# Package 'MSCquartets'

# October 6, 2019

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Title Analyzing gene trees through quartets under the multispecies coalescent model

**Description** A package for analyzing and using quartets displayed on a collection of gene trees, primarily to make inferences about the species tree or network under the multispecies coalescent (MSC) model.

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# **R** topics documented:

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# Description

Create a list of all taxa appearing on a collection of trees, with no repeats.

# Usage

AllTaxonNames(trees)

# Arguments

trees a multiphylo object containing a collection of trees

# Value

a vector of unique names of taxa appearing on the trees

CollapseQuartetTable 3

#### **Examples**

```
gtrees=read.tree(file=system.file("genetreeSample",package="MSCquartets"))
taxonnames=AllTaxonNames(gtrees)
```

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

#### **Description**

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

### Usage

```
CollapseQuartetTable(RQT, taxaA, taxaB)
```

### **Arguments**

RQT a resolved quartet table, as from ResolvedQuartetTable taxaA a vector of taxon names in RQT to be included in new table

taxaB a vector of taxon names in RQT to form new composite taxon in new 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).

#### 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

WODCrec

DominantQuartetTable Produce table of dominant quartets, with ML estimates of internal edge length under the MSC model

#### **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 multispecies coalescent model.

# Usage

```
DominantQuartetTable(RQT, bigweights = "infinite")
```

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#### **Arguments**

RQT array as produced by ResolvedQuartetTable of size (n choose 4)x(n+3);

bigweights "infinite" or "finite", determines if the weight of a quartet for which only one

topology appears is given as "Inf" or a finite, but large, numerical value

#### 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. Column "weight" contains ML estimate under MSC model of quartets central edge length, in coalescent units.

#### See Also

QuartetTable, ResolvedQuartetTable

### **Examples**

```
gtrees=read.tree(file=system.file("genetreeSample",package="MSCquartets"))
taxonnames=AllTaxonNames(gtrees)
QT=QuartetTable(gtrees, taxonnames[1:5])
RQT=ResolvedQuartetTable(QT)
DQT=DominantQuartetTable(RQT)
```

HolmBonferroni

Adjust p-values for multiple tests by Holm-Bonferroni method

#### **Description**

When p-values are computed for each quartet using MultiIndepQuartetTest or MultiIndepStarTest, multiple comparisons are being done for one dataset. The Holm-Bonferroni method adjusts these p-values upward, controlling the familywise error rate. The probability of at least one false discovery is no more than the significance level.

#### Usage

```
HolmBonferroni(pTable, columnname, alpha)
```

### Arguments

pTable a table of quartets with p-values, as computed by MultiIndepQuartetTest or

MultiIndepStarTest

columname a name of a column of pTable containing p-values, such as "p\_T3", "p\_T1", "p\_star"

alpha a critical value, for rejection of adjusted p-values below alpha

#### Value

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

log10Hist 5

#### See Also

 ${\tt MultiIndepQuartetTreeTest}, {\tt MultiIndepQuartetStarTest}$ 

### **Examples**

```
gtrees=read.tree(file=system.file("genetreeSample",package="MSCquartets"))
taxanames=AllTaxonNames(gtrees)
QT=QuartetTable(gtrees,taxanames)
RQT=ResolvedQuartetTable(QT)
pTable=MultiIndepQuartetTreeTest(RQT,"T3")
HBpTable=HolmBonferroni(pTable,"p_T3",.05)
HBpTable
```

log10Hist

Plot histogram of log base 10 of p-values in table

### Description

Graphical exploration of extreme p-values from quartet hypothesis tests, to aid in choosing critical values for use in NANUQ algorithm

### Usage

```
log10Hist(pTable, pcol, pmin = 0)
```

# Arguments

pTable	a table of quartet p-values such as from MultiIndepQuartetTreeTest or from MultiIndepQuartetStarTest
pcol	name of column of pTable containing p-values, "p_T1", "p_T3", or "p_star"
pmin	omit all p-values below pmin

```
pTable=NANUQ(system.file("yeastRokas",package="MSCquartets"), alpha=0, beta=.95) \\ log10Hist(pTable,"p_T3") \\ NANUQdist(pTable, alpha=10^-5, beta=.95) \\ NANUQdist(pTable, alpha=10^-3, beta=.95) \\
```

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MSCquartets

Multispieces Coalescent Model Quartet Package

### **Description**

A package for analyzing quartets displayed on gene trees, under the multispecies coalscent (MSC) model.

