Package: MSCquartets (via r-universe)

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Type Package

Title Analyzing Gene Tree Quartets under the Multi-Species Coalescent

Version 2.0.1

Description Methods for analyzing and using quartets displayed on a collection of gene trees, primarily to make inferences about the species tree or network under the multi-species coalescent model. These include quartet hypothesis tests for the model, as developed by Mitchell et al. (2019) <doi:10.1214/19-EJS1576>, simplex plots of quartet concordance factors as presented by Allman et al. (2020) <doi:10.1101/2020.02.13.948083>, species tree inference methods based on quartet distances of Rhodes (2019) <doi:10.1109/TCBB.2019.2917204> and Yourdkhani and Rhodes (2019) <doi:10.1007/s11538-020-00773-4>, the NANUQ algorithm for inference of level-1 species networks of Allman et al. (2019) <doi:10.1186/s13015-019-0159-2>, and the TINNIK algorithm for inference of the tree of blobs of an arbitrary network of Allman et al.(2022) <doi:10.1007/s00285-022-01838-9>. Software announcement by Rhodes et al. (2020) <doi:10.1093/bioinformatics/btaa868>.

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Imports zipfR, graphics, stats, Rdpack, foreach, doParallel, methods, Rcpp (>= 1.0.10), igraph (>= 2.0.0)

RdMacros Rdpack

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LazyData true

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NeedsCompilation yes

LinkingTo Rcpp, RcppProgress

Depends R (>= 3.5.0), ape (>= 5.0), phangorn

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Suggests knitr, rmarkdown

VignetteBuilder knitr

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Contents

`MSCquartets-package` *Multispecies Coalescent Model Quartet Package*

Description

A package for analyzing quartets displayed on gene trees, under the multispecies coalescent (MSC) model and network multispecies coalescet model (NMSC).

Details

This package contains routines to analyze a collection of gene trees through the displayed quartets on them.

A quartet count concordance factor (qcCF) for a set of 4 taxa is the triple of counts of the three possible resolved quartet trees on those taxa across some set of gene trees. The major routines in this package can:

1. Tabulate all qcCFs for a collection of gene trees.

2. Perform hypothesis tests of whether one or more qcCFs are consistent with the MSC model on a species tree (Mitchell et al. 2019).
3. Produce simplex plots showing all estimated CFs as well as results of hypothesis tests (Allman et al. 2021).
4. Infer a species tree using the qcCFs via the QDC and WQDC methods (Rhodes 2020; Yourdkhani and Rhodes 2020).
5. Infer a level-1 species network via the NANUQ method (Allman et al. 2019).
6. Infer the tree of blobs for a species network via the TINNiK method (Allman et al. 2022),(Allman et al. 2024).

As discussed in the cited works, the inference methods for species trees and networks are statistically consistent under the MSC and Network MSC respectively.

This package, and the theory on which it is based, allows gene trees to have missing taxa (i.e., not all gene trees display all the taxa). It does require that each subset of 4 taxa is displayed on at least one of the gene trees.

Several gene tree data sets, simulated and empirical, are included.

In publications please cite the software announcement (Rhodes et al. 2020), as well as the appropriate paper(s) above developing the theory behind the routines you used.

Author(s)

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References

Rhodes JA, Baños H, Mitchell JD, Allman ES (2020). "MSCquartets 1.0: Quartet methods for species trees and networks under the multispecies coalescent model in R." *Bioinformatics*. doi:10.1093/bioinformatics/btaa868.

Mitchell J, Allman ES, Rhodes JA (2019). "Hypothesis testing near singularities and boundaries." *Electron. J. Statist.*, **13**(1), 2150-2193. doi:10.1214/19EJS1576.

Allman ES, Mitchell JD, Rhodes JA (2021). "Gene Tree Discord, Simplex Plots, and Statistical Tests under the Coalescent." *Systematic Biology*, **71**(4), 929-942. ISSN 1063-5157, doi:10.1093/sysbio/syab008, https://academic.oup.com/sysbio/article-pdf/71/4/929/44114555/syab008.pdf.

Rhodes JA (2020). "Topological metrizations of trees, and new quartet methods of tree inference." *IEEE/ACM Trans. Comput. Biol. Bioinform.*, **17**(6), 2107-2118. doi:10.1109/TCBB.2019.2917204.

Yourdkhani S, Rhodes JA (2020). "Inferring metric trees from weighted quartets via an intertaxon distance." *Bul. Math. Biol.*, **82**(97). doi:10.1007/s11538020007734.

Allman ES, Baños H, Rhodes JA (2019). "NANUQ: A method for inferring species networks from gene trees under the coalescent model." *Algorithms Mol. Biol.*, **14**(24), 1-25. doi:10.1186/s13015-01901592.

Allman ES, Baños H, Mitchell JD, Rhodes JA (2022). "The tree of blobs of a species network: identifiability under the coalescent." *Journal of Mathematical Biology*, **86**(1), 10. doi:10.1007/s00285022018389.

Allman ES, Baños H, Mitchell JD, Rhodes JA (2024). "TINNiK: Inference of the Tree of Blobs of a Species Network Under the Coalescent." *bioRxiv*. doi:10.1101/2024.04.20.590418, `https://www.biorxiv.org/content/10.1101/2024.04.20.590418v1`.

`BQinference` *Main loop of B-quartet inference*

Description

This is a C++ function, called from `TINNIKdist`, to infer B and T quartets.

Usage

```
BQinference(pTable, C, Cn4, n, Bquartets, L1, lenL1, Nrule1, Nrule2, cuttops)
```

Arguments

`pTable`	a quartet table with p-values
`C`	precomputed binomial coefficients
`Cn4`	precomputed binomial coefficient
`n`	number of taxa
`Bquartets`	0/1 vector of initial Bquartets
`L1`	vector of recently inferred B quartets
`lenL1`	lnegth of L1
`Nrule1`	count of inference from rule 1
`Nrule2`	count of inference from rule 2
`cuttops`	inferred cut topologies

See Also

`quartetTable`, `quartetTableParallel`

`collapseEdges` *Collapse short tree edges*

Description

Set all edges of a tree with short lengths to be zero.

Usage

```
collapseEdges(tree, delta)
```

Arguments

`tree`	a phylo object
`delta`	minimum edge length to retain

Value

a phylo object

Examples

```
tree=read.tree(text="((a:1,b:1):.5,(c:.5,d:2):1);")
newtree=collapseEdges(tree,delta=1)
write.tree(newtree)
```

`compatibleSplits` *Extract compatible splits*

Description

Given an object of class splits, first discards any with weight less than a tolerance, and then further removes all remaining splits that are incompatible with any other remaining one.

Usage

```
compatibleSplits(sp, tol = 0, plot = FALSE)
```

Arguments

`sp`	an object of class splits
`tol`	splits with weights below tol are dropped
`plot`	a logical; if TRUE plots tree displaying remaining spilts

Value

splits objects containing only those that are compatible and high weight

See Also

`treeFromSplits`, `TINNIK`

Examples

```
data(pTableYeastRokas)
dist=NANUQdist(pTableYeastRokas, alpha=.05, beta=.95,outfile=NULL)
nn=neighborNet(dist)
plot(nn,"2D")
tob=treeFromSplits(compatibleSplits(nn$splits),plot=TRUE) #produce tree of blobs of splits graph
```

`cutDensity` *Probability density function for Cut Model*

Description

Value of probability density function for Cut Model of Allman et al. (2024), Section 3.

Usage

```
cutDensity(lambda, mu0, alpha0, beta0)
```

Arguments

`lambda`	statistic value (e.g., likelihood ratio statistic, or other power divergence statistic)
`mu0`	parameter of density function
`alpha0`	parameter of density function
`beta0`	parameter of density function

Value

value of density function

References

Allman ES, Baños H, Mitchell JD, Rhodes JA (2024). “TINNiK: Inference of the Tree of Blobs of a Species Network Under the Coalescent.” *bioRxiv*. doi:10.1101/2024.04.20.590418, `https://www.biorxiv.org/content/10.1101/2024.04.20.590418v1`.

See Also

`T1density`,`T3density`

`dataGeneTreeSample` *Simulated gene tree dataset from species tree*

Description

A text file dataset containing 1000 gene trees on 9 taxa simulated under the MSC on a species tree

Format

A text file with 1000 metric Newick gene trees on the taxa t1-t9

Details

This simulated dataset was produced by SimPhy (Mallo et al. 2016), using the species tree

((((t5:5000,t6:5000):5000,t4:10000):2500,t7:12500):7500,((t8:3000,t9:3000):5000,
((t1:4000,t2:4000):2500,t3:6500):1500):12000);

with a population size of 10,000 throughout the tree.

File is accessed as `system.file("extdata","dataGeneTreeSample",package="MSCquartets")`, for example via the ape command:

```
gts=read.tree(file = system.file("extdata","dataGeneTreeSample",package="MSCquartets")
)
```

References

Mallo D, De Oliveira Martins L, Posada D (2016). "SimPhy: Phylogenomic Simulation of Gene, Locus, and Species Trees." *Syst. Biol.*, **65**(2), 334-344. doi:10.1093/sysbio/syv082, `http://dx.doi.org/10.1093/sysbio/syv082`.

`dataHeliconiusMartin` *Heliconius gene tree dataset*

Description

A text file dataset for Heliconius butterflies containing 2909 gene trees on 7 taxa, with 4 individuals sampled for each of 3 of the taxa, for a total of 16 leaves per gene tree. This is a subset of the data of Martin et al. (2013).

Format

A text file with 2909 metric Newick gene trees each with 16 leaves labelled:
chioneus.553, chioneus.560, chioneus.564, chioneus.565,
ethilla.67, hecale.273, melpomeneFG.13435, melpomeneFG.9315,
melpomeneFG.9316, melpomeneFG.9317, pardalinus.371, rosina.2071,
rosina.531, rosina.533, rosina.546, sergestus.202

Details

File is accessed as `system.file("extdata","dataHeliconiusMartin",package="MSCquartets")`, for example via the ape command:

`gts = read.tree(file=system.file("extdata","dataHeliconiusMartin",package="MSCquartets"))`

Source

doi:10.5061/dryad.dk712

References

Martin SH, K.K. D, Nadeau NJ, Salazar C, Walters JR, Simpson F, Blaxter M, Manica A, Mallet J, Jiggins CD (2013). "Genome-wide evidence for speciation with gene flow in Heliconius butterflies." *Genome Res*, **23**, 1817-1828.

`dataPapioniniVanderpool` *Papionini gene tree dataset*

Description

A text file dataset for Papionini containing 1730 gene trees on 7 taxa. This is a subset of the data of Vanderpool et al. (2020).

Format

A text file with 1703 metric Newick gene trees each with 7 leaves labelled:
Cercocebus_atys, Mandrillus_leucophaeus, Papio_anubis, Theropithecus_gelada, Macaca_fascicularis, Macaca_mulatta, Macaca_nemestrina

Details

File is accessed as `system.file("extdata","dataPapioniniVanderpool",package="MSCquartets")`, for example via the ape command:

`gts = read.tree(file=system.file("extdata","dataPapioniniVanderpool",package="MSCquartets"))`

Source

doi:10.5061/dryad.rfj6q577d

References

Vanderpool D, Minh BQ, Lanfear R, Hughes D, Murali S, Harris RA, Raveendran M, Muzny DM, Hibbins MS, Williamson RJ, Gibbs RA, Worley KC, Rogers J, Hahn MW (2020). "Primate phylogenomics uncovers multiple rapid radiations and ancient interspecific introgression." *PLOS Biology*, **18**(12), 1-27. doi:10.1371/journal.pbio.3000954.

`dataYeastRokas` *Yeast gene tree dataset*

Description

A text file dataset for Yeast containing 106 gene trees on 8 taxa (7 Saccharomyces and 1 Candida outgroup). This is a subset of the data of Rokas et al. (2003).

