Package 'MSCquartets'

March 7, 2025

```
Type Package
```

Title Analyzing Gene Tree Quartets under the Multi-Species Coalescent

Version 3.1

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>, 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>, and NANUQ+ routines for resolving multifurcations in the tree of blobs to cycles as in Allman et al.(2024) (forthcoming).

Software announcement by Rhodes et al. (2020) <doi:10.1093/bioinformatics/btaa868>.

```
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```

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MSCau	Jantets-nackage Multispecies Coglescent 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).
- Infer the tree of blobs for a species network via the TINNiK method (Allman et al. 2022),(Allman et al. 2024).
- 7. Resolove multifurcations in a tree of blobs to cycles via NANUQ+ routines (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.

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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.

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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.

Allman ES, Baños H, Rhodes JA, Wicke K (2024). "NANUQ+: A divide-and-conquer approach to network estimation." draft.

allPerms

Generate permutations

Description

Generate all permutations of 1 to n, as rows of a matrix

Usage

allPerms(n)

Arguments

n

size of permutations

Value

an n!xn matrix whose rows give permutations

Examples

allPerms(4)

BQinference

blobDistance	Compute empirical distance between taxon groups.

Description

From gene quartet counts, computes NANUQ or modNANUQ distances between groups of taxa (which should be those around a multifurcation in a tree of blobs. If these groups are not singletons, averaging is done over group elements.

Usage

```
blobDistance(pTable, taxa, groupvec, test = "T3", alpha, beta, dist = "NANUQ")
```

Arguments

pTable table of giving empirical gene quartet counts for the taxa on tree, with columns

p_star and p_test

taxa a list of taxon names, who positions are used in 'groups'

groupvec taxon groups encoded in vector

test to be used for detecting hybridizations in quartete ("T3" or "cut")

alpha test level for p_test beta test level for p_star

dist the distance to compute, either "NANUQ" or "modNANUQ"

Value

the distance matrix, ordered by taxon group number

BOinference	Main loop of B-quartet inference	
DQTITI CI CIICC	main toop of B quarter injerence	

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)
```

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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

circHybOrders

Generate all circular orders with designated hybrid

Description

Generate a matrix whose rows give all circular orders with a designated hybrid. The order is encoded as a vector with entries from 1 to n, where the position corresponds to a node/group of taxa. The location in the vector of the 1 indicates the hybrid, the positions of 2, n its neighbors, etc.

Usage

circHybOrders(n)

Arguments

n

size of order, with n>3

Details

To avoid duplication of circular orders, the entry 2 in each vector always occurs before the entry n. Since in using first-order quartet-based methods to infer 4-cycles the hybrid node is not identifiable, for n=4 only 3 orders are given, with 1 as hybrid for each

Value

an (n!/2)xn (or 3xn if n=4) matrix whose rows give all circular orders.

Examples

```
circHybOrders(4)
circHybOrders(5)
```

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

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

combineCycleResolutions

Combine several cycle resolutions on a tree of blobs to create a network

Description

Given a list of resolutions of different multifurcations on a tree of blobs (each as produced by resolveCycle), combine these with the tree of blobs to form a network.

Usage

```
combineCycleResolutions(ToB, resolutions, plot = 1, titletext = NULL)
```

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Arguments

ToB an unrooted tree of blobs for the network, with multifurcating nodes labelled by

labelIntNodes

resolutions a list of resolutions (each of which may be a list) for different nodes with ele-

ments in format described in output of resolveCycle

plot if FALSE (0), no plots; if TRUE (>0) plot networks

titletext a string of text for plot

Details

This function is useful for forming near-optimal networks when there are several resolutions that have similar fit for some of the multifurcations.