#### **Details**

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

Recall that 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, as in [MAR19]
- 3. Infer a species tree using the QCCFs via the methods of [R19] and [YR19]
- 4. Infer a level-1 species network via the NANUQ method of [ABR19]

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

Two data sets are included as text files. The file "genetreeSample" contains a sample of 10000 gene trees sampled under the MSC from the species tree ((a,b),(c,(d,e)));. The file "yeastRokas" contains 106 gene trees for a subset of 7 yeast and one outgroup taxa, subtrees of the [Rokas et al., 2003] data set.

### References

[R19] Toplogical metrizations of trees and new quartet methods of tree inference, J.A. Rhodes, IEEE/ACM Trans. Comput. Biol. Bioinf., early access, 2019

[MAR19] Hypothesis testing near singularities and bondaries, J.D. Mitchell, E.S. Allman, J.A. Rhodes, Electron. J. Statist., 13 (1) 2019

[YR19] Metrizing trees with weighted quartets, and species tree inference, S. Yourdkhani, J.A. Rhodes, ??draft??, 2019

[ABR19] NANUQ: A method for inferring species networks from gene trees under the coalescent model,, E.S. Allman, H. Banos, J.A. Rhodes, submitted, 2019

MultiIndepQuartetStarTest

Mutiple independent hypothesis tests for gene quartet counts fitting a star species tree under the multispecies coalescent model

### **Description**

Perform hypothesis test for star species tree for all quartet counts in an input table, as if the quartets are independent. Assumes all quartets are resolved. The test performed is described in QuartetTreeTest.

### Usage

MultiIndepQuartetStarTest(T)

#### **Arguments**

Τ

Table of resolved quartet counts, as produced by ResolvedQuartetTable, or MultiIndepQuartetTreeTest

#### Value

The same table as the input T with column "p\_star" appended, containing p-values for judging fit to MSC on a star tree

### See Also

 ${\tt QuartetStarTest,\,QuartetTreeTest,\,MultiIndepQuartetTreeTest,\,ResolvedQuartetTable,\,PlotQuartetTest}$ 

#### **Examples**

```
gtrees=read.tree(file=system.file("genetreeSample",package="MSCquartets"))
taxanames=AllTaxonNames(gtrees)
QT=QuartetTable(gtrees,taxanames)
RQT=ResolvedQuartetTable(QT)
pTable=MultiIndepQuartetStarTest(RQT)
pTable
```

MultiIndepQuartetTreeTest

Mutiple independent hypothesis tests for quartet counts fitting multispecies coalescent model on a tree

#### **Description**

Perform hypothesis test for tree for all quartets in a table, as if the quartets are independent. Assumes all quartets are resolved. The test performed is described in more detail in QuartetTreeTest and fully in the [MAR19].

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#### Usage

```
MultiIndepQuartetTreeTest(T, model = "T3", lambda = 0,
   smallcounts = "approximate", bootstraps = 10^4, method = "MLest",
   speciestree = NULL)
```

### **Arguments**

T table of resolved quartet counts, as produced by ResolvedQuartetTable, or

MultiIndepQuartetStarTest

model "T1" or "T3", for the models of [MAR19]

lambda power divergence statistic parameter (0 for likelihood ratio stat)

smallcounts "bootstrap" or "approximate", method of obtaining p-value when some counts

are small

bootstraps number of samples for bootstrapping
method "MLest", "conservative", or "bootstrap"

species tree species tree, in Newick as text, to determine quartet for T1 test; required for

model="T1", ignored for model="T3"