Format

A text file with 106 topological Newick gene trees on the taxa: Sbay, Scas, Scer, Sklu, Skud, Smik, Spar, and Calb (outgroup).

Details

File is accessed as `system.file("extdata","dataYeastRokas",package="MSCquartets")`, for example via the ape command:

```
gts=read.tree(file = system.file("extdata","dataYeastRokas",package="MSCquartets"))
```

Source

https://wiki.rice.edu/confluence/download/attachments/8898533/yeast.trees?version=1&modificationDate=1360603275797&api=v2

References

Rokas A, Williams B, Carrol S (2003). “Genome-scale approaches to resolving incongruence in molecular phylogenies.” *Nature*, **425**, 798–804.

`estimateEdgeLengths` *Estimate edge lengths on a species tree from gene tree quartet counts*

Description

Estimate edge lengths, in coalescent units, on an unrooted species tree from a table of resolved quartet counts from a collection of gene trees.

Usage

```
estimateEdgeLengths(tree, rqt, terminal = 1, method = "simpleML", lambda = 1/2)
```

Arguments

`tree`	a phylo object, giving a resolved tree on which to estimate edge lengths
`rqt`	a resolved quartet table, as from `quartetTableResolved`, in which all taxa on `tree` appear
`terminal`	an edge length to assign to terminal edges, whose lengths cannot be estimated
`method`	`"simpleML"` or `"simpleBayes"`
`lambda`	a positive parameter for the `"simpleBayes"` method

Details

While the argument `tree` may be supplied as rooted or unrooted, metric or topological, only its unrooted topology will be used for determining new metric estimates.

Counts of quartets for all those quartets which define a single edge on the tree (i.e., whose internal edge is the single edge on the unrooted input tree) are summed, and from this an estimate of the branch length is computed. If `method= "simpleML"` this is the maximum likelihood estimate. If `method="simpleBayes"` this is the Bayesian estimate of Theorem 2 of Sayyari and Mirarab (2016), using parameter `lambda`. Using `lambda=1/2` gives a flat prior on [1/3,1] for the probability of the quartet displayed on the species tree.

These methods are referred to as ‘simple’ since they use only the quartets defining a single edge of the species tree. Quartets with central edges composed of several edges in the species tree are ignored.

Note that branch length estimates may be 0 (if the count for the quartet displayed on the input tree is not dominant), positive, or `Inf` (if the counts for quartet topologies not displayed on the input tree are all 0, and `method="simpleML"`).

Value

an unrooted metric tree with the same topology as `tree`, of type phylo

References

Sayyari E, Mirarab S (2016). “Fast Coalescent-Based Computation of Local Branch Support from Quartet Frequencies.” *Mol. Biol. Evol.*, **33**(7), 1654-1668.

Examples

```
gtrees=read.tree(file=system.file("extdata","dataGeneTreeSample",package="MSCquartets"))
taxanames=taxonNames(gtrees)
QT=quartetTable(gtrees,taxanames[1:6])
RQT=quartetTableResolved(QT)
DQT=quartetTableDominant(RQT)
tree=QDS(DQT)
write.tree(tree)
plot(tree)
metricMTree=estimateEdgeLengths(tree,RQT,method="simpleML")
write.tree(metricMTree)
plot(metricMTree)
metricBTree=estimateEdgeLengths(tree,RQT,method="simpleBayes")
```

```
write.tree(metricBTree)
plot(metricBTree)
```

`expectedCFs` *Produce table of expected quartet concordance factors for a species tree*

Description

Compiles table of expected quartet concordance factors (CFs) for gene trees under the MSC model on a metric species tree.

Usage

```
expectedCFs(speciestree, plot = TRUE, model = "T1", cex = 1)
```

Arguments

`speciestree`	phylo or character object specifying un/rooted metric species tree
`plot`	`TRUE` (default) to produce simplex plot of CFs, or `FALSE` to omit plot
`model`	"T1" or "T3" specifying model for plot
`cex`	scaling factor for size of plotted symbols

Details

The species tree may be rooted or unrooted, but must have edge lengths given in coalescent units. Note that while the MSC requires a rooted metric species tree parameter, as shown in (Allman et al. 2011) the quartet CFs are independent of the root.

In the returned table, columns are labeled by taxon names and quartet names ("12|34", etc.). 1s and 0s in taxon columns indicate the taxa in a quartet. Quartet 12|34 means the first and second indicated taxa form a cherry, 13|24 means the first and third form a cherry, and 14|23 means the first and fourth form a cherry. Unresolved quartets always have expectation 0 under the MSC.

If a simplex plot is produced, for the `T1` model all CFs will lie on the vertical model line, and many choices of 4 taxa will give the same CFs. For model `T3` the model lines the CFs are plotted on depend on taxon names and are essentially arbitrary.

Value

an (`n` choose 4)x(`n`+3) matrix encoding 4 taxon subsets of taxa and expectation of each of the quartets 12|34, 13|24, 14|23 across gene trees

References

Allman ES, Degnan JH, Rhodes JA (2011). “Identifying the rooted species tree from the distribution of unrooted gene trees under the coalescent.” *Journal of Mathematical Biology*, **62**(6), 833–862. doi:10.1007/s0028501003557.

See Also

quartetTable, quartetTableResolved

Examples

```
stree="((((t5:5000,t6:5000):5000,t4:10000):2500,t7:12500):7500,((t8:3000,t9:3000):5000,
((t1:4000,t2:4000):2500,t3:6500):1500):12000);"
st=read.tree(text=stree)
st$edge.length=st$edge.length/10000
expectedCFs(st)
```

`HolmBonferroni` *Apply Holm-Bonferroni method to adjust for multiple tests*

Description

Apply the Holm-Bonferroni method to adjust for multiple hypothesis tests performed on quartets from a data set of gene trees.

Usage

```
HolmBonferroni(pTable, model, alpha = 0.05)
```

Arguments

`pTable`	a table of quartets with p-values, as computed by `quartetTreeTestInd` or `quartetStarTestInd`
`model`	one of `"T1"`, `"T3"`, or `"star"`, where `pTable` contains a column `p_model` of p-values
`alpha`	a critical value, for rejection of adjusted p-values less than or equal to `alpha`

Details

When p-values are computed for each quartet using `quartetTreeTestInd` or `quartetStarTestInd`, multiple comparisons are being done for one dataset. The Holm-Bonferroni method (Holm 1979) adjusts these p-values upward, controlling the familywise error rate. The probability of at least one false discovery (rejection of the null hypothesis) is no more than the significance level.

The Holm-Bonferroni method does not require that test hypotheses are independent, which is important for its application to quartet counts presumed to have arisen on a single species tree.

This can be a low power test (often failing to reject when the null hypothesis is false). In particular for the T1 and T3 tests, it does not consider the relationships between edge lengths for different sets of four taxa.

Warning: Output of this function should not be used as input for other MSCquartets functions, as it reorders the quartets in the table.

Value

the same table, with rows reordered, and 2 new columns of 1) adjusted p-values, and 2) "Y" or "N" for indicating "reject" or "fail to reject"

References

Holm S (1979). “A simple sequentially rejective multiple test procedure.” *Scand. J. Statist.*, **6**(2), 65-70.

See Also

`quartetTreeTestInd`, `quartetStarTestInd`

Examples

```
gtrees=read.tree(file=system.file("extdata","dataGeneTreeSample",package="MSCquartets"))
taxanames=taxonNames(gtrees)
QT=quartetTable(gtrees,taxanames[1:6])
RQT=quartetTableResolved(QT)
pTable=quartetTreeTestInd(RQT,"T3")
pTable[1:10,]
HBpTable=HolmBonferroni(pTable,"T3",.05)
HBpTable[1:10,]
```

`initBquartets` *Initialize vector of B quartets*

Description

This is a C++ function, called from `TINNIKdist`, to initialize for inference of B and T quartets.

Usage

```
initBquartets(pTable, m, alpha, beta, colptest, colpstar, Bquartets)
```

Arguments

`pTable`	a quartet table with p-values
`m`	number of rows in pTable
`alpha`	critical value for tree test
`beta`	critical value for star tree test
`colptest`	column with p value for tree test
`colpstar`	column with p value for star tree test
`Bquartets`	0/1 vector encoding initial B quartets

See Also

`quartetTable`, `quartetTableParallel`

`M0` *Modified Struve function*

Description

This function is used in computing the probability density for Model T1. The code is closely based on the `I0L0` function implemented in Python for the package RandomFieldUtils, which was previously on CRAN up to 12/2022).

Usage

```
M0(x)
```

Arguments

`x`	function argument

Value

value of negative modified Struve function function

`NANUQ` *Apply NANUQ network inference algorithm to gene tree data*

Description

Apply the NANUQ algorithm of Allman et al. (2019) to infer a hybridization network from a collection of gene trees, under the level-1 network multispecies coalescent (NMSC) model.

Usage

```
NANUQ(
  genedata,
  outfile = "NANUQdist",
  omit = FALSE,
  epsilon = 0,
  alpha = 0.05,
  beta = 0.95,
  taxanames = NULL,
  plot = TRUE
)
```

Arguments

`genedata`	gene tree data that may be supplied in any of 3 forms: 1. as a character string giving the name of a file containing Newick gene trees, 2. as a multiPhylo object containing the gene trees, or 3. as a table of quartets on the gene trees, as produced by a previous call to `NANUQ` or `quartetTableResolved`, which has columns only for taxa, resolved quartet counts, and possibly p_T3 and p_star
`outfile`	a character string giving an output file name stub for saving a `NANUQ` distance matrix in nexus format; to the stub `outfile` will be appended an `alpha` and `beta` value and ".nex"; if `NULL` then then no file is written
`omit`	`FALSE` to treat unresolved quartets as 1/3 of each resolution; `TRUE` to discard unresolved quartet data; ignored if gene tree data given as quartet table
`epsilon`	minimum for branch lengths to be treated as non-zero; ignored if gene tree data given as quartet table
`alpha`	a value or vector of significance levels for judging p-values testing a null hypothesis of no hybridization vs. an alternative of hybridization, for each quartet; a smaller value applies a less conservative test for a tree (more trees), hence a stricter requirement for desciding in favor of hybridization (fewer reticulations)
`beta`	a value or vector of significance levels for judging p-values testing a null hypothesis of a star tree (polytomy) for each quartet vs. an alternative of anything else; a smaller value applies a less conservative test for a star tree (more polytomies), hence a stricter requirement for deciding in favor of a resolved tree or network; if vectors, `alpha` and `beta` must have the same length
`taxanames`	if `genedata` is a file or a multiPhylo object, a vector of a subset of the taxa names on the gene trees to be analyzed, if `NULL` all taxa on the first gene tree are used; if `genedata` is a quartet table, this argument is ignored and all taxa in the table are used
`plot`	`TRUE` produces simplex plots of hypothesis test results, `FALSE` omits plots

Details

This function

1. counts displayed quartets across gene trees to form quartet count concordance factors (qcCFs),
2. applies appropriate hypothesis tests to judge qcCFs as representing putative hybridization, resolved trees, or unresolved (star) trees using `alpha` and `beta` as significance levels,
3. produces a simplex plot showing results of the hypothesis tests for all qcCFs
4. computes the appropriate NANUQ distance table, writing it to a file.

The distance table file can then be opened in the external software SplitsTree (Huson and Bryant 2006) (recommended) or within R using the package `phangorn` to obtain a circular split system under the Neighbor-Net algorithm, which is then depicted as a splits graph. The splits graph should be interpreted via the theory of Allman et al. (2019) to infer the level-1 species network, or to conclude the data does not arise from the NMSC on such a network.

If `alpha` and `beta` are vectors, they must have the same length k. Then the i-th entries are paired to produce k plots and k output files. This is equivalent to k calls to `NANUQ` with scalar values of `alpha` and `beta`.

A call of `NANUQ` with `genedata` given as a table previously output from `NANUQ` is equivalent to a call of `NANUQdist`. If `genedata` is a table previously output from `quartetTableResolved` which lacks columns of p-values for hypothesis tests, these will be appended to the table output by `NANUQ`.

