# Package 'ClockstaRG'

July 29, 2014

Type Package

Title ClockstaRG: An implementation of ClockstaR for genomic data  Version 0.1  Date 2014-07-28  Author Sebastian Duchene  Maintainer Sebastian Duchene <sebastian.duchene@sydney.edu.au>  Description ClockstaRG is an implementation of ClockstaR for large data sets. Some steps of the analysis can be run in parallel. It also includes a fast clustering algorithm, CLARA.  Depends R (&gt;= 2.15.0), ape (&gt;= 3.0-8), cluster (&gt;= 1.14.4), phangorn (&gt;= 1.7-4), ClockstaR2 (&gt;= 2.0)  License GPL (&gt;=2)  R topics documented:  ClockstaRG-package boot.clara fill.matrix fold.sbsd get.gap get.sbsd make.tree.comps optim.trees.g</sebastian.duchene@sydney.edu.au>
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ClockstaRG-package

ClockstaRG: An implementation of ClockstaR for genomic data

## **Description**

CLockstaRG is an implementation of ClockstaR for large genomic data sets. Some of the steps in the algorithm, such as optimising the branch lengths of the trees, and estimating the tree distances can be run in parallel. This implementation also includes an fast clustering algorithm, CLARA, for large data sets.

#### **Details**

Package: ClockstaRG
Type: Package
Version: 1.0

Date: 2014-07-28 License: GPL (<= 2)

#### Author(s)

Sebastian Duchene

Maintainer: Sebastian Duchene <sebastian.duchene@sydney.edu.au>

#### References

Duchêne, S, Molak, M., and Ho, SYW. "ClockstaR: choosing the number of relaxed-clock models in molecular phylogenetic analysis." Bioinformatics (2014) 30 (7):1017-1019

#### See Also

github.com/sebastianduchene/clockstar github.com/sebastianduchene/nelsi

boot.clara

boot.clara performs a parametric bootstrap of the sBSDmin distances among trees. For every bootstrap replicate it calculates the cluster width (Wk) or the silhouette width (Sk), depending on whether run.clara.sk, or run.clara.sil is used. See the tutorial for details and instructions.

#### **Description**

boot.clara performs a parametric bootstrap of the sBSDmin distances among trees. For every bootstrap replicate it calculates the cluster width (Wk) or the silhouette width (Sk), depending on whether run.clara.sk, or run.clara.sil is used. See the tutorial for details and instructions.

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#### Usage

boot.clara(clus.matrix.name, out.boot.name = "out\_boot.txt", nboot = 10, k.range = NULL, boot.te

#### Arguments

clus.matrix.name

The name of the file with the matrix with the MDS points, obtained with run.mds

out.boot.name Name of the output file.

nboot Number of bootstrap replicates to perform for every value of 'k'.

k.range Range of values of 'k'

boot.temp.name Name of temporary files of the bootstrap data. This is deleted after runing

CLARA for the range of 'k' specified.

FUNboot The function to use. run.clara.wk for cluster width, or run.clara.sil for silhouette

width.

## **Details**

Please see the tutorial for instructions.

#### Value

This function does not return a value to the console. It writes a text file with the statistic, Wk or Sk, for the bootstrap replicates

#### Author(s)

Sebastian Duchene

## References

Kaufman, L., & Rousseeuw, P. J. (2009). Finding groups in data: an introduction to cluster analysis (Vol. 344). John Wiley & Sons.

fill.matrix fills the NA values in the pairwise sBSDmin matrix obtained with fold.sbsd

## **Description**

fill.matirx fills the NA values in the pairwise sBSDmin matrix obtained with fold.sbsd

## Usage

```
fill.matrix(matrix.name, new.matrix.name = NULL)
```

# **Arguments**

matrix.name The name of the text file of the matrix obtained with fold.sbsd. new.matrix.name

The file name of the matrix with filled NA values.

4 fold.sbsd

#### **Details**

Please see the tutorial for instructions on how to use this function.

#### Value

This function does not return a value to the prompt. The output is text file. Please see the tutorial for instructions on how to use this function.

#### Note

None. Please see the tutorial for instructions on how to use this function.

## Author(s)

Sebastian Duchene

fold.sbsd	fold.sbsd formats the sBSDmin distances calculated with get.sbsd to
	be used in clustering algorithms.

## **Description**

fold.sbsd folds the output of get.sbsd into a pairwise matrix that can be used in clustering algorithms.