#### Value

If model="T3", a copy of T with a new column "p\_T3" appended with p-values for each quartet; If model="T1", a copy of T with 2 columns appended: "p\_T1" with p-values, and "qindex" giving index of quartet consistent with specified species tree, i.e., 1 if ablcd on species tree, 2 if aclbd, 3 if adlbc

#### See Also

Quartet TreeTest, Plot Quartet Test, MultiIndep Quartet StarTest, Resolved Quartet Table

```
gtrees=read.tree(file=system.file("genetreeSample",package="MSCquartets"))
taxanames=AllTaxonNames(gtrees)
QT=QuartetTable(gtrees,taxanames)
RQT=ResolvedQuartetTable(QT)
pTable3=MultiIndepQuartetTreeTest(RQT,"T3")
pTable3
stree="((a,b),(c,(d,e)));"
pTable1=MultiIndepQuartetTreeTest(RQT,"T1",speciestree=stree)
pTable1
```

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#### **Description**

The NANUQ algorithm of [ABR19] infers a hybridization network from a collection of gene trees, under the level-1 network multispecies coalescent (NMSC) model. This function

- 1. counts displayed quartets across gene trees,
- 2. applies appropriate hypothesis tests to judge quartet CFs as representing putative hybridization, resolved trees, or unresolved (star) trees using alpha and beta as significance levels, and
- 3. computes the appropriate distance table under the level-1 network quartet distance, writing it to a file.

The distance table file can then be opened in SplitsTree to obtain a circular split system under the Neighbor-Net algorithm, which is then depicted as a splits graph. The splits graph should be interpretted via the theory in [ABR19] to infer the level-1 species network, or to conclude the data does not arise from the NMSC on such a network.

### Usage

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

#### **Arguments**

guinents	
genedata	gene tree data that may be supplied in one of 3 ways:
	<ol> <li>as a character string giving the name of a file containing Newick gene trees,</li> <li>as a multiPhylo object containing the gene trees, or</li> </ol>
	3. as a table of quartets on the gene trees, as produced by a previous call to NANUQ or ResolvedQuartetTable, which has columns only for taxa, quartet counts, and possibly p_T3 and p_star.
outfile	a character string giving an output file name stub, to which will be appended an alpha and beta value and ".nex", for saving the NANUQ distance matrix; if NULL then distance matrix not computed
alpha	a value or vector of significance levels for judging p-values indicating hybridization on quartet, one for each output file; smaller values mean fewer calls of hybridization
beta	a value or vector of significance levels for judging p-values indicating star quartet tree, one for each output file; smaller values result in fewer calls of resolved tree; alpha and beta should be vectors of the same length
taxanames	if genedata is a file or multiphylo object, a subset of taxa on the gene trees, which will be the only ones analyzed, if NULL all taxa on the first gene tree are

### Details

plot

In most instances of NANUQ, 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 quartet counts and p-values to be saved, for input to further calls of NANUQ with new choices of alpha and beta.

used; if genedata is a quartet table, this argument is ignored

TRUE produces simplex plots of hypothesis test results, FALSE omits plots

If alpha and beta are vectors, they must be of same length, k. Then the i-th entries are paired to produce k plots and k output files.

NANUQdist

A call of NANUQ with genedata given as a table previously output from NANUQ is equivalent to a call of NANUQdist.

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

#### Value

a table of quartets and p-values for judging fit to the MSC on quartet trees (returned invisibly); this table can be used as input to NANUQ or NANUQdist with new choices of alpha and beta, without re-tallying quartets on the gene trees. A distance table to be used as input for SplitsTree is written to a nexus file.