If plots are produced, each point represents an empirical quartet concordance factor, color-coded to represent test results.

In general, `alpha` should be chosen to be small and `beta` to be large so that most quartets are interpreted as resolved trees.

Usually, an initial call to `NANUQ` will not give a good analysis, as values of `alpha` and `beta` are likely to need some adjustment based on inspecting the data. Saving the returned table from `NANUQ` will allow for the results of the time-consuming computation of qcCFs to be saved, along with p-values, for input to further calls of `NANUQ` with new choices of `alpha` and `beta`.

See the documentation for `quartetNetworkDist` for an explanation of a small, rarely noticeable, stochastic element of the algorithm.

For data sets of many gene trees, user time may be reduced by using parallel code for counting displayed quartets. See `quartetTableParallel`, where example commands are given.

Value

a table `$pTable` of quartets and p-values for judging fit to the MSC on quartet trees, and a distance table `$dist`, or list of distance tables, giving NANUQ distance (returned invisibly); the table can be used as input to `NANUQ` or `NANUQdist` with new choices of alpha and beta, without re-tallying quartets on gene trees; the distance table is to be used as input to NeighborNet.

References

Allman ES, Baños H, Rhodes JA (2019). “NANUQ: A method for inferring species networks from gene trees under the coalescent model.” *Algorithms Mol. Biol.*, **14**(24), 1-25. doi:10.1186/s13015-01901592.

Huson DH, Bryant D (2006). “Application of Phylogenetic Networks in Evolutionary Studies.” *Molecular Biology and Evolution*, **23**(2), 254-267.

See Also

`quartetTable`, `quartetTableParallel`, `quartetTableDominant`, `quartetTreeTestInd`, `quartetStarTestInd`, `NANUQdist`, `quartetTestPlot`, `pvalHist`, `quartetNetworkDist`

Examples

```
data(pTableYeastRokas)
out=NANUQ(pTableYeastRokas, alpha=.05, beta=.95, outfile = NULL)
# Specifying an outfile would write the distance table to it for opening in SplitsTree.
# Alternately, to use the phangorn implementation of NeighborNet
# within R, enter the following additional lines:
nn=neighborNet(out$dist)
plot(nn,"2D")
```

`NANUQdist` *Compute NANUQ distance and write to file*

Description

Computes the quartet distance tables for the NANUQ algorithm of Allman et al. (2019), using precomputed p-values for quartets, for each of several levels specified. Distance tables are written to files, in nexus format.

Usage

```
NANUQdist(
  pTable,
  outfile = "NANUQdist",
  alpha = 0.05,
  beta = 0.95,
  plot = TRUE
)
```

Arguments

`pTable`	a table of resolved quartets and p-values, as previously computed by `NANUQ`, or by both `quartetTreeTestInd` and `quartetStarTestInd`, with columns `"p_T3"` and `"p_star"`
`outfile`	a character string giving an output file name stub for saving a `NANUQ` distance matrix in nexus format; to the stub `outfile` will be appended an `alpha` and `beta` value and ".nex"; if `NULL` then not written to file
`alpha`	a value or vector of significance levels for judging p-values testing a null hypothesis of no hybridization for each quartet; a smaller value applies a more liberal test for a tree (more trees), hence a stricter requirement for suspecting hybridization (fewer reticulations)
`beta`	a value or vector of significance levels for judging p-values testing a null hypothesis of a star tree for each quartet; a smaller value applies a more liberal test for a star tree (more polytomies), hence a stricter requirment for suspecting a resolved tree; if vectors, `alpha` and `beta` must have the same length
`plot`	`TRUE` produces simplex plots of hypothesis tests, `FALSE` omits plots

Details

If plots are produced, each point represents an empirical quartet concordance factor, color-coded to represent test results giving interpretation as network, resolved tree, or star tree.

If `alpha` and `beta` are vectors, they must be of the same length k. Then the i-th entries are paired to produce k plots and k distance tables/output files. This is equivalent to k calls to `NANUQdist` with paired scalar values from the vectors of `alpha` and `beta`.

See the documentation for `quartetNetworkDist` for an explanation of a small, rarely noticeable, stochastic element of the algorithm.

Value

a NANUQ distance table, or a list of such tables if `alpha` and `beta` are vectors (returned invisibly)

References

Allman ES, Baños H, Rhodes JA (2019). "NANUQ: A method for inferring species networks from gene trees under the coalescent model." *Algorithms Mol. Biol.*, **14**(24), 1-25. doi:10.1186/s13015-01901592.

See Also

`NANUQ`, `quartetTreeTestInd`, `quartetStarTestInd`

Examples

```
data(pTableYeastRokas)
dist=NANUQdist(pTableYeastRokas, alpha=.05, beta=.95, outfile = NULL)
```

`nexusDist` *Write a distance table to a file in nexus format*

Description

Write a distance table to a file in nexus format.

Usage

```
nexusDist(distMatrix, outfilename)
```

Arguments

`distMatrix`	a square matrix giving a distance table, with rows and columns labeled by taxon names
`outfilename`	the name of an output file

Examples

```
gtrees=read.tree(file=system.file("extdata","dataGeneTreeSample",package="MSCquartets"))
tnames=taxonNames(gtrees)
QT=quartetTable(gtrees,tnames[1:6])
RQT=quartetTableResolved(QT)
DQT=quartetTableDominant(RQT)
Dist=quartetDist(DQT)
nexusDist(Dist,outfile = file.path(tempdir(), "NANUQdist"))
```

`nodeGroups` *Groups taxa by deleting a node in a tree*

Description

Finds groups of taxa determined by the connected components of the graph resulting from deleting an internal node in a tree.

Usage

```
nodeGroups(tree, nodeNum)
```

Arguments

`tree`	a tree, of class "phylo"
`nodeNum`	a node number, representing an internal node in the phylo representation

Details

When applied to a rooted tree, the last group returned is the set of tips that are non-descendants of the node (provided any exist).

Value

a list of lists of tree tip numbers for each group. The union of the groups is the set of all tips.

Examples

```
tree=read.tree(text="((a,b),((c,d,e),(f,g)));")
nodeGroups(tree,8)
nodeGroups(tree,10)
nodeGroups(tree,11)
```

`powerDivStat` *Power divergence statistic of Cressie & Read*

Description

Computes any of the family of power-divergence statistics for multinomial data of Cressie and Read (1984), to compare observed and expected counts. Includes Likelihood Ratio and Chi-squared statistics as special cases.

Usage

```
powerDivStat(obs, expd, lambda)
```

Arguments

`obs`	observation vector
`expd`	expected vector
`lambda`	statistic parameter (e.g., 0=Likelihood Ratio, 1=Chi-squared)

Value

value of statistic

References

Cressie N, Read TRC (1984). “Multinomial Goodness-Of-Fit Tests.” *J. Royal Stat. Soc. B*, **46**(3), 440-464.

Examples

```
obs=c(10,20,30)
expd=c(20,20,20)
powerDivStat(obs,expd,0)
```

`pTableYeastRokas` *pTable for Yeast dataset*

Description

An .rda file dataset for the "dataYeastRokas" dataset. This is a subset of the data of Rokas et al. (2003).

Usage

```
data(pTableYeastRokas)
```

Format

an R data file

Details

This is provided primarily so that examples of other functions run more quickly. It can be reproduced by the following example code below.

Source

`https://wiki.rice.edu/confluence/download/attachments/8898533/yeast.trees?version=1&modificationDate=1360603275797&api=v2`

References

Rokas A, Williams B, Carrol S (2003). “Genome-scale approaches to resolving incongruence in molecular phylogenies.” *Nature*, **425**, 798–804.

Examples

```
gtrees=read.tree(file = system.file("extdata","dataYeastRokas",package="MSCquartets"))
QT=quartetTable(gtrees)
RQT=quartetTableResolved(QT)
pTable=quartetCutTestInd(RQT)
pTable=quartetTreeTestInd(pTable)
pTableYeastRokas=quartetStarTestInd(pTable)
```

`pvalHist` *Plot histogram of log p-values in table*

Description

Graphical exploration of extreme p-values from quartet hypothesis tests, to aid in choosing critical values for hypothesis tests. Log base 10 of p-values exceeding some minimum are plotted, to explore gaps in the tail of the distribution.

Usage

```
pvalHist(pTable, model, pmin = 0)
```

Arguments

`pTable`	a quartet table with p-values, such as from `NANUQ`, `quartetTreeTestInd`, or `quartetStarTestInd`
`model`	one of `"T1"`, `"T3"`, or `"star"`, where `pTable` contains a column `p_model` of p-values
`pmin`	include only p-values above `pmin` in the histogram

Details

Since logarithms are plotted, p-values close to 0 will appear as negative numbers of large magnitude, putting the tail of the distribution to the left in the histogram.

When exploring possible critical values for the hypothesis tests in the NANUQ algorithm, use `model= "T3"` to choose values for `alpha` which distinguish treelikeness from hybridization, and `model= "star"` to choose values for `beta` which distinguish polytomies from resolved trees. In general, `alpha` should be chosen to be small and `beta` to be large so that most quartets are interpreted as resolved trees.

See Also

`NANUQ`, `NANUQdist`

Examples

```
data(pTableYeastRokas)
pvalHist(pTableYeastRokas,"T3")
```

QDC *Compute Quartet Distance Consensus tree from gene tree data*

Description

Compute the Quartet Distance Consensus (Rhodes 2020) estimate of an unrooted topological species tree from gene tree data.

Usage

```
QDC(
  genetreedata,
  taxanames = NULL,
  method = fastme.bal,
  omit = FALSE,
  metric = FALSE
)
```

Arguments

`genetreedata`	gene tree data that may be supplied in any of 3 forms: 1. a character string giving the name of a file containing gene trees in Newick, 2. a multiPhylo object containing gene trees, or 3. a resolved quartet table, such as produced by `quartetTableResolved`
`taxanames`	if `genetreedata` is a file or a multiPhylo object, a vector of a subset of the taxa names on the gene trees to be analyzed, if `NULL` all taxa on the first gene tree are used; if `genetreedata` is a quartet table, this argument is ignored and all taxa in the table are used
`method`	a distance-based tree building function, such as `fastme.bal` or `nj`
`omit`	`TRUE` ignores unresolved quartets; `FALSE` treats them as 1/3 of each resolution; ignored if `genetreedata` is supplied as a quartet table
`metric`	if `FALSE` return topological tree; if `TRUE` return metric tree with internal edge lengths estimated by `estimateEdgeLengths` with `lambda=0`, and terminal branches of length 1

Details

This function is a wrapper which performs the steps of reading in a collection of gene trees, tallying quartets, computing the quartet distance between taxa, building a tree which consistently estimates the unrooted species tree topology under the MSC, and then possibly estimating edge lengths using the "simpleML" method.

Value

an unrooted tree of type phylo

References

Rhodes JA (2020). "Topological metrizations of trees, and new quartet methods of tree inference." *IEEE/ACM Trans. Comput. Biol. Bioinform.*, **17**(6), 2107-2118. doi:10.1109/TCBB.2019.2917204.

See Also

`quartetTable`, `quartetTableResolved`, `quartetTableDominant`, `quartetDist`, `QDS`, `WQDC`, `WQDCrecursive` `estimateEdgeLengths`

Examples

```
gtrees=read.tree(file=system.file("extdata","dataGeneTreeSample",package="MSCquartets"))
tnames=taxonNames(gtrees)
stree=QDC(gtrees,tnames[1:6])
write.tree(stree)
plot(stree)
streeMetric=QDC(gtrees, tnames[1:6],metric=TRUE)
write.tree(streeMetric)
plot(streeMetric)
```

`QDS` *Compute Quartet Distance Supertree*

Description

Apply the Quartet Distance Supertree method of Rhodes (2020) to a table specifying a collection of quartets on `n` taxa.

