a leaf y is an S-distance Q, then the path from x to y will go through the distal side of the edge and we will need to add d_d to Q to get the distance from x to y. If the distance from x to a leaf y is a P-distance Q, then the path from x to y will go through the proximal side of the edge, and we will need to subtract off d_d from Q to get the distance from x to y. In either case, we always need to add the length of the pendant edge, which is the second column.

To review, say the values of the two leftmost columns are a and b for a given placement x, and that it is on an edge i. We are interested in the distance of x to a leaf y, which is on edge j. We look at the distance matrix, entry (i,j), and say it is an S-distance Q. Then our distance is Q+a+b. If it is a P-distance Q, then the distance is Q-a+b.

The distances between leaves should always be P-distances, and there we need no trickery.

(thanks to Erick Matsen for this description)

Value

A list with the following elements:

`dists`	rectangular matrix of distances with rows corresponding to all nodes in pplacer order, and columns corresponding to tips in the order of the corresponding `phylo{ape}` object.
`paths`	rectangular matrix in the same configuration as `dists` with values of 1 or -1 if the path between nodes is serial or parallel, respectively (see Details)
`dmat`	square matrix containing distances between pairs of tips.

Note

The output of this function is required for `classifyPlacements`.

Author(s)

Noah Hoffman

References

Documentation for `pplacer` and `guppy` can be found here: `http://matsen.fhcrc.org/pplacer/`

See Also

`classifyPlacements`

Examples

```
placefile <- system.file('extdata','merged.json', package='clstutils')
distfile <- system.file('extdata','merged.distmat.bz2', package='clstutils')
treedists <- treeDists(placefile, distfile)

## coordinates of a single placement
placetab <- data.frame(at=49, edge=5.14909e-07, branch=5.14909e-07)

## dvects is a matrix in which each row corresponds to a vector of
## distances between a single placement along the edge of the reference
## tree used to generate 'distfile', and each column correspons to a
## reference sequence (ie, a terminal node).

dvects <- with(placetab, {
treedists$dists[at+1,,drop=FALSE] + treedists$paths[at+1,,drop=FALSE]*edge + branch
})
```

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