### See Also

Quartet Table, Dominant Quartet Table, MultiIndep Quartet Tree Test, MultiIndep Quartet Star Test, NANUQ dist

### **Examples**

```
pTable=NANUQ(system.file("yeastRokas",package="MSCquartets"), alpha=.0001, beta=.95)
NANUQ(pTable, alpha=.05, beta=.95)
```

NANUQdist	Compute NANUQ distance and write to file

### **Description**

Computes the quartet distance tables for NANUQ of [ABR19], using precomputed p-values for quartets, for each of several levels specified. Distance tables are written to files, in nexus format.

### Usage

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

#### **Arguments**

pTable	a table of quartets and p-values, as computed by NANUQ, or by MultiInde-pQuartetTreeTest and MultiIndepQuartetStarTest, with columns "p_T3" and "p_star"
outfile	a character string giving an output file name stub, to which will be appended an alpha and beta value and ".nex", for saving distance matrix; if NULL then distance matrix not written to file
alpha	a value or vector of significance levels for judging p-values indicating hybridization on quartet, one for each distance table/output file; smaller values mean fewer calls of hybridization
beta	a value or vector of significance levels for judging p-values indicating star quartet tree, one for each distance/table output file; smaller values result in fewer calls of resolved tree; alpha and beta should be vectors of the same length
plot	TRUE produces simplex plots of hypothesis tests, FALSE omits plots

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#### **Details**

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

If alpha and beta are vectors, they must be of same length, k. Then the i-th entries are paired to produce k plots and k distance tables/output files.

### Value

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

#### See Also

NANUQ, MultiIndepQuartetTreeTest, MultiIndepQuartetStarTest

#### **Examples**

```
pTable=NANUQ(system.file("yeastRokas",package="MSCquartets"), alpha=.0001, beta=.95) NANUQdist(pTable, alpha=.05, beta=.95)
```

NexusDist

Write a distance table to a file in nexus format

### **Description**

Write a distance table to a file in nexus format

#### Usage

```
NexusDist(D, outfilename)
```

### Arguments

D a square matrix giving a distance table, with rows and columns labeled by taxon

names

outfilename the name of an output file

### Value

None

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PlotQuartetTest	Produce simplex plot of results of MultiIndepQuartetTreeTest, Multi-IndepQuartetStarTest, or NANUQ
-----------------	--

### Description

Plot is of 2-d simplex, with points for all quartet count vectors. Color of point indicates rejection or failure to reject of tests, at specified level.

#### Usage

```
PlotQuartetTest(pTable, test, alpha = 0, beta = 1)
```

### **Arguments**

pTable	table of quartets and p-values, as produced by $MultiIndepQuartetTreeTest$ (extra columm if $model=T1$ ), $MultiIndepQuartetStarTest$ , or $NANUQ$
test	model to use, options are "T1", "T3" (NANUQ uses "T3")
alpha	significance level for H0="T1" or "T3" test
beta	significance level for H0=star tree test (test shown only if beta<1)

#### **Details**

This function must be supplied with a table of quartets and p-values. The plot may show results of either the T1 or T3 test, with or without a star tree test (depending on whether a p\_star column is in the table). The p-values must be supplied by previous calls to MultiIndepQuartetTreeTest (for T1 or T3 p-values) and MultiIndepQuartetStarTest (for star tree). The NANUQ functions include calls for the T3 and star tests

#### Value

None

### See Also

 ${\tt MultiIndepQuartetTreeTest, MultiIndepQuartetStarTest, NANUQ, NANUQdist}$ 

```
gtrees=read.tree(file=system.file("genetreeSample",package="MSCquartets"))
taxanames=AllTaxonNames(gtrees)
QT=QuartetTable(gtrees,taxanames)
RQT=ResolvedQuartetTable(QT)
stree="((a,b),(c,(d,e)));"
pTable=MultiIndepQuartetTreeTest(RQT,"T1",speciestree=stree)
pTable=MultiIndepQuartetStarTest(pTable)
PlotQuartetTest(pTable, "T1", alpha=.05, beta=.95)
```

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Power Divergence statistic of Cressie & Read

### **Description**

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

### Usage

```
power.div.stat(obs, expd, lambda)
```

#### **Arguments**

obs observation vector expd expected vector

lambda statistic parameter (0=Likelihood Ratio, 1=Chi-squared)