Usage

```
QDS(dqt, method = fastme.bal)
```

Arguments

`dqt`	an (`n` choose 4) x `n` (or `n+1`) matrix of form output by `quartetTableDominant`; (Note: If present, the `n+1`th column of `dqt` is ignored)
`method`	tree building function (e.g., fastme.bal, nj)

Details

This function is a wrapper which runs `quartetDist` and then builds a tree.

Value

an unrooted metric tree of type phylo. Edge lengths are not in interpretable units

References

Rhodes JA (2020). "Topological metrizations of trees, and new quartet methods of tree inference." *IEEE/ACM Trans. Comput. Biol. Bioinform.*, **17**(6), 2107-2118. doi:10.1109/TCBB.2019.2917204.

See Also

`quartetTableDominant`, `quartetDist`, `QDC`, `WQDS`, `WQDC`, `WQDCrecursive`

Examples

```
gtrees=read.tree(file=system.file("extdata","dataGeneTreeSample",package="MSCquartets"))
tnames=taxonNames(gtrees)
QT=quartetTable(gtrees,tnames[1:6])
RQT=quartetTableResolved(QT)
DQT=quartetTableDominant(RQT)
tree=QDS(DQT)
write.tree(tree)
plot(tree)
```

`quartetBTinferencePlot` *Produce simplex plot with results of B/T-quartet inference*

Description

Plot a 2-d probability simplex, with points for all normalized quartet count vectors. Colors indicate B- or T-quartets from TINNIK algorithm, at specified test levels.

Usage

```
quartetBTinferencePlot(pTable, Bquartets, test, alpha, beta, cex = 1)
```

Arguments

`pTable`	table of quartets and p-values
`Bquartets`	indicator vector for B-quartets (1=B, 0=T), ordered as in pTable
`test`	test model used for tree null hypothesis; options are `"cut"`, `"T3"`
`alpha`	significance level used by TINNIK for test `test`
`beta`	significance level used by TINNIK for star tree test
`cex`	scaling factor for size of plotted symbols

Details

The first argument of this function is a table of quartets and p-values. The plot may show results using either the T3, or 2-cut test, and a star tree test. The p-values must be computed by or before previous calls to `TINNIK`. The second argument is the indicator vector for B/T quartets produced by `TINNIK`.

See Also

`TINNIK`, `quartetTestPlot`

Examples

```
data(pTableYeastRokas)
out=TINNIKdist(pTableYeastRokas,test="T3",alpha=.05,beta=.05)
quartetBTinferencePlot(pTableYeastRokas,out$B,test="T3",alpha=.05,beta=.05)
```

`quartetCutMLE` *Maximum likelihood estimate of quartet tree of blobs topology and CF under Cut model*

Description

Computes Maximum likelihood estimate of quartet tree of blobs topology and CF under the Cut model of Allman et al. (2024), Section 3. In case of ties, the topology and CF estimate are chosen randomly among those maximizing the likelihood. In particular, a resolved tree of blobs is always returned.

Usage

```
quartetCutMLE(qcCF)
```

Arguments

`qcCF`	a quartet count Concordance Factor (a 3-element vector)

Value

output with `output$topology` = 1, 2, or 3 indicating topology of tree of blobs in accord with ordering of qcCF entries, and `output$CFhat` the ML estimate for the CF

References

Allman ES, Baños H, Mitchell JD, Rhodes JA (2024). "TINNiK: Inference of the Tree of Blobs of a Species Network Under the Coalescent." *bioRxiv*. doi:10.1101/2024.04.20.590418, `https://www.biorxiv.org/content/10.1101/2024.04.20.590418v1`.

Examples

```
quartetCutMLE(c(17,72,11))
quartetCutMLE(c(48,11,41))
quartetCutMLE(c(11,48,41))
quartetCutMLE(c(48,41,11))
```

`quartetCutTest` *Hypothesis test for quartet counts fitting a resolved quartet tree of blobs under NMSC*

Description

Test the hypothesis H_0=Cut model of Allman et al. (2024), Section 3., vs. H_1= everything else. Returns p-value and estimate of tree of blobs topology.

Usage

```
quartetCutTest(
  obs,
  lambda = 0,
  method = "MLest",
  smallcounts = "approximate",
  bootstraps = 10^4
)
```

Arguments

`obs`	vector of 3 counts of resolved quartet frequencies
`lambda`	parameter for power-divergence statistic (e.g., 0 for likelihood ratio statistic, 1 for Chi-squared statistic)
`method`	`"MLtest"`,`"conservative"`, or `"bootstrap"`
`smallcounts`	`"bootstrap"` or `"approximate"`, method of obtaining p-value when some counts are small
`bootstraps`	number of samples for bootstrapping

Details

The Cut model for quartet CFs is the NMSC combined with the quartet species network having a cut edge separating two of the taxa from the other two.

This function implements the test described in Allman et al. (2024) as well as parametric bootstrapping, with other procedures for when some expected counts are small. These are more accurate tests than, say, a Chi-square with one degree of freedom, which is not theoretically justified near the singularity of the model, nor for small counts.

If `method="MLtest"`, this uses the test for the Cut model described in Section 3 of Allman et al. (2024), using the ML estimate of the generating parameter. As shown in simulations in that paper, the test is conservative when small critical values are used for rejection. Although the test generally performs well in practice, it lacks a uniform asymptotic guarantee over the full parameter space.

If `method="conservative"`, the test uses the Chi-square distribution with 1 degree of freedom (the "least favorable" approach). This is asymptotically guaranteed to reject the null hypothesis at most at a specified level, but at the expense of increased type II errors.

If `method="bootstrap"`, then parametric bootstrapping is performed, based on ML estimates of the CF. The bootstrap sample size is given by the `bootstrap` argument.

When some expected topology counts are small, the methods `"MLest"` and `"conservative"` are not appropriate. The argument `smallcounts` determines whether bootstrapping or a faster approximate method is used. These use ML estimates of the CF under the Cut model.

If two of the three counts are small (so the estimated CF is near a vertex of the simplex), The approximate approach returns a precomputed p-value, found by replacing the largest observed count with 1e+6 and performing 1e+8 bootstraps. When n is sufficiently large (at least 30) and some expected counts are small, the probability of topological error is small and the bootstrap p-value is approximately independent of the largest observed count.

If one of the three counts is small (so the estimated CF is near an edge of the simplex), a chi-squared test using the binomial model for the larger counts is used, as described by Allman et al. (2024).

The returned p-value should be taken with caution when there is a small sample size, e.g. less than 30 gene trees.

Value

output where `output$p.value` is a p-value and `output$topology` = 1, 2, or 3 indicates the ML estimate of the topology of the quartet tree of blobs in accord with ordering of qcCF entries.

References

Allman ES, Baños H, Mitchell JD, Rhodes JA (2022). “The tree of blobs of a species network: identifiability under the coalescent.” *Journal of Mathematical Biology*, **86**(1), 10. doi:10.1007/s002850022018389.

Allman ES, Baños H, Mitchell JD, Rhodes JA (2024). “TINNiK: Inference of the Tree of Blobs of a Species Network Under the Coalescent.” *bioRxiv*. doi:10.1101/2024.04.20.590418, `https://www.biorxiv.org/content/10.1101/2024.04.20.590418v1`.

Mitchell J, Allman ES, Rhodes JA (2019). “Hypothesis testing near singularities and boundaries.” *Electron. J. Statist.*, **13**(1), 2150-2193. doi:10.1214/19EJS1576.

See Also

`quartetCutTestInd`

Examples

```
quartetCutTest(c(17,72,11))
quartetCutTest(c(48,11,41))
quartetCutTest(c(11,48,41))
quartetCutTest(c(48,41,11))
```

`quartetCutTestInd` *Multiple independent hypothesis tests for quartet counts fitting the Cut model under the NMSC*

Description

Perform a hypothesis test for all quartet counts in an input table, as if the counts for different choices of 4 taxa are independent.

Usage

```
quartetCutTestInd(
  rqt,
  lambda = 0,
  method = "MLest",
  smallcounts = "approximate",
  bootstraps = 10^4
)
```

Arguments

`rqt`	table of resolved quartet counts, as produced by `quartetTableResolved`, or `quartetStarTestInd`
`lambda`	power divergence statistic parameter (e.g., 0 for likelihood ratio statistic, 1 for Chi-squared statistic)
`method`	`"MLest"`, `"conservative"`, or `"bootstrap"`; see `quartetCutTest` for explanation
`smallcounts`	`"bootstrap"` or `"approximate"`, method of obtaining p-value when some counts are small, so the chosen `method` is inappropriate
`bootstraps`	number of samples for bootstrapping

Details

This function assumes all quartets are resolved. The test performed and the arguments are described more fully in `quartetCutTest`.

Value

a copy of `rqt` with two columns appended: `"p_cut"` with p-values and `"cutindex"` giving index 1,2, or 3 of ML estimate of quartet tree of blobs (1 if 12|34, 2 if 13|24, 3 if 14|23) under Cut model.

References

Allman ES, Baños H, Mitchell JD, Rhodes JA (2024). “TINNiK: Inference of the Tree of Blobs of a Species Network Under the Coalescent.” *bioRxiv*. doi:10.1101/2024.04.20.590418, `https://www.biorxiv.org/content/10.1101/2024.04.20.590418v1`.

See Also

`quartetCutTest`, `quartetTestPlot`, `quartetStarTestInd`, `quartetTableResolved`

Examples

```
data(pTableYeastRokas)
pT=pTableYeastRokas[1:10,1:11]
pTable=quartetCutTestInd(pT)
```

`quartetDist` *Compute quartet distance between taxa*

Description

Compute the Quartet Distance of Rhodes (2020) from a table specifying a collection of quartets on `n` taxa.

Usage

```
quartetDist(dqt)
```

Arguments

`dqt`	an (`n` choose 4) x `n` (or `n+1`) matrix of form output by `quartetTableDominant`; (Note: If present, the `n+1`th column of `dqt` is ignored.)

Value

a pairwise distance matrix on `n` taxa

References

Rhodes JA (2020). “Topological metrizations of trees, and new quartet methods of tree inference.” *IEEE/ACM Trans. Comput. Biol. Bioinform.*, **17**(6), 2107-2118. doi:10.1109/TCBB.2019.2917204.

See Also

`quartetTableDominant`, `QDS`, `QDC`, `quartetWeightedDist`

Examples

```
gtrees=read.tree(file=system.file("extdata","dataGeneTreeSample",package="MSCquartets"))
tnames=taxonNames(gtrees)
QT=quartetTable(gtrees,tnames[1:6])
RQT=quartetTableResolved(QT)
DQT=quartetTableDominant(RQT)
Dist=quartetDist(DQT)
tree=NJ(Dist)
```

```
write.tree(tree)
plot(tree)
```

`quartetNetworkDist` *Compute network quartet distance between taxa*

Description

Produce network quartet distance table for the NANUQ algorithm, from a table of quartets and p-values, and specified levels of quartet hypothesis tests. The network quartet distance, which is described more fully by Allman et al. (2019), generalizes the quartet distance of Rhodes (2020).

Usage

```
quartetNetworkDist(pTable, alpha, beta)
```

Arguments

`pTable`	a table of quartets and p-values, as computed by NANUQ, or `quartetTreeTestInd` and `quartetStarTestInd`
`alpha`	a scalar significance level for judging p-values `p_T3` indicating hybridization on quartet; smaller value gives fewer hybridization decisions
`beta`	a scalar significance level for judging p-values `p_star` indicating quartet star tree; smaller value gives fewer resolved tree decisions

Details

In case of a triple of quartet counts with the two largest equal and the third slighltly smaller, along with `alpha` and `beta` leading to a star quartet being rejected and a tree not being rejected, this function chooses a resolved quartet topology uniformly at random from the two largest counts. This is the only stochastic element of the code, and its impact is usually negligible.