## Usage

```
fold.sbsd(trees.file, comps.file, out.name = "test.fold.txt", method = "lite", comps.range = NUL
```

## **Arguments**

trees.file	The file with the gene trees, as produced in optim.trees.g
comps.file	The file with the sBSDmin distances among pairs of trees.
out.name	The name of the output file.
method	There are two methods available: 'memory' and 'lite'. The 'memory' method loads all the sBSDmin distances into RAM, while the 'lite' method reads one at a time. The 'memory' method is faster, but with 'lite' it is possible to overcome memory limitations from very large files.
comps.range	A sequence of integers. This is the range of sBSDmin distances to read and format into the pairwise matrix. Use this for very large files that are difficult to read into RAM.

# **Details**

None. See the tutorial for instructions and deatails on some of the settings.

## Value

This function does not return a value to the prompt. Instead, it writes a text file with the pairwise distance matrix. Note that it only prints the below diagonal values of the matrix, and the rest is filled with NA. To complete these values in the matrix use fill.matrix. This is a requirement of some clusteing algorithms.

get.gap 5

#### Note

See the tutorial for instructions and deatails on some of the settings.

#### Author(s)

Sebastian Duchene

get.gap

Get gap statistic.

## **Description**

get.gap obtains the gap statistic for a range of Wk and bootstrap replicates.

#### Usage

```
get.gap(true.data, boot.data)
```

#### **Arguments**

true.data The data with Wk for a range of k. Note that this is not the file name, but the

data loaded as a matrix or data fram in R.

boot.data The data with Wk for bootstrap replicates for a range of k. Note that this is not

the file name, but the data loaded as a matrix or data fram in R.

## **Details**

Please see the tutorial for instructions.

#### Value

A matrix with the Gap statistic and the standard errors (SE). The first column is the Gap, and the second is the SE.

#### Note

Please see the tutorial and the documentation for 'clusGap' function of the 'cluster' package for more details.

# Author(s)

Sebastian Duchene

#### References

Tibshirani, R., Walther, G. and Hastie, T. (2001). Estimating the number of data clusters via the Gap statistic. \_Journal of the Royal Statistical Society B\_, \*63\*, 411-423.

Tibshirani, R., Walther, G. and Hastie, T. (2000). Estimating the number of clusters in a dataset via the Gap statistic. Technical Report. Stanford.

Per Broberg (2006). SAGx: Statistical Analysis of the GeneChip. R package version 1.9.7. <URL: http://home.swipnet.se/pibroberg/expression\_hemsida1.html>

get.sbsd

get.sbsd	get.sbsd calculates the sBSDmin distance for pairs of trees. It is sim-
	ilar to the function bsd.dist in ClockstaR2, but it can handle data sets with many trees.

# Description

get.sbsd calculates the sBSDmin distance for pairs of trees. It is similar to the function bsd.dist in ClockstaR2, but it can handle data sets with many trees.

# Usage

```
get.sbsd(trees.file, comps.file, method = "lite", range.comps = NULL, out.file = "sbsd.txt")
```

# Arguments

trees.file	The name of the file with the gene trees. This is a newick with a list of the gene trees with branch lengths. The trees can include names. See the tutorial and example files for details.
comps.file	The name of the file with the tree comparissons.
method	There are two methods available: 'memory' and 'lite'. Use 'memory' to load all the trees in RAM. Use 'lite' to read the trees one at a time, so it can be parallelised over different machines or processors. The method 'memory' is faster, i the analysis is not run in parallel.
range.comps	This is useful for the 'lite' method. In this case it is possible to run several instances of the analysis, each for a range of sBSDmin distances among trees.
out.file	The name of the file to write the output.

# **Details**

Please see the tutorial for instructions.

## Value

This function does not return a value to the prompt. It saves the output to a text file.

# Note

NONE

# Author(s)

Sebastian Duchene

## See Also

NONE

make.tree.comps 7

make.tree.comps This function creates a file with the names of the pairwise comparissons for all trees.	
---	--

# Description

This function creates a file with the names of the pairwise comparissons for all trees.

## Usage

```
make.tree.comps(trees.file, tree.comps = "treecomps.txt")
```

# **Arguments**

trees.file Name of file with the trees

tree.comps Name of file to write the list of tree comparissons

## **Details**

None. See the tutorial for instructions on how to run.

#### Value

This function does not return values on the command prompt. It creates a text file with the tree comparissons. See the tutorial for instructions on how to run.

#### Note

See the tutorial for instructions on how to run.

## Author(s)

Sebastian Duchene

#### References

**NONE** 

optim.trees.g is can be used to optimise the branch lengths for a tree topology over many alignments. Please see the tutorial for instructions to use.
nons to use.