#### Value

value of statistic

QDC

Compute Quarter Distance Consensus tree from gene tree data

### **Description**

Compute the Quartet Distance Consensus [R19] estimate of a species tree from a file of gene trees

#### Usage

```
QDC(genetreedata, taxanames = NULL, omit = FALSE)
```

### **Arguments**

genetreedata gene tree data either in the form of 1) a multiphylo object containing gene trees,

or 2) a character string giving the name of a file containing gene trees in Newick

taxanames list of taxa to construct tree on, can be subset of those on trees; if NULL, uses

taxa on first gene tree in file

omit TRUE ignores unresolved quartets, FALSE treats them as 1/3 of each resolution.

#### **Details**

This function is a wrapper which performs the the steps of reading in a collection of gene trees, tallying quartets, computing the quartet distanace between taxa, and building a tree which consistently estimates the species tree topology under the multispecies coalescent model.

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#### Value

an unrooted tree

#### See Also

QuartetTable, ResolvedQuartetTable, DominantQuartetTable, Qdist, QDS, WQDC, WQDCrec

### **Examples**

```
stree=QDC(system.file("genetreeSample",package="MSCquartets"))
```

Qdist

Compute Quartet Distance between taxa

### Description

Compute the Quartet Distance of [R19] from a table specifying a collection of quartets on n taxa.

### Usage

Qdist(DQT)

### **Arguments**

DQT

an (n choose 4) x n (or n+1) matrix of form output by DominantQuartetTable (Note: n+1th column of DQT is ignored)

### Value

a pairwise distance matrix on n taxa

#### See Also

DominantQuartetTable, QDS, QDC, WQdist

```
gtrees=read.tree(file=system.file("genetreeSample",package="MSCquartets"))
taxanames=AllTaxonNames(gtrees)
QT=QuartetTable(gtrees,taxanames[1:5])
RQT=ResolvedQuartetTable(QT)
DQT=DominantQuartetTable(RQT)
Dist=Qdist(DQT)
tree=NJ(Dist)
```

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QDS

Compute Quartet Distance Supertree

#### **Description**

Apply the Quartet Distance Supertree method of [R19] 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 DominantQuartetTable

(Note: n+1th column of DQT is ignored)

method tree building method function (fastme.bal, nj, etc.)

#### **Details**

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

#### Value

An unrooted metric tree (type phylo)

### See Also

```
DominantQuartetTable, Qdist, QDC, WQDS, WQDC, WQDCrec
```

### **Examples**

```
gtrees=read.tree(file=system.file("genetreeSample",package="MSCquartets"))
taxanames=AllTaxonNames(gtrees)
QT=QuartetTable(gtrees,taxanames[1:5])
RQT=ResolvedQuartetTable(QT)
DQT=DominantQuartetTable(RQT)
tree=QDS(DQT)
```

QNdist

Produce network quartet distance table for NANUQ, as in [ABR19], from a table of p-values and specified levels

### Description

Produce network quartet distance table for NANUQ, as in [ABR19], from a table of p-values and specified levels

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#### Usage

```
QNdist(pTable, alpha0, beta0)
```

### **Arguments**

pTable a table of quartets and p-values, as computed by NANUQ, or MultiIndepQuartetTreeTest

and MultiIndepQuartetStarTest

alpha0 a scalar significance level for judging p\_T3 indicating hybridization on quartet;

smaller value gives fewer hybridization calls

beta0 a scalar significance level for judging p\_star indicating star quartet tree; smaller

value gives fewer resolved tree calls

#### Value

a NANUQ distance table

#### See Also

NANUQ, NANUQdist

quartet.table.print *Print a quartet table with nice formatting* 

#### **Description**

Print a quartet table with nice formatting

# Usage

```
quartet.table.print(QT)
```

### **Arguments**

QT a table such as returned by QuartetTable, ResolvedQuartetTable, or DominantQuartetTable,

possibly with extra columns added by other functions

```
gtrees=read.tree(file=system.file("genetreeSample",package="MSCquartets"))
taxonnames=AllTaxonNames(gtrees)
QT=QuartetTable(gtrees,taxonnames)
quartet.table.print(QT)
RQT=ResolvedQuartetTable(QT)
quartet.table.print(RQT)
pTable=MultiIndepQuartetTreeTest(RQT,"T3")
quartet.table.print(pTable)
DQT=DominantQuartetTable(RQT)
quartet.table.print(DQT)
```