Value

a list of Newick strings for the networks, with all edge lengths 1

See Also

```
TINNIK, labelIntNodes, resolveCycle, resolveLevel1
```

Examples

```
data(pTableYeastRokas)
out=TINNIK(pTableYeastRokas, alpha=.01, beta=.05)
ToB=labelIntNodes(out$ToB)
R9=resolveCycle(ToB, node=9, pTable=out$pTable, alpha=.01, beta=.05, distance="NANUQ")
R10=resolveCycle(ToB, node=10, pTable=out$pTable, alpha=.01, beta=.05, distance="NANUQ")
combineCycleResolutions(ToB, resolutions=list(R9,R10),plot=TRUE)
```

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

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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
```

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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: <math display="block"> \\ \text{gts=read. tree} (\text{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.

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

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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 13

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.

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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

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)
```

expmodNANUQCycleDist Expected modNANUQ cycle distance

Description

Compute expected modNANUQ distance for a sunlet network with 4 or more taxa. This is used in a hueristic method for resolving multifurcation in a tree of blobs to a cycle by NANUQ+ commands.

Usage

```
expmodNANUQCycleDist(n)
```

Arguments

n

number of edges in cycle (at least 4)

Value

an nxn distance matrix with rows/columns ordered from hybrid following circular order

Examples

```
expmodNANUQCycleDist(5)
#'@seealso \code{\link{resolveCycle}} \code{\link{ordersHeuristicmodNANUQ}}
```

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expNANUQCycleDist

Expected NANUQ cycle distance

Description

Compute expected NANUQ distance for a sunlet network with 4 or more taxa. This is used to resolve multifurcations in a tree of blobs by NANUQ+ functions

Usage

```
expNANUQCycleDist(n)
```

Arguments

n

number of edges in cycle

Value

an nxn distance matrix with rows/columns ordered from hybrid following circular order

See Also

```
resolveCycle
```

Examples

```
expNANUQCycleDist(5)
```

fitCycleOrders

Compute fit of circular orders to distance with least squares

Description

Compute residual sum of squares (RSS) comparing empirical distance for a blob to an expected one for a cycle with each given order/designated hybrid. This is used in NANAUQ+ commands for resolving multifurcations in a tree of blobs to a cycle

Usage

```
fitCycleOrders(D, E, orders)
```

Arguments

D an empirical distance table

E an expected distance table, to be reordered

orders a vector indicating an order, or matrix whose rows give orders, to fit

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Value

vector of RSSs, one for each order

See Also

resolveCycle, resolveLevel1

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	s, as computed by quartetTreeTestInd or
--------	-----------------------------------	---

quartetStarTestInd

model one of "T1", "T3", or "star", where pTable contains a column p_model of

p-values

alpha test level, 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"

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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
```

labelIntNodes 19

labelIntNodes	Label internal nodes on tree	
Tabelliitiodes	Easet internat nodes on tree	

Description

Label all internal nodes of tree, as "Node NN" where NN is the node number, and plot tree with labels

Usage

```
labelIntNodes(tree, plot = TRUE, type = "unrooted")
```

Arguments

tree a rooted or unrooted tree (phylo object)
plot TRUE for plot, FALSE for no plot

type plot type (e.g., "unrooted") to be passed to ape plot command

Value

a phylo object with internal node labels

See Also

```
resolveCycle, combineCycleResolutions, resolveLevel1
```

Examples

```
data(pTableYeastRokas)
out=TINNIK(pTableYeastRokas,test="T3",alpha=.01, beta=.05)
labelIntNodes(out$ToB)
```

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)

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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

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alpha a value or vector of significance levels for judging p-values testing a null hy-

pothesis 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 describing in favor of hybridization (fewer reticulations)

beta a value or vector of significance levels for judging p-values testing a null hy-

pothesis 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.

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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.

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Usage

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

Arguments

pTable

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)

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 requirement for suspecting a resolved tree if vectors alpha and hata must have the same level.

a table of resolved quartets and p-values, as previously computed by NANUQ, or

resolved tree; if vectors, alpha and beta must have the same length

plot TRUE produces simplex plots of hypothesis tests, FALSE omits plots

Details

beta

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.

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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 25

nodeGroups	
HOUEGI OUDS	

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)
```

ordersHeuristicmodNANUQ

Choose cycle orders heuristically from empirical modNANUQ distance

Description

Find candidates for best hybrid node and circular order fitting the modNANUQ distance.