Value

a distance table

References

Allman ES, Baños H, Rhodes JA (2019). “NANUQ: A method for inferring species networks from gene trees under the coalescent model.” *Algorithms Mol. Biol.*, **14**(24), 1-25. doi:10.1186/s13015-01901592.

Rhodes JA (2020). “Topological metrizations of trees, and new quartet methods of tree inference.” *IEEE/ACM Trans. Comput. Biol. Bioinform.*, **17**(6), 2107-2118. doi:10.1109/TCBB.2019.2917204.

See Also

`NANUQ`, `NANUQdist`

Examples

```
data(pTableYeastRokas)
dist=quartetNetworkDist(pTableYeastRokas, alpha=.05, beta=.95)
```

`quartetStarTest` *Hypothesis test for quartet counts fitting a star tree under the MSC*

Description

Perform hypothesis test for star tree for a vector of quartet counts to fit expected frequencies of (1/3,1/3,1/3). The test performed is a standard Chi-square with 2 degrees of freedom.

Usage

```
quartetStarTest(obs)
```

Arguments

`obs`	vector of 3 counts of resolved quartet frequencies

Value

p-value

Examples

```
obs=c(16,72,12)
quartetStarTest(obs)
```

`quartetStarTestInd` *Multiple independent hypothesis tests for gene quartet counts fitting a species quartet star tree under the MSC*

Description

Perform hypothesis tests for a species quartet star tree vs. any alternative for all quartet counts in an input table, as if the quartets are independent.

Usage

```
quartetStarTestInd(rqt)
```

Arguments

`rqt`	Table of resolved quartet counts, as produced by `quartetTableResolved`, or `quartetTreeTestInd`

Details

This function assumes all quartets are resolved. The test performed is described in `quartetStarTest`.

Value

the same table as the input `rqt` with column `"p_star"` appended, containing p-values for judging fit to MSC on a star tree

See Also

`quartetStarTest`, `quartetTreeTest`, `quartetTreeTestInd`, `quartetTableResolved`, `quartetTestPlot`

Examples

```
gtrees=read.tree(file=system.file("extdata","dataGeneTreeSample",package="MSCquartets"))
tnames=taxonNames(gtrees)
QT=quartetTable(gtrees,tnames[1:6])
RQT=quartetTableResolved(QT)
pTable=quartetStarTestInd(RQT)
quartetTablePrint(pTable[1:6,])
```

`quartetTable` *Produce table of counts of quartets displayed on trees*

Description

Compiles table of quartet count concordance factors (qcCFs) for topological quartets displayed on a collection of trees.

Usage

```
quartetTable(
  trees,
  taxonnames = NULL,
  epsilon = 0,
  random = 0,
  progressbar = FALSE
)
```

Arguments

`trees`	multiphylo object containing un/rooted metric/topological trees
`taxonnames`	vector of `n` names of taxa of interest; if `NULL` then taken from taxa on `trees[[1]]`
`epsilon`	minimum for branch lengths to be treated as non-zero (default 0)
`random`	number of random subsets of 4 taxa to consider; if 0, use all `n` choose 4 subsets
`progressbar`	FALSE, set to TRUE if want to see tally progress

Details

The names in `taxonnames` may be any subset of those on the trees. Branch lengths of non-negative size less than or equal to `epsilon` are treated as zero, giving polytomies.

In the returned table, columns are labeled by taxon names and quartet names ("12|34", etc.). 1s and 0s in taxon columns indicate the taxa in a quartet. Quartet 12|34 means the first and second indicated taxa form a cherry, 13|24 means the first and third form a cherry, 14|23 means the first and fourth form a cherry, and 1234 means the quartet is unresolved.

An error occurs if any branch length is negative. Warnings are given if some of `taxonnames` are missing on some trees, or if some 4-taxon set is not on any tree.

If `random`>0, then for efficiency `random` should be much smaller then the number of possible 4 taxon subsets.

This function calls an Rcpp function for tallying quartets, for much shorter computational time than can be achieved in R alone.

Value

an (`n` choose 4)x(n+4) matrix (or (`random`)x(n+4) matrix) encoding 4 taxon subsets of `taxonnames` and counts of each of the quartets 12|34, 13|24, 14|23, 1234 across the trees

See Also

`quartetTableParallel`, `quartetTableResolved`, `quartetTableDominant`, `taxonNames`

Examples

```
gtrees=read.tree(file=system.file("extdata","dataGeneTreeSample",package="MSCquartets"))
tnames=taxonNames(gtrees)
QT=quartetTable(gtrees,tnames[1:6])
RQT=quartetTableResolved(QT)
DQT=quartetTableDominant(RQT)
```

`quartetTableCollapse` *Reduce quartet table by combining some taxa*

Description

Form a smaller resolved quartet table by lumping some taxa into a composite taxon.

Usage

```
quartetTableCollapse(rqt, taxaA, taxaB)
```

Arguments

`rqt`	a resolved quartet table, as from `quartetTableResolved`
`taxaA`	a vector of taxon names in `rqt` to be included in the output table
`taxaB`	a vector of taxon names in `rqt` to form new composite taxon in the output table

Details

This function is needed for the recursive calls in `WQDSrec`. It should only be applied to a resolved quartet table which includes counts for all possible quartets on the taxa (though counts can be zero).

The sets `taxaA` and `taxaB` must be disjoint. Their union need not be all taxa in `rqt`.

Value

a resolved quartet table with `length(taxaA)+1` taxa; the composite taxon is named as the concatenation of the sorted names in `taxaB`

See Also

`WQDCrecursive`

`quartetTableDominant` *Produce table of dominant quartets, with estimates of internal edge lengths*

Description

Converts table of counts of resolved quartets on `n` taxa to show only dominant one, with maximum likelihood estimate of internal edge weight under the MSC.

Usage

```
quartetTableDominant(rqt, bigweights = "infinite")
```

Arguments

`rqt`	a table, as produced by `quartetTableResolved` of size (n choose 4)x(n+3);
`bigweights`	`"infinite"` or `"finite"`, to indicate whether the weight (internal edge length) of a quartet for which only one topology appears is given as `Inf` or a finite, but large, numerical value

Details

If `bigweights="finite"`, when for a set of 4 taxa the quartet counts are (m,0,0) then the edge weight is computed as if the relative frequency of the dominant topology were m/(m+1).

Value

an (n choose 4)x(n+1) array with dominant quartet topology encoded by 1,1,-1,-1 in taxon columns, with signs indicating cherries; the (n+1)th column `"weight"` contains the maximum likelihood estimates, under MSC on a 4-taxon tree, of the quartets' central edge lengths, in coalescent units

See Also

`quartetTable`, `quartetTableResolved`

Examples

```
gtrees=read.tree(file=system.file("extdata","dataGeneTreeSample",package="MSCquartets"))
tnames=taxonNames(gtrees)
QT=quartetTable(gtrees,tnames[1:6])
RQT=quartetTableResolved(QT)
RQT[1:6,]
DQT=quartetTableDominant(RQT)
DQT[1:6,]
```

`quartetTableParallel` *Produce table of counts of quartets displayed on trees, in parallel for large data sets*

Description

Compiles table of quartet count concordance factors (qcCFs) for topological quartets displayed on a collection of trees. Gives the same output as `quartetTable`, but operates in parallel.

Usage

```
quartetTableParallel(trees, taxonnames = NULL, epsilon = 0, numCores)
```

Arguments

`trees`	multiphylo object containing un/rooted metric/topological trees
`taxonnames`	vector of `n` names of taxa of interest; if `NULL` then taken from taxa on `trees[[1]]`
`epsilon`	minimum for branch lengths to be treated as non-zero
`numCores`	number of cores to use for parallel calls

Details

The number of available cores can be determined by `parallel::detectCores()`. With overhead, tabulating quartets for a large data set (many taxa and/or many gene trees) on a 4-core computer using `numCores=4` may require less than half the elapsed time of the sequential `quartetTable`.

The names in `taxonnames` may be any subset of those on the trees. Branch lengths of non-negative size less than or equal to `epsilon` are treated as zero, giving polytomies.

In the returned table, columns are labeled by taxon names and quartet names ("12|34", etc.). 1s and 0s in taxon columns indicate the taxa in a quartet. Quartet 12|34 means the first and second indicated taxa form a cherry, 13|24 means the first and third form a cherry, 14|23 means the first and fourth form a cherry, and 1234 means the quartet is unresolved.

An error occurs if any branch length is negative. Warnings are given if some of `taxonnames` are missing on some trees, or if some 4-taxon set is not on any tree.

If `random`>0, then for efficiency `random` should be much smaller then the number of possible 4 taxon subsets.

If the quartet counts are to be used for NANUQ, or any other routines requiring resolved quartet counts, `quartetTableResolved` must be run following `quartetTableParallel`. See example below.

Value

an (`n` choose 4)x(n+4) matrix (or (`random`)x(n+4) matrix) encoding 4 taxon subsets of `taxonnames` and counts of each of the quartets 12|34, 13|24, 14|23, 1234 across the trees

See Also

`quartetTable`, `quartetTableResolved`, `quartetTableDominant`, `taxonNames`

Examples

```
gtrees=read.tree(file=system.file("extdata","dataHeliconiusMartin",package="MSCquartets"))
QT=quartetTableParallel(gtrees,numCores=2)
RQT=quartetTableResolved(QT)
pTable=NANUQ(RQT,alpha=1e-40, beta=1e-30, outfile = file.path(tempdir(), "NANUQdist"))
```

`quartetTablePrint` *Print a quartet table with nice formatting*

Description

Print a quartet table with the taxa in each quartet shown by name.

Usage

```
quartetTablePrint(qt)
```

Arguments

`qt`	a table such as returned by `quartetTable`, `quartetTableResolved`, or `quartetTableDominant`, possibly with extra columns added by other functions

Examples

```
gtrees=read.tree(file=system.file("extdata","dataGeneTreeSample",package="MSCquartets"))
tnames=taxonNames(gtrees)
QT=quartetTable(gtrees,tnames[1:6])
QT[1:6,]
quartetTablePrint(QT[1:6,])
RQT=quartetTableResolved(QT)
RQT[1:6,]
quartetTablePrint(RQT[1:6,])
pTable=quartetTreeTestInd(RQT,"T3")
pTable[1:6,]
quartetTablePrint(pTable[1:6,])
DQT=quartetTableDominant(RQT)
DQT[1:6,]
quartetTablePrint(DQT[1:6,])
```

`quartetTableResolved` *Modify quartet table to show only resolved quartets*

Description

Converts table of all quartet counts, including unresolved ones, by either dropping unresolved ones, or distributing them uniformly among the three resolved counts.

Usage

```
quartetTableResolved(qt, omit = FALSE)
```

Arguments

`qt`	table, as produced by `quartetTable` for `n` taxa, with `n+4` columns
`omit`	`TRUE` deletes unresolved quartets column; `FALSE` deletes the column but redistributes unresolved counts as (1/3,1/3,1/3) to resolved counts

Value

a table of quartet counts similar to `qt`, but with columns showing only resolved quartet counts

See Also

`quartetTable`, `quartetTableDominant`

Examples

```
gtrees=read.tree(file=system.file("extdata","dataGeneTreeSample",package="MSCquartets"))
tnames=taxonNames(gtrees)
QT=quartetTable(gtrees,tnames[1:6])
QT[1:6,]
RQT=quartetTableResolved(QT)
RQT[1:6,]
```

`quartetTallyCpp` *Build quartet table from distances*

Description

This is a C++ function, called from quartetTable, to fill in the quartet counts. From a list of topological distance matrices (1 for each gene tree) it determines all gene quartets. It is not intended to be used as a stand-alone function, and hence not fully documented. The faster looping in C++ over R gives substantial time improvements

Usage

```
quartetTallyCpp(dList, M, nt, Q, random, progressbar = FALSE)
```

Arguments

`dList`	a list of distance matrices
`M`	number of sets of 4 taxa
`nt`	number of gene trees/distance matrices
`Q`	matrix to fill out as table of quartet counts
`random`	if 0 compute for all sets of 4 taxa, otherwise for M random ones
`progressbar`	if TRUE, display progress bar

See Also

`quartetTable`, `quartetTableParallel`

`quartetTestPlot` *Produce simplex plot with results of quartet hypothesis tests*

Description

Plot a 2-d probability simplex, with points for all quartet count vectors. Colors indicate rejection or failure to reject for tests at specified levels.