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QuartetStarTest	Hypothesis tests for fit of quartet counts to star tree multispecies coa-
	lescent model

# 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 squared.

### Usage

```
QuartetStarTest(obs)
```

### **Arguments**

obs vector of 3 counts of resolved quartet frequencies

#### Value

p-value

### **Examples**

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

OuartetTable	٥

Produce table of counts of quartets displayed on trees

### Description

Compiles table of counts of topological quartets displayed on a collection of trees.

### Usage

```
QuartetTable(trees, taxonnames, epsilon = 0, random = 0)
```

### **Arguments**

trees multiphylo object containing un/rooted metric/topological trees

taxonnames vector of names of taxa of interest, of length n

epsilon minimum for branch lengths to be treated as non-zero

random number of random subsets of 4 taxa to consider; if 0, use all n choose 4 subsets

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#### **Details**

The taxa on the trees may be any set overlapping with taxonnames. Branch lengths of non-negative size less than or equal to epsilon are treated as zero, giving polytomies.

Error if any branch length <0; Warnings if some of taxonnames are missing on some trees, or if some 4-taxon set is on no trees.

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

#### Value

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

#### See Also

ResolvedQuartetTable, DominantQuartetTable

#### **Examples**

```
gtrees=read.tree(file=system.file("genetreeSample",package="MSCquartets"))
taxonnames=AllTaxonNames(gtrees)
QT=QuartetTable(gtrees,taxonnames[1:5])
RQT=ResolvedQuartetTable(QT)
DQT=DominantQuartetTable(RQT)
```

QuartetTreeErrorProb Bayesian posterior probability of error in 4-taxon unrooted species tree topology estimate

### Description

Bayesian posterior probability that ML estimate of 4-taxon species tree topology from gene quartet topology counts is incorrect, under the assumption that the counts arises from some species tree. Uses Jeffreys prior for internal branch length, and uniform prior on the resolved topology.

# Usage

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

### Arguments

obs vector of counts for 3 topologies

model "T3" or "T1", for the models of [MAR19] describing an unspecified species tree

topology ("T3"), or the topology corresponding to the first entry of obs ("T1")

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#### Value

posterior probability

#### **Examples**

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

QuartetTreeTest

Hypothesis test for fit of a quartet counts to multispecies coalescent model.

### **Description**

Test the hypothesis H\_0= T1 or T3 model of [MAR19], vs. H\_1 = everything else. This function implements two of the versions of the test given in [MAR19] as well as parametric boostrapping, with other procedures for when some counts are small. Due to the singularity and boundary of the models, when the topology and/or the internal quartet branch length is unknown these are more accurate tests than, say, a chi-squared with one degree of freedom which assumes no model boundary or singularity near the data

### Usage

```
QuartetTreeTest(obs, model = "T3", lambda = 0,
   smallcounts = "approximate", bootstraps = 10^4, method = "MLest")
```

#### **Arguments**

obs vector of 3 counts of resolved quartet frequncies,

model "T1" or "T3", for the models of [MAR19],

lambda parameter for power-divergence statistic (0 for LR stat, 1 for Chi-squared stat)

smallcounts "bootstrap" or "approximate", method of obtaining p-value when some counts

are small

bootstraps number of samples for bootstrapping
method "MLtest", "conservative", or "bootstrap"

#### **Details**

If method="MLtest", this uses the test by that name described in Section 7 of [MAR19]. For model T1 this test is slightly anticonservative if the true internal edge of the quartet species tree is very short. Although the test generally performs well in practice, it lacks a uniform asymptotic guarantee over the full parameter space.