Usage

```
ordersHeuristicmodNANUQ(M, delta = 10^-6)
```

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Arguments

M an empirical modNANUQ distance table

delta cutoff for relative difference in distances for determining near ties for "best"

orders

Details

Candidadte orders are obtained by first picking the hybrid node (from the minimum column sum of the distance matrix), then ordering nodes by distance from the hybrid, and for each consecutive pair picking nodes in the cycle closest to the previous node. This constructs one or more orders since ties may occur. For more details, see Allman et al. (2024).

This function is used by NANUQ+ commands to resolve multifurcations in a tree of blobs of high degree.

Value

a list of circular orders

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

expmodNANUQCycleDist resolveCycle resolveLevel1

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)

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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.

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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")
```

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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

QDS

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

quartet Table, quartet Table Resolved, quartet Table Dominant, quartet Dist, QDS, WQDC, WQDC recursive estimate Edge Lengths

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+1th 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

quartetBTinferencePlot

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.

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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 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.

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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 33

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 levels 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.

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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/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.

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 35

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 $\footnote{\colored}$
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.

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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+1th 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

```
\verb"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)
```

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```
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

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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.

```
quartetStarTestInd(rqt)
```

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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.

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

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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

```
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)
```

quartet Table Collapse 41

quartetTableCollapse	Reduce quartet table by combining some taxa
qual tetrablecollapse	Reduce quarter 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.

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

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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.

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

quartetTableParallel 43

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

```
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,])
```

Description

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

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

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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 redis-

tributes 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

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See Also

quartetTable, quartetTableParallel

quartetTestPlot	Produce simplex plot with results of quartet hypothesis tests
qual tet lesti 10t	Troduce simplex plot with results of quarter hypothesis tesis

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 quartet Tree Test Ind, quartet Star Test Ind, or NANUQ
test	model to use, for tree null hypothesis; options are "T1", "T3", "cut", "NANUQ"
alpha	level for tree test with null hypothesis given by test
beta	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

```
\verb| quartetTreeTestInd|, \verb| quartetStarTestInd|, \verb| NANUQ|, \verb| NANUQdist| \\
```

```
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 47

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.

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

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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.

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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

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

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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 quartet Table Resolved, or quartet Star Test Ind
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 $\footnote{\colored}$
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.

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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,])
```

quartet Weighted Dist

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

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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)
```

resolveCycle

Resolve a node on a tree of blobs as a cycle

Description

Given a Tree of Blobs and quartet Concordance Factor data, resolve a specific polytomy to a cycle. Resolution is performed by finding a least-squares best-fit of an empirical distance to an expected distance related to the cycle, as described in Allman et al. (2024).

```
resolveCycle(
  ToB,
  node,
  pTable,
  test = "T3",
  alpha,
  beta,
  distance = "NANUQ",
  hdegree = 10,
  plot = TRUE,
  delta = 10^-6
)
```

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Arguments

ТоВ	an unrooted tree of blobs (phylo object), as determined by TINNIK or another method, with multifurcations labelled by labelIntNodes
node	number of an internal node to be resolved
pTable	a table of qcCFs, with columns p_star and p_test
test	either "T3" or "cut", indicating the test to use for determining what qcCFs indicate hybridization
alpha	test level for p_test
beta	test level for p_star
distance	cycle resolution distance to be used; one of "NANUQ" or "modNANUQ"
hdegree	resolve a multifurcation of this degree or larger by a heuristic method; must be at least 5
plot	if FALSE (0), no plots; if TRUE (>0), make plots of resolved cycle(s) considered best and histogram of measure of fit for all hybrid/orders considered
delta	$cutoff for relative \ difference \ in \ squared \ residuals \ and \ smallest, (RSS-minRSS)/minRSS,$

Details

Possible distances to use are the NANUQ distance and a modified NANUQ distance that weights quartet trees differently, but from which the cycle structure is still identifiable.

for determining near ties as "best" fit resolutions

For multifucations of degree less than a designated cutoff, all possible circular orders and choices of hybrid nodes are considered in choosing the best. Above that cutoff, a heuristic method built on the modified NANUQ distance is used to obtain a small number of orders likely to be good fits, with the least-squares fitting applied only to those.