Usage

```
quartetTestPlot(pTable, test, alpha = 0.05, beta = 1, cex = 1)
```

Arguments

`pTable`	table of quartets and p-values, as produced by `quartetTreeTestInd`, `quartetStarTestInd`, or `NANUQ`
`test`	model to use, for tree null hypothesis; options are `"T1"`, `"T3"`, `"cut"`, `"NANUQ"`
`alpha`	significance level for tree test with null hypothesis given by `test`
`beta`	significance level for test with null hypothesis star tree; test results plotted only if `beta<1` and `"p_star"` column present in `pTable`
`cex`	scaling factor for size of plotted symbols

Details

The first argument of this function is a table of quartets and p-values. The plot may show results of either the T1, T3, or 2-cut test, with or without a star tree test (depending on whether a `"p_star"` column is in the table and/or `beta =1`). The p-values must be computed by previous calls to `quartetTreeTestInd` (for `"T1"` or `"T3"` p-values) and `quartetStarTestInd` (for `"star"` p-values). The `NANUQ` and `NANUQdist` functions include calls to these tree test functions.

See Also

`quartetTreeTestInd`, `quartetStarTestInd`, `NANUQ`, `NANUQdist`

Examples

```
gtrees=read.tree(file=system.file("extdata","dataGeneTreeSample",package="MSCquartets"))
tnames=c("t1","t2","t3","t4","t5","t6")
QT=quartetTable(gtrees,tnames[1:6])
RQT=quartetTableResolved(QT)
stree="(((t5,t6),t4),((t1,t2),t3));"
pTable=quartetTreeTestInd(RQT,"T1",speciestree=stree)
pTable=quartetStarTestInd(pTable)
quartetTestPlot(pTable, "T1", alpha=.05, beta=.95)
```

`quartetTreeErrorProb` *Bayesian posterior probability of error in 4-taxon unrooted species tree topology estimate*

Description

From a gene quartet count concordance factor (qcCF), computes Bayesian posterior probabilities of the three 4-taxon species tree topologies and the Bayesian posterior probability that the assumed topology is incorrect, under the assumption that the counts arise from the MSC on some species tree.

Usage

```
quartetTreeErrorProb(obs, model = "T3")
```

Arguments

`obs`	vector of counts for 3 topologies
`model`	`"T3"` or `"T1"`, for the models of Mitchell et al. (2019) describing an unspecified species tree topology (`"T3"`), or the topology whose count is the first entry of `obs` (`"T1"`)

Details

The Jeffreys prior is used for internal branch length, along with the uniform prior on the resolved topology.

Value

`(error.prob, top.probs)` where `error.prob` is the species tree error probability and `top.probs` is a vector of the three species tree topology probabilities in the order of `obs`; for model `"T1"` the species tree used is the one corresponding to the first count; for model `"T3"` the species tree is the one corresponding to the largest count

References

Mitchell J, Allman ES, Rhodes JA (2019). “Hypothesis testing near singularities and boundaries.” *Electron. J. Statist.*, **13**(1), 2150-2193. doi:10.1214/19EJS1576.

Examples

```
obs <- c(28,32,30)
quartetTreeErrorProb(obs,model="T1")
quartetTreeErrorProb(obs,model="T3")
```

`quartetTreeTest` *Hypothesis test for quartet counts fitting a tree under the MSC*

Description

Test the hypothesis H_0= T1 or T3 model of Mitchell et al. (2019), vs. H_1 = everything else. T1 is for a specific species quartet topology, and T3 for any species quartet topology.

Usage

```
quartetTreeTest(
  obs,
  model = "T3",
  lambda = 0,
  method = "MLest",
  smallsample = "precomputed",
  smallcounts = "precomputed",
  bootstraps = 10^4
)
```

Arguments

`obs`	vector of 3 counts of resolved quartet frequencies
`model`	`"T1"` or `"T3"`, for the models of Mitchell et al. (2019)
`lambda`	parameter for power-divergence statistic (e.g., 0 for likelihood ratio statistic, 1 for Chi-squared statistic)
`method`	`"MLtest"`,`"conservative"`, or `"bootstrap"`
`smallsample`	`"precomputed"` or `"bootstrap"`, method of obtaining p-value when sample is small (<30)
`smallcounts`	`"precomputed"` or `"bootstrap"`, method of obtaining p-value when some (but not all) counts are small
`bootstraps`	number of samples for bootstrapping

Details

This function implements two of the versions of the test given by Mitchell et al. (2019) as well as parametric bootstrapping, with other procedures for when some expected counts are small. When the topology and/or the internal quartet branch length is not specified by the null hypothesis these are more accurate tests than, say, a Chi-square with one degree of freedom, which is not theoretically justified near the singularities and boundaries of the models.

If `method="MLtest"`, this uses the test by that name described in Section 7 of Mitchell et al. (2019). For both the T1 and T3 models the test is slightly anticonservative over a small range of true internal edges of the quartet species tree. Although the test generally performs well in practice, it lacks a uniform asymptotic guarantee over the full parameter space for either T1 or T3.

If `method="conservative"`, a conservative test described by Mitchell et al. (2019) is used. For model T3 this uses the Chi-square distribution with 1 degree of freedom (the "least favorable" approach), while for model T1 it uses the Minimum Adjusted Bonferroni, based on precomputed values from simulations with n=1e+6. These conservative tests are asymptotically guaranteed to reject the null hypothesis at most at a specified level, but at the expense of increased type II errors.

If `method="bootstrap"`, then parametric bootstrapping is performed, based on parameter estimates of the quartet topology and internal edge length. The bootstrap sample size is given by the `bootstrap` argument.

When some or all expected topology counts are small, the methods `"MLest"` and `"conservative"` are not appropriate. The argument `smallsample` determines whether a precomputed bootstrap of 1e+8 samples, or actual boostrapping with the specified size, is used when the total sample is small (<30). The argument `smallcounts` determines whether bootstrapping or a faster approximate method is used when only some counts are small. The approximate approach returns a precomputed p-value, found by replacing the largest observed count with 1e+6 and performing 1e+8 bootstraps for the model T3. When n >30 and some expected counts are small, the quartet tree error probability is small and the bootstrap p-value is approximately independent of the choice of T3 or T1 and of the largest observed count.

For model T1, the first entry of `obs` is treated as the count of gene quartets concordant with the species tree.

The returned p-value should be taken with caution when there is a small sample size, e.g. less than 30 gene trees. The returned value of `$edgelength` is a consistent estimator, but not the MLE, of the internal edge length in coalescent units. Although consistent, the MLE for this length is biased. Our consistent estimator is still biased, but with less bias than the MLE. See Mitchell et al. (2019) for more discussion on dealing with the bias of parameter estimates in the presence of boundaries and/or singularities of parameter spaces.

Value

`output` where `output$p.value` is the p-value and `output$edgelength` is a consistent estimator of the internal edge length in coalescent units, possibly `Inf`.

References

Mitchell J, Allman ES, Rhodes JA (2019). “Hypothesis testing near singularities and boundaries.” *Electron. J. Statist.*, **13**(1), 2150-2193. doi:10.1214/19EJS1576.

See Also

`quartetTreeTestInd`

Examples

```
quartetTreeTest(c(17,72,11),"T3")
quartetTreeTest(c(17,72,11),"T1")
quartetTreeTest(c(72,11,17),"T1")
quartetTreeTest(c(11,17,72),"T1")
```

`quartetTreeTestInd` *Multiple independent hypothesis tests for quartet counts fitting a species tree under the MSC*

Description

Perform a tree hypothesis test for all quartet counts in an input table, as if the counts for different choices of 4 taxa are independent.

Usage

```
quartetTreeTestInd(
  rqt,
  model = "T3",
  lambda = 0,
  method = "MLest",
  smallsample = "precomputed",
  smallcounts = "precomputed",
  bootstraps = 10^4,
  speciestree = NULL
)
```

Arguments

`rqt`	table of resolved quartet counts, as produced by `quartetTableResolved`, or `quartetStarTestInd`
`model`	`"T1"` for a specific species tree topology, or `"T3"` for any species tree topology, with these models explained more fully by Mitchell et al. (2019)
`lambda`	power divergence statistic parameter (e.g., 0 for likelihood ratio statistic, 1 for Chi-squared statistic)
`method`	`"MLest"`, `"conservative"`, or `"bootstrap"`; see `quartetTreeTest` for explanation
`smallsample`	`"precomputed"` or `"bootstrap"`, method of obtaining p-value when sample is small (<30)
`smallcounts`	`"precomputed"` or `"bootstrap"`, method of obtaining p-value when some counts are small, so the chosen `method` is inappropriate
`bootstraps`	number of samples for bootstrapping
`speciestree`	species tree, in Newick as text, to determine quartet for T1 test; required for `model="T1"`, ignored for `model="T3"`

Details

This function assumes all quartets are resolved. The test performed and the arguments are described more fully in `quartetTreeTest`.

Value

if `model="T3"`, a copy of `rqt` with a new column `"p_T3"` appended with p-values for each quartet; if `model="T1"`, a copy of `rqt` with 2 columns appended: `"p_T1"` with p-values, and `"qindex"` giving index of quartet consistent with specified species tree, i.e., 1 if 12|34 on species tree, 2 if 13|24, 3 if 14|23

References

Mitchell J, Allman ES, Rhodes JA (2019). “Hypothesis testing near singularities and boundaries.” *Electron. J. Statist.*, **13**(1), 2150-2193. doi:10.1214/19EJS1576.

See Also

`quartetTreeTest`, `quartetTestPlot`, `quartetStarTestInd`, `quartetTableResolved`

Examples

```
gtrees=read.tree(file=system.file("extdata","dataGeneTreeSample",package="MSCquartets"))
tnames=c("t1","t2","t3","t4","t5","t6")
QT=quartetTable(gtrees,tnames)
RQT=quartetTableResolved(QT)
stree="(((t5,t6),t4),((t1,t2),t3));"
pTable3=quartetTreeTestInd(RQT,"T3")
quartetTablePrint(pTable3[1:6,])
stree="((((t5,t6),t4),t7),((t8,t9),((t1,t2),t3)));"
pTable1=quartetTreeTestInd(RQT,"T1",speciestree=stree)
quartetTablePrint(pTable1[1:6,])
```

`quartetWeightedDist` *Compute the Weighted Quartet Distance between taxa*

Description

Compute the Weighted Quartet Distance between taxa of Yourdkhani and Rhodes (2020) from a table specifying a collection of quartets on `n` taxa and the quartets' internal branch lengths.

Usage

```
quartetWeightedDist(dqt)
```

Arguments

`dqt`	an (`n` choose 4) x (`n`+1) matrix of the form output by `quartetTableDominant`

Value

a pairwise distance matrix on `n` taxa

References

Yourdkhani S, Rhodes JA (2020). “Inferring metric trees from weighted quartets via an intertaxon distance.” *Bul. Math. Biol.*, **82**(97). doi:10.1007/s11538020007734.

See Also

`quartetTableDominant`, `WQDSAdjustLengths`, `WQDS`, `WQDC`, `WQDCrecursive`, `quartetWeightedDist`

Examples

```
gtrees=read.tree(file=system.file("extdata","dataGeneTreeSample",package="MSCquartets"))
tnames=taxonNames(gtrees)
QT=quartetTable(gtrees,tnames[1:6])
RQT=quartetTableResolved(QT)
DQT=quartetTableDominant(RQT,bigweights="finite")
D=quartetWeightedDist(DQT)
tree=NJ(D)
stree=WQDSAdjustLengths(tree)
write.tree(stree)
```

`simplexCoords` *Convert 3-d coordinates to 2-d probability simplex coordinates*

Description

Convert from 3-d Cartesian coordinates to 2-d coordinates suitable for plotting in the probability simplex.