If method="conservative", a more conservative test described in [MAR19] is used. For model T3 this uses the chi^2\_1 distribution (the "least favorable" approach), while for model T1 it uses the Minimum Adjusted Bonferroni, based on precomputed values from simulations. These conservative test are 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 bootsrapping is done, based on parameter estimates of the quartet topology and internal edge length. 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 an approximate method that uses precomputed p-values is used. These both involve estimates of the quartet topology and internal edge length.

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

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

The returned value of t is a consistent estimator, but not the MLE, of the internal edge length in coalescent units. Although consistent, the MLE for t is biased. Our consistent estimator is still biased, but with less bias than the MLE. See [MAR19] for more discussion on dealing with the bias of parameter estimates in the presence of boundaries and/or singularities of parameter spaces.

#### Value

(p-value, t) where t is a consistent estimator of the internal edge length in coalescent units, possibly Inf.

### See Also

MultiIndepQuartetTreeTest

### **Examples**

```
obs=c(17,72,11)
QuartetTreeTest(obs,"T3")
QuartetTreeTest(obs,"T1")
```

### **Description**

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

#### Usage

```
ResolvedQuartetTable(QT, omit = FALSE)
```

# Arguments

omit

QT table as produced by QuartetTable of size (n choose 4)x(n+4)

TRUE deletes unresolved quartets column; FALSE redistributes unresolved counts

as (1/3,1/3,1/3) to resolved counts

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#### Value

A table of size (n choose 4)x(n+3), similar to QuartetTable

#### See Also

```
QuartetTable, DominantQuartetTable
```

### **Examples**

```
gtrees=read.tree(file=system.file("genetreeSample",package="MSCquartets"))
taxonnames=AllTaxonNames(gtrees)
QT=QuartetTable(gtrees,taxonnames[1:5])
RQT=ResolvedQuartetTable(QT)
DQT=DominantQuartetTable(RQT)
```

SLabels

2-d simplex plotting routine to label vertices of simplex

### **Description**

2-d simplex plotting routine to label vertices of simplex

### Usage

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

### **Arguments**

top label for top

left label for left bottom
right label for right bottom

### Value

None

### See Also

```
SPoint, SPrepare, SSegment, SText, StoP
```

```
SPrepare("T3","Example Plot")
SLabels("ab|cd","ac|bd","ad|bc")
```

SPrepare SPrepare

SPoint

Plot point in 2-d simplex

### **Description**

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

### Usage

```
SPoint(v, ...)
```

### **Arguments**

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

#### Value

None

#### See Also

```
SLabels, SPrepare, SSegment, SText, StoP
```

### **Examples**

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

SPrepare

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

### Description

Outline the planar 2-d simplex, and draw the models for 1-tree or 3-tree models as in [MAR19].

### Usage

```
SPrepare(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

### Value

None

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#### See Also

```
SLabels, SPoint, SSegment, SText, StoP
```

# **Examples**

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

SSegment

Plot line segment in 2-d simplex

### Description

Normalizes two points in 3-d, and draws segment between them in simplex

# Usage

```
SSegment(v, w, ...)
```

# Arguments

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

#### Value

None

#### See Also

```
SLabels, SPoint, SPrepare, SText, StoP
```

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

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SText

Add text at a point in 2-d simplex

### Description

Add text at a point in 2-d simplex

### Usage

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

#### **Arguments**

v a 3-d point in non-negative orthant, coords not summing to 0

label text

... other options to pass to graphics text function

#### Value

None

#### See Also

```
SLabels, SPoint, SPrepare, SSegment, StoP
```

### **Examples**

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

StoP

Convert 3-d coordinates to planar 2-d simplex coordinates, for plot-

### **Description**

Convert 3-d coordinates to planar 2-d simplex coordinates, for plotting

### Usage

StoP(v)

### Arguments

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

### Value

2-d coordinates to plot normalized point in simplex

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#### See Also