# Description

This function is practical for large data sets. For data sets with less than 20 genes, it may be sufficient to use the standard version of ClockstaR. Please see the tutorial for instructions on how to use.

8 optim.trees.g

## Usage

```
optim.trees.g(data.folder, init.alin = NULL, end.alin = NULL, out.trees = "out.trees", model.tes
```

## **Arguments**

data.folder	This is the folder with the individual alignments in fasta files and a tree topology to optimise the branch lengths.
init.alin	The number of the first alignment. This is useful for runing several instances of this function. Please see the tutorial for instructions on how to use.
end.alin	The number of the first alignment. This is useful for runing several instances of this function. Please see the tutorial for instructions on how to use.
out.trees	A character. The name of the file to write the optimised trees.
model.test	A logical. Select T for model selection. The default is F. It is recommended to leave the default because it can be very slow to run
out.models	The name of the file to write the models to.

## **Details**

Please see the tutorial for instructions on how to use

## Value

The function does not return anything to the prompt. It saves the trees with optimised branch lenghts to the file specified.

## Author(s)

Sebastian Duchene

#### References

Duchêne, S, Molak, M., and Ho, SYW. "ClockstaR: choosing the number of relaxed-clock models in molecular phylogenetic analysis." Bioinformatics (2014) 30 (7):1017-1019

#### See Also

optim.trees.interactive in ClockstaR

# **Examples**

```
## Not run:
optim.trees.g(data_folder)
## End(Not run)
```

run.clara.sil

run.clara.sil	run.clara is used to run the CLARA algorithm from package 'cluster'. For values of 'k' from 2:N, it estimates the average silhouette width.

## **Description**

run.clara is used to run the CLARA algorithm from package 'cluster'. For values of 'k' from 2:N, it estimates the average silhouette width.

# Usage

```
run.clara.sil(clus.matrix.name, out.clus.name = "out_clus_sil.txt", k.range = NULL)
```

#### **Arguments**

clus.matrix.name

This is the filename of the MDS of the sBSDmin distances for pairs of trees.

of k in k.range.

k. range The range of 'k' values to calculate Wk.

... Other arguments passed to the 'clara' function from pacakge 'cluster'.

#### **Details**

Please see the tutorial for instructions.

#### Value

This function does not return a value to the prompt. It writes a text file with the average silhouette width for values of k.

# Author(s)

Sebastian Duchene

## References

Kaufman, L., & Rousseeuw, P. J. (2009). Finding groups in data: an introduction to cluster analysis (Vol. 344). John Wiley & Sons.

10 run.clara.wk

run.clara.wk	run.clara is used to run the CLARA algorithm on the MDS of the sB-SDmin distances for pairs of trees. For every value of 'k' it estimates the cluster width, 'Wk'.
	the cluster width, wk.

## **Description**

run.clara is a raper from the CLARA algorithm ,implemented in the package 'cluster. It can be run for a range of values of k.

# Usage

```
run.clara.wk(clus.matrix.name, out.clus.name = "out_clus_wk.txt", k.range = NULL, ...)
```

## **Arguments**

clus.matrix.name

This is the filename of the MDS of the sBSDmin distances for pairs of trees.

out.clus.name

The name of the out put name of the avearage cluster width (Wk) for the values

of k in k.range.

k.range

The range of 'k' values to calculate Wk.

. . .

Other arguments passed to the 'clara' function from pacakge 'cluster'.

## **Details**

Please see the tutorial for instructions.

# Value

This function does not return a value to the prompt. It writes a text file with Wk for values of k.

# Author(s)

Sebastian Duchene

## References

Kaufman, L., & Rousseeuw, P. J. (2009). Finding groups in data: an introduction to cluster analysis (Vol. 344). John Wiley & Sons.

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run.mds	run.mds obtains a multidimensional scaling (MDS) of the pariwise sB- SDmin distances between trees.
	22 mm distances convectivities.

# Description

run.mds obtains a multidimensional scaling (MDS) of the pariwise sBSDmin distances between trees.

# Usage

```
run.mds(matrix.name, out.mds.name = "test_mds.txt")
```

## **Arguments**

matrix.name The path and name of the file with the pairwise sBSDmin distances between trees.

out.mds.name The name of the output files. Please see the tutorial for instructions.

# **Details**

None. Please see the tutorial for instructions.

#### Value

This function does not return an object to the prompt. Instead, it returns two text files: The points of the MDS of the sBSDmin distances, and the eigen values.

## Author(s)

Sebastian Duchene

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