Usage

```
simplexCoords(v)
```

Arguments

`v`	vector of 3 non-negative numbers, not summing to 0

Details

Applies an affine coordinate trandformation that maps the centroid (1/3,1/3,1/3) to the origin (0,0), and rescales so that the line segments between (1,0,0), (0,1,0), and (0,0,1) are mapped to segments of length 1.

An input vector `v` is first normalized so its component sum to 1 before the map is applied.

Value

2-d coordinates to plot normalized point in simplex

See Also

`simplexLabels`, `simplexPoint`, `simplexPrepare`, `simplexSegment`, `simplexText`

Examples

```
simplexCoords(c(15,65,20))
```

`simplexLabels` *Label vertices of 2-d probability simplex*

Description

Add labels to vertices of the probability simplex.

Usage

```
simplexLabels(top = "", left = "", right = "")
```

Arguments

`top`	label for top
`left`	label for left bottom
`right`	label for right bottom

See Also

`simplexPoint`, `simplexPrepare`, `simplexSegment`, `simplexText`, `simplexCoords`

Examples

```
simplexPrepare("T3","Example Plot")
simplexLabels("ab|cd","ac|bd","ad|bc")
```

`simplexPoint` *Plot point in 2-d probability simplex*

Description

Normalizes a point given in 3-d non-normalized coordinates, then plots it in the 2-d probability simplex.

Usage

```
simplexPoint(v, ...)
```

Arguments

`v`	a 3-d point in non-negative orthant, coordinates not summing to 0
`...`	other options to pass to graphics::points function

See Also

`simplexLabels`, `simplexPrepare`, `simplexSegment`, `simplexText`, `simplexCoords`

Examples

```
simplexPrepare("T3","Example Plot")
simplexPoint(c(15,65,20),pch=3,col="blue")
```

`simplexPrepare` *Draw 2-d probability simplex, with model lines for T3 or T1 model*

Description

Outline the 2-d probability simplex, and draw the T1 or T3 model points for quartet frequencies. The models "T1" and "T3" are described more fully by Mitchell et al. (2019).

Usage

```
simplexPrepare(model = "T3", maintitle = NULL, titletext = NULL)
```

Arguments

`model`	`"T1"` or `"T3"`, for 1-tree or 3-tree model
`maintitle`	main title for plot
`titletext`	additional text for title

References

Mitchell J, Allman ES, Rhodes JA (2019). "Hypothesis testing near singularities and boundaries." *Electron. J. Statist.*, **13**(1), 2150-2193. doi:10.1214/19EJS1576.

See Also

`simplexLabels`, `simplexPoint`, `simplexSegment`, `simplexText`, `simplexCoords`

Examples

```
simplexPrepare("T3",maintitle="Main title",titletext="further text")
```

`simplexSegment` *Plot line segment in 2-d probability simplex*

Description

Normalizes two points in 3-d, and draws line segment between them in 2-d probability simplex.

Usage

```
simplexSegment(v, w, ...)
```

Arguments

`v, w`	3-d endpoints of line segment in non-negative orthant, coords not summing to 0
`...`	other options to pass to graphics::segments function

See Also

`simplexLabels`, `simplexPoint`, `simplexPrepare`, `simplexText`, `simplexCoords`

Examples

```
simplexPrepare("T3","Example Plot")
simplexSegment(c(15,65,20),c(15,70, 15),col="green")
```

`simplexText` *Add text at a point in 2-d probability simplex*

Description

Add text to a 2-d probability simplex plot, at specified location.

Usage

```
simplexText(v, label = "", ...)
```

Arguments

`v`	a 3-d point in non-negative orthant, coordinates not summing to 0
`label`	text to add to plot
`...`	other options to pass to graphics::text function

See Also

`simplexLabels`, `simplexPoint`, `simplexPrepare`, `simplexSegment`, `simplexCoords`

Examples

```
simplexPrepare("T3","Example Plot")
simplexText(c(15,65,20),"tree ac|bd")
```

`sortQuartetTableRows` *Sort quartet table rows by lex order*

Description

Sort the rows of a quartet table so they are in MSCquartet's standard lex order. This is the order produced by the `quartetTable` function. The only exceptions to this order produced in the package are when `quartetTable` is called with the `random` argument non-zero, or when the `HolmBonferoni` function is called. However, for tables made outside this package, it can be useful.

Usage

```
sortQuartetTableRows(qT)
```

Arguments

`qT`	a quartet Table to be sorted

Value

sorted table

See Also

`quartetTable`, `HolmBonferroni`

`T1density` *Probability density function for Model T1*

Description

Value of probability density function for Model T1 of Mitchell et al. (2019), Proposition 5.2.

Usage

```
T1density(x, mu0)
```

Arguments

`x`	statistic value (e.g., likelihood ratio statistic, or other power divergence statistic)
`mu0`	parameter of density function

Value

value of density function

References

Mitchell J, Allman ES, Rhodes JA (2019). “Hypothesis testing near singularities and boundaries.” *Electron. J. Statist.*, **13**(1), 2150-2193. doi:10.1214/19EJS1576.

See Also

`T3density`

`T3density` *Probability density function for Model T3*

Description

Value of probability density function for Model T3 of Mitchell et al. (2019), Proposition 4.2.

Usage

```
T3density(x, mu0, alpha0, beta0)
```

Arguments

`x`	statistic value (e.g., likelihood ratio statistic, or other power divergence statistic)
`mu0`	parameter of density function
`alpha0`	parameter of density function
`beta0`	parameter of density function

Value

value of density function

References

Mitchell J, Allman ES, Rhodes JA (2019). “Hypothesis testing near singularities and boundaries.” *Electron. J. Statist.*, **13**(1), 2150-2193. doi:10.1214/19EJS1576.

See Also

`T1density`

`taxonNames` *Get all taxon names from a collection of trees*

Description

Create a vector of all taxon names appearing on a collection of trees, with no repeats.

Usage

```
taxonNames(trees)
```

Arguments

`trees`	a multiPhylo object containing a collection of trees

Value

a vector of unique names of taxa appearing on the trees

Examples

```
gtrees=read.tree(file=system.file("extdata","dataGeneTreeSample",package="MSCquartets"))
tnames=taxonNames(gtrees)
```

TINNIK *TINNIK algorithm to infer species tree of blobs*

Description

Apply the TINNIK algorithm of Allman et al. (2024) (see also Allman et al. (2022)) to infer a tree of blobs for the species network from a collection of gene trees, under the network multispecies coalescent (NMSC) model.

Usage

```
TINNIK(
  genedata,
  omit = FALSE,
  epsilon = 0,
  test = "T3",
  alpha = 0.05,
  beta = 0.95,
  treemethod = fastme.bal,
  delta = 2,
  taxanames = NULL,
  plot = TRUE
)
```

Arguments

`genedata`	gene tree data that may be supplied in any of 3 forms: 1. as a character string giving the name of a file containing Newick gene trees, 2. as a multiPhylo object containing the gene trees, or 3. as a table of quartets on the gene trees, as produced by a previous call to `TINNIK` or `quartetTableResolved`, which has columns only for taxa, resolved quartet counts, and possibly p_T3, p_cut, and p_star
`omit`	`FALSE` to treat unresolved quartets as 1/3 of each resolution; `TRUE` to discard unresolved quartet data; ignored if gene tree data given as quartet table
`epsilon`	minimum for branch lengths to be treated as non-zero; ignored if gene tree data given as quartet table
`test`	a hypothesis test to perform, either "cut" or "T3" (default)

`alpha`	a value or vector of significance levels for judging p-values for test specified by "test"; testing a null hypothesis of no hybridization vs. an alternative of hybridization, for each quartet; a smaller value applies a less conservative test for a tree (more trees), hence a stricter requirement for deciding in favor of hybridization (fewer reticulations)
`beta`	a value or vector of significance levels for judging p-values testing a null hypothesis of a star tree (polytomy) for each quartet vs. an alternative of anything else; a smaller value applies a less conservative test for a star tree (more polytomies), hence a stricter requirement for deciding in favor of a resolved tree or network; if vectors, `alpha` and `beta` must have the same length
`treemethod`	a function implementing a method of tree inference from a distance table, e.g. the ape package's fastme.bal or nj
`delta`	a minimum edge length to retain in tree of blobs (see (Allman et al. 2024) for related theory); shorter edges are collapsed
`taxanames`	if `genedata` is a file or a multiPhylo object, a vector of a subset of the taxa names on the gene trees to be analyzed, if `NULL` all taxa on the first gene tree are used; if `genedata` is a quartet table, this argument is ignored and all taxa in the table are used
`plot`	`TRUE` produces simplex plots of hypothesis test results and plots the tree of blobs `FALSE` omits plots

Details

This function

1. counts displayed quartets across gene trees to form quartet count concordance factors (qcCFs),
2. applies appropriate hypothesis tests to judge qcCFs as representing putative hybridization, resolved trees, or unresolved (star) trees using `alpha` and `beta` as significance levels,
3. produces a simplex plot showing results of the hypothesis tests for all qcCFs
4. computes the appropriate TINNIK distance table, and infers the tree of blobs from the distance.

A call of `TINNIK` with `genedata` given as a table previously output from `TINNIK` is equivalent to a call of `TINNIKdist` followed by tree construction from the distance table. If `genedata` is a table previously output from `quartetTableResolved` which lacks columns of p-values for hypothesis tests, these will be appended to the table output by `TINNIK`. This table must contain a row with quartet counts for every 4 taxon set.

If plots are produced, there are 2 simplex plots: The first shows the hypothesis test results, and the second shows inferred B-quartets and T-quartets. In both, each point in the simplex plot corresponds to an empirical quartet concordance factor, color-coded to represent test or inference results.

In general, `alpha` should be chosen to be small and `beta` to be large so that most quartets are interpreted as resolved trees. More quartets judges to have either blob or unresolved relationships will lead to a less resolved blob tree.

Usually, an initial call to `TINNIK` will not give a good analysis, as values of `alpha` and `beta` are likely to need some adjustment based on inspecting the data. Saving the returned table of test results from `TINNIK` will allow for the results of the time-consuming computation of qcCFs to be saved, along with p-values, for input to further calls of `TINNIK` with new choices of `alpha` and `beta`.

See the documentation for `TINNIKdist` for an explanation of a small, rarely noticeable, stochastic element of the algorithm.

For data sets of many gene trees, user time may be reduced by using parallel code for counting displayed quartets. See `quartetTableParallel`.

Value

`output` (returned invisibly), with `output$ToB` the TINNIK tree of blobs, `output$pTable` the table of quartets and p-values for judging fit to the MSC on quartet trees, and `output$Bquartets` a TRUE/FALSE indicator vector of B-quartets; if `alpha, beta` are vectors, `output$ToB` is a vector of trees; the table can be used as input to `TINNIK` or `TINNIKdist` with new choices of `alpha, beta`, without re-tallying quartets on gene trees

References

Allman ES, Baños H, Mitchell JD, Rhodes JA (2022). "The tree of blobs of a species network: identifiability under the coalescent." *Journal of Mathematical Biology*, **86**(1), 10. doi:10.1007/s002850220218389.

Allman ES, Baños H, Mitchell JD, Rhodes JA (2024). "TINNiK: Inference of the Tree of Blobs of a Species Network Under the Coalescent." *bioRxiv*. doi:10.1101/2024.04.20.590418, `https://www.biorxiv.org/content/10.1101/2024.04.20.590418v1`.