Value

a list of resolution information, given as a list of:

- \$node number,
- \$cycleRes list [[1]]-[[k]] of best resolutions,
- \$RSSs RSSs from all cycle resolutions considered in choosing best.

Each resolution is itself a 5-element list with entries:

- \$cycleNet Newick network with 1 cycle (with all edge lengths 1)
- \$cycleRSS RSS for cycle,
- \$taxonGroups taxon groups for cycle,
- \$order order of groups around cycle,
- \$nonRootEdges logical vector indicating edges of ToB where root cannot be.

(Items \$taxonGroups, \$order, \$nonRootEdges are needed to combine resolutions to form networks with multiple cycles using combineCycleResolutions, and otherwise may not be of interest to users).

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References

Allman ES, Baños H, Rhodes JA, Wicke K (2024). "NANUQ+: A divide-and-conquer approach to network estimation." draft.

See Also

TINNIK, labelIntNodes, combineCycleResolutions, resolveLevel1

Examples

```
data(pTableYeastRokas)
out=TINNIK(pTableYeastRokas, alpha=.01, beta=.05)
TOB=labelIntNodes(out$TOB)
resolveCycle(ToB, node=9, pTable=out$pTable, alpha=.01, beta=.05, distance="NANUQ")
```

resolveLevel1

Resolve Tree of Blobs to Level-1 network

Description

Given a Tree of Blobs and qcCF information, resolve all multifurcations to cycles. Resolution is performed by finding a least-squares best-fit of an empirical distance to an expected distance related to the cycle, as described in Allman et al. (2024).

Usage

```
resolveLevel1(
   ToB,
   pTable,
   test = "T3",
   alpha,
   beta,
   distance = "NANUQ",
   hdegree = 10,
   plot = 2,
   delta = 10^-6,
   fullResMax = 10
)
```

Arguments

ToB an unrooted tree of blobs (phylo object) as determined by TINNIK or another

method

pTable a table of qcCFs, with columns p_star and p_test

test either "T3" or "cut", indicating test to use for determining what qcCFs indicate

hybridization

resolveLevel1 55

alpha test level for p_test beta test level value for p_star

distance cycle resolution distance to be used ("NANUQ" or "modNANUQ")

hdegree resolve a multifurcation of this degree or larger by a heuristic method; must be

at least 5

plot if 0, no plots; if 1, plot only possible root locations on ToB and full resolution;

if 2, include plots of each individual blob resolution, if 3 include histograms of

measure of fit for all hybrid/orders considered in choosing best

delta cutoff for relative difference in squared residuals and smallest, (RSS-minRSS)/minRSS,

for determining near ties as "best" fit resolutions

fullResMax maximum number of full resolutions (all multifurcations at once) to form; if the

product of the number of resolutions of individual multifurcations exceeds this, no full resolutions are produced, although combineCycleResolutions can be

applied to produce them.

Details

Possible distances to use are the NANUQ distance and a modified NANUQ distance that weights quartet trees differently, but from which the cycle structure is still identifiable.

For multifucations of degree less than a designated cutoff, all possible circular orders and choices of hybrid nodes are considered in choosing the best. Above that cutoff, a heuristic method is used to obtain a small number of orders likely to be good fits, with the least-squares fitting applied only to those.

Value

a list of resolutions and squared residuals:

- [[1]] is a list of Newick resolutions of entire network, with all edge lengths 1 (NULL if one cannot be produced or fullResMax is exceeded),
- [[2]]-[[n]] are individual resolutions of each multifurcation on ToB, each given as a list as output from resolveCycle.

References

Allman ES, Baños H, Rhodes JA, Wicke K (2024). "NANUQ+: A divide-and-conquer approach to network estimation." draft.