See Also

`quartetTable`, `quartetTableParallel`, `quartetTableDominant`, `quartetCutTestInd`,`quartetTreeTestInd`, `quartetStarTestInd`, `TINNIKdist`, `quartetTestPlot`, `pvalHist`

Examples

```
data(pTableYeastRokas)
out=TINNIK(pTableYeastRokas, alpha=.01, beta=.05)
```

`TINNIKdist` *Compute TINNIK distance from quartets and hypothesis test p-values*

Description

Apply the B-quartet inference algorithm of Allman et al. (2022), Allman et al. (2024) to infer all B-quartets from results of hypothesis tests, and then compute an estimate of an intertaxon distance fitting the topological tree of blobs of the species network.

Usage

```
TINNIKdist(pTable, test = "T3", alpha = 0.05, beta = 0.05)
```

Arguments

`pTable`	table of resolved quartet counts, as produced by `quartetTableResolved`, with extra columns from both star hypothesis test, and either cut or T3 hypothesis tests
`test`	either "cut" or "T3"
`alpha`	critical value for cut or T3 test
`beta`	critical value for star test

Details

This function assumes `pTable` has columns for taxa and resolved quartet counts as originally produced by `quartetTable`, and hypothesis test results as produced by `quartetStarTestInd`, and either `quartetTreeTestInd` for the `T3` test or `quartetCutTestInd`. Rows must be present for every 4-taxon subset. (Note: Of functions in this package, only `HolmBonferroni` might modify the row order from the required one.)

This function uses the Rcpp package for significant speed up in computation time.

Value

a distance table `output$dist` and a vector `output$Bquartets` with TRUE/FALSE entries indicating B-quartets ordered as rows of `pTable`.

References

Allman ES, Baños H, Mitchell JD, Rhodes JA (2022). “The tree of blobs of a species network: identifiability under the coalescent.” *Journal of Mathematical Biology*, **86**(1), 10. doi:10.1007/s00285022018389.

Allman ES, Baños H, Mitchell JD, Rhodes JA (2024). “TINNiK: Inference of the Tree of Blobs of a Species Network Under the Coalescent.” *bioRxiv*. doi:10.1101/2024.04.20.590418, `https://www.biorxiv.org/content/10.1101/2024.04.20.590418v1`.

See Also

`quartetTable`, `quartetTableResolved`, `quartetStarTest`, `quartetCutTest`, `quartetStarTestInd`, `quartetCutTestInd`

Examples

```
data(pTableYeastRokas)
out=TINNIKdist(pTableYeastRokas,test="T3",alpha=.05,beta=.05)
```

`topDist` *Topological distances on a tree*

Description

Compute a pairwise table of topological distances from a tree, after contracting short edges

Usage

```
topDist(tree, epsilon = 0)
```

Arguments

`tree`	a phylo object, with or without edge lengths
`epsilon`	a tolerance, so all edges shorter than epsilon are contracted

Value

a distance table, with rows and columns named by taxa

`treeFromSplits` *Produce tree from compatible splits*

Description

Produce tree from compatible splits

Usage

```
treeFromSplits(sp, plot = FALSE)
```

Arguments

`sp`	a compatible split system, as produced by compatibleSplits
`plot`	a logical, if TRUE, plot tree

Value

a phylo object for tree displaying splits

See Also

`compatibleSplits`, `TINNIK`

Examples

```
data(pTableYeastRokas)
dist=NANUQdist(pTableYeastRokas, alpha=.05, beta=.95,outfile=NULL)
nn=neighborNet(dist)
plot(nn,"2D")
tob=treeFromSplits(compatibleSplits(nn$splits),plot=TRUE) #produce tree of blobs of splits graph
```

`treeOfBlobs` *Tree of blobs for a network*

Description

Given extended newick, an evonet object, or an igraph object for a network, return its reduced, unrooted tree of blobs. Here 'reduced' means all nodes resulting from 2-blobs are suppressed, as are edges above the network's LSA.

Usage

```
treeOfBlobs(net, plot = FALSE)
```

Arguments

`net`	A network, supplied as an extended Newick string, an evonet object, or an igraph object
`plot`	if TRUE (default), plot the tree of blobs.

Value

An object of class `phylo` containing the unrooted topological tree derived from the network by contracting all blobs. All edge lengths are 1.

See Also

`TINNIK`

Examples

```
network = "(((a:1,d:1):1,(b:1)#H1:1):1,(#H1,c:1):2);"
plot(read.evonet(text=network))
treeOfBlobs(network, plot=TRUE)
```

`WQDC` *Compute Weighted Quartet Distance Consensus tree from gene tree data*

Description

Compute the Weighted Quartet Distance Consensus (Yourdkhani and Rhodes 2020) estimate of a species tree from gene tree data. This is a consistent estimator of the unrooted species tree topology and all internal branch lengths.

Usage

```
WQDC(
  genetreedata,
  taxanames = NULL,
  method = fastme.bal,
  omit = FALSE,
  terminal = 1
)
```

Arguments

`genetreedata`	gene tree data that may be supplied in any of 3 forms: 1. a character string giving the name of a file containing gene trees in Newick 2. a multiPhylo object containing gene trees 3. a resolved quartet table, as produced by `quartetTableResolved`
`taxanames`	if `genetreedata` is a file or a multiPhylo object, a vector of a subset of the taxa names on the gene trees to be analyzed, if `NULL` all taxa on the first gene tree are used; if `genetreedata` is a quartet table, this argument is ignored and all taxa in the table are used
`method`	a distance-based tree building function, such as `fastme.bal` or `nj`
`omit`	`TRUE` leaves out unresolved quartets, `FALSE` treats them as 1/3 of each resolution; ignored if `genetreedata` is given as a resolved quartet table
`terminal`	non-negative branch length to supply for terminal branches whose length cannot be inferred by `WQDC`

Details

This function is a wrapper which performs the steps of reading in a collection of gene trees, tallying quartets, estimating quartet internal branch lengths, computing the weighted quartet distance between taxa, building a tree, and adjusting edge lengths, to give a consistent estimate of the metric species tree in coalescent units under the MSC.

If the gene tree data indicates some quartets experienced little to no incomplete lineage sorting, this algorithm tends to be less topologically accurate than `QDC` (which infers no metric information) or `WQDCrecursive` (which gives better topologies, and reasonably accurate lengths for short edges, though long edge lengths may still be unreliable).

Value

an unrooted metric tree of type phylo

References

Yourdkhani S, Rhodes JA (2020). “Inferring metric trees from weighted quartets via an intertaxon distance.” *Bul. Math. Biol.*, **82**(97). doi:10.1007/s11538020007734.

See Also

quartetTable, quartetTableResolved, quartetTableDominant, quartetWeightedDist, WQDCrecursive, WQDS, QDC

Examples

```
gtrees=read.tree(file=system.file("extdata","dataGeneTreeSample",package="MSCquartets"))
tnames=taxonNames(gtrees)
stree=WQDC(gtrees,tnames[1:6])
write.tree(stree)
plot(stree)
```

`WQDCrecursive` *Compute the Recursive Weighted Quartet Distance Consensus tree from gene tree data*

Description

Infer a metric species tree from counts of quartets displayed on a collection of gene trees, as described by Yourdkhani and Rhodes (2020). Edge lengths are in coalescent units.

Usage

```
WQDCrecursive(rqt, method = fastme.bal, stopAt = 2, terminal = 1)
```

Arguments

`rqt`	a resolved quartet table as produced by `quartetTableResolved`
`method`	a distance-based tree building function, such as `fastme.bal` or `nj`
`stopAt`	a non-negative branch length in coalescent units; recursive calls stop when the longest branch in a recursively examined subtree is smaller than this value
`terminal`	non-negative branch length to supply for terminal branches, whose lengths cannot be inferred by `WQDCrecursive`

Details

The algorithm counts quartets displayed on the gene trees, builds a tree using `WQDS`, determines the split corresponding to the longest edge in that tree, and then recursively builds trees on the taxa in each split set together with a 'composite taxon' formed by all taxa in the other split set. This approach is slower than non-recursive `WQDC`, but increases topological accuracy. Shorter branch lengths tend to be more accurately estimated.

This function must be called with its argument a resolved quartet table of size (n choose 4)x(n+3). Its recursive nature requires building smaller resolved quartet tables on split sets with an additional composite taxon.

Value

an unrooted metric tree, of type phylo

References

Yourdkhani S, Rhodes JA (2020). "Inferring metric trees from weighted quartets via an intertaxon distance." *Bul. Math. Biol.*, **82**(97). doi:10.1007/s11538020007734.

See Also

`quartetTableResolved`,`quartetTable`, `QDC`, `QDS`, `quartetTableCollapse`

Examples

```
gtrees=read.tree(file=system.file("extdata","dataGeneTreeSample",package="MSCquartets"))
tnames=taxonNames(gtrees)
QT=quartetTable(gtrees,tnames[1:6])
RQT=quartetTableResolved(QT)
stree=WQDCrecursive(RQT)
write.tree(stree)
plot(stree)
```

`WQDS` *Compute the Weighted Quartet Distance Supertree*

Description

Apply the Weighted Quartet Distance Supertree method of Yourdkhani and Rhodes (2020) to a collection of quartets on `n` taxa together with internal quartet branch lengths, specified by a table.

Usage

```
WQDS(dqt, method = fastme.bal)
```

Arguments

`dqt`	an (`n` choose 4) x `n+1`) matrix of form output by `quartetTableDominant`
`method`	a distance-based tree building function (e.g., fastme.bal, NJ, etc.)

Details

This function is a wrapper which runs `quartetWeightedDist`, builds a tree, and then adjusts edge lengths with `WQDSAdjustLengths`.

Value

an unrooted metric tree, of type phylo

References

Yourdkhani S, Rhodes JA (2020). "Inferring metric trees from weighted quartets via an intertaxon distance." *Bul. Math. Biol.*, **82**(97). doi:10.1007/s11538020007734.

See Also

`quartetTableDominant`, `quartetWeightedDist`, `WQDSAdjustLengths`, `WQDC`, `WQDCrecursive`, `QDS`

Examples

```
gtrees=read.tree(file=system.file("extdata","dataGeneTreeSample",package="MSCquartets"))
tnames=taxonNames(gtrees)
QT=quartetTable(gtrees,tnames[1:6])
RQT=quartetTableResolved(QT)
DQT=quartetTableDominant(RQT,bigweights= "finite")
tree=WQDS(DQT)
write.tree(tree)
plot(tree)
```

`WQDSAdjustLengths` *Adjust edge lengths on tree built from Weighted Quartet distance to estimate metric tree*

Description

Modify edge lengths of a tree built from a distance table produced by `quartetWeightedDist`, to remove scaling factors related to the size of the split associated to the edge.

Usage

```
WQDSAdjustLengths(tree)
```

Arguments

`tree`	an unrooted metric tree, of type phylo

Details

As explained by Yourdkhani and Rhodes (2020), a metric tree produced from the weighted quartet distance has edge lengths inflated by a factor dependent on the associated split size. Removing these factors yields a consistent estimate of the metric species tree displaying the weighted quartets, if such a tree exists.

This function should not be used on trees output from `WQDS`, `WQDC`, or `WQDCrecursive`, as their edges are already adjusted. It can be used on trees built from the distance computed by `quartetWeightedDist`.

Value

an unrooted metric tree, of type phylo

References

Yourdkhani S, Rhodes JA (2020). "Inferring metric trees from weighted quartets via an intertaxon distance." *Bul. Math. Biol.*, **82**(97). doi:10.1007/s11538020007734.

See Also

`WQDS`, `WQDC`

Examples

```
gtrees=read.tree(file=system.file("extdata","dataGeneTreeSample",package="MSCquartets"))
tnames=taxonNames(gtrees)
QT=quartetTable(gtrees,tnames[1:6])
RQT=quartetTableResolved(QT)
DQT=quartetTableDominant(RQT,bigweights="finite")
D=quartetWeightedDist(DQT)
tree=NJ(D)
write.tree(tree)
plot(tree)
stree=WQDSAdjustLengths(tree)
write.tree(stree)
plot(stree)
```

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