See Also

TINNIK, labelIntNodes, resolveCycle, combineCycleResolutions

```
data(pTableYeastRokas)
out=TINNIK(pTableYeastRokas, alpha=.01, beta=.05)
ToB=labelIntNodes(out$ToB)
resolveLevel1(ToB, pTable=out$pTable, alpha=.01, beta=.05, distance="NANUQ")
```

56 simplexLabels

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 transformation 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.

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

simplexPoint 57

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\\
```

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

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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.

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

simplexText 59

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
```

```
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

suppressNetBinaryNodes

Suppress Network Binary Nodes

Description

Suppress any non-root binary nodes in a phylogenetic network.

Usage

```
suppressNetBinaryNodes(net, addlength = TRUE)
```

Arguments

net a phylogenetic network, of class "evonet"

addlength if TRUE (default), add lengths of two incident edges for new edge.

Details

This function is similar to ape's collapse.singles which only works on phylo objects that are trees.

T1density 61

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

Х	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

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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

tableHeliconiusMartin Quartet table for Heliconius gene tree dataset

Description

An .rda file containing a quartet table summarizing the "Heleconius" gene trees of Martin et al. (2013). This table contains quartet counts from 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.

Usage

data(tableHeliconiusMartin)

Format

an R data file

Details

This table is provided rather than the original gene trees to save storage space. If used, please cite Martin et al. (2013).

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.

tableLeopardusLescroart

Quartet table for Leopardus dataset

Description

An .rda file containing a quartet table summarizing the "Leopardus" gene trees of Lescroart et al. (2023). This table contains quartet counts for 16,338 "gene" trees for 16 taxa, inferred from sliding widows across genomic sequences.

Usage

data(tableLeopardusLescroart)

Format

an R data file

Details

This table is provided rather than the original gene trees to save storage space. If used, please cite Lescroart J, Bonilla-Sánchez A, Napolitano C, Buitrago-Torres DL, Ramírez-Chaves HE, Pulido-Santacruz P, Murphy WJ, Svardal H, Eizirik E (2023). "Extensive Phylogenomic Discordance and the Complex Evolutionary History of the Neotropical Cat Genus Leopardus." *Molecular Biology and Evolution*, **40**(12), msad255. doi:10.1093/molbev/msad255, https://academic.oup.com/mbe/article-pdf/40/12/msad255/56555032/msad255.pdf..

References

Lescroart J, Bonilla-Sánchez A, Napolitano C, Buitrago-Torres DL, Ramírez-Chaves HE, Pulido-Santacruz P, Murphy WJ, Svardal H, Eizirik E (2023). "Extensive Phylogenomic Discordance and the Complex Evolutionary History of the Neotropical Cat Genus Leopardus." *Molecular Biology and Evolution*, **40**(12), msad255. doi:10.1093/molbev/msad255, https://academic.oup.com/mbe/article-pdf/40/12/msad255/56555032/msad255.pdf.

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)

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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

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epsilon minimum for branch lengths to be treated as non-zero; ignored if gene tree data given as quartet table a hypothesis test to perform, either "cut" or "T3" (default) test a value or vector of significance levels for judging p-values for test specified alpha 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 ni delta a minimum edge length to retain in tree of blobs (see (Allman et al. 2024) for related theory); shorter edges are collapsed if genedata is a file or a multiPhylo object, a vector of a subset of the taxa taxanames 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

Details

plot

This function

1. counts displayed quartets across gene trees to form quartet count concordance factors (qcCFs),

TRUE produces simplex plots of hypothesis test results and plots the tree of blobs

- 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

FALSE omits plots

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.

66 TINNIKdist

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/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, 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.

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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 level for cut or T3 test

beta level 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

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

68 treeFromSplits

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
```

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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

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

70 WQDC

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).

WQDCrecursive 71

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

quartet Table, quartet Table Resolved, quartet Table Dominant, quartet Weighted Dist, WQDC recursive, 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

72 WQDS

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)
```

WODS

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.

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

WQDSAdjustLengths 73

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

 ${\tt quartetTableDominant,\ quartetWeightedDist,\ WQDSAdjustLengths,\ WQDC,\ WQDCrecursive,\ QDS}$

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.

```
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

```
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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