```
SLabels, SPoint, SPrepare, SSegment, SText
```

### **Examples**

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

T1density

Probability density function for Model T1 of [MAR19], Proposition 5.2

### **Description**

Probability density function for Model T1 of [MAR19], Proposition 5.2

### Usage

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

### **Arguments**

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

#### Value

value of density function

### See Also

T3density

T3density	Probability density	function for	· Model T3	of [MAR19],	Proposition
	4.2				

# Description

Probability density function for Model T3 of [MAR19], Proposition 4.2

# Usage

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

### Arguments

X	statistic value (e.g., LR stat, or other power divergence stat)
mu0	parameter
alpha0	parameter
beta0	parameter

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#### Value

value of density function

#### See Also

T1density

WQDC	Compute Weighted Quartet Distance Consensus tree from gene tree
	aara

### **Description**

Compute the Weighted Quartet Distance Consensus [YR19] estimate of a species tree from a file of gene trees, adjusting so internal edge lengths estimate those on species tree

### Usage

```
WQDC(genetreedata, taxanames = NULL, omit = FALSE, terminal = 1)
```

### **Arguments**

genetreedata	gene tree data in one of the 3 forms

1. a multiphylo object containing gene trees,

2. a character string giving the name of a file containing gene trees in Newick

3. a resolved quartet table, as produced by ResolveQuartetTable

taxanames list of taxa to construct tree on; may be subset of those on gene trees; ignored if

genetreedata given as resolved quartet table

omit TRUE leaves out unresolved quartets, FALSE treats them as 1/3 of each resolu-

tion.

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 the steps of reading in a collection of gene trees, tallying quartets, estimating quartet internal branch lengths, computing the weighted quartet distanace between taxa, building a tree, and adjusting edge lengths, to give a consistent estimate of the metric species tree under the multispecies coalescent model.

#### Value

an unrooted tree, with internal edge lengths the inferred lengths for the species tree

#### See Also

```
QuartetTable, ResolvedQuartetTable, DominantQuartetTable, WQdist, WQDCrec WQDS, QDC
```

```
stree= \verb"WQDC" (system.file("genetreeSample", package="MSC quartets"))
```

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WQDCrec	Compute the Recursive Weighted Quartet Distance Consensus tree
	from gene tree data

### Description

As described in [YR2019], this algorithm infers a metric species tree from counts of quartets displayed on a collection of gene trees. It first builds a tree using WQDS, determines the split corrsponding 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 the WQDS, but gives better topological accuracy.

### Usage

```
WQDCrec(RQT, terminal = 1)
```

#### **Arguments**

RQT a resolved quartet table as produced by ResolvedQuartetTable

terminal non-negative branch length to supply for terminal branches, whose length cannot

be inferred by WQDCrec

### **Details**

This function must be called with its argument a resolved quartet table (not a dominant 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

#### See Also

Resolved Quartet Table, Quartet Table, QDC, QDS, Collapse Quartet Table

```
gtrees=read.tree(file=system.file("genetreeSample",package="MSCquartets"))
taxanames=AllTaxonNames(gtrees)
QT=QuartetTable(gtrees,taxanames[1:5])
RQT=ResolvedQuartetTable(QT)
stree=WQDCrec(RQT)
plot(stree)
stree
```

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WQdist

Compute the Weighted Quartet Distance between taxa

#### **Description**

Compute the Weighted Quartet Distance between taxa of [YR19] from a table specifying a collection of quartets on n taxa and the quartets' internal branch lengths.

### Usage

```
WQdist(DQT)
```

### **Arguments**

DQT

an (n choose 4) x n+1) matrix of form output by DominantQuartetTable

#### Value

A pairwise distance matrix on n taxa

#### See Also

DominantQuartetTable, WQDSAdjustLengths, WQDS, WQDC, WQDCrec, WQdist

### **Examples**

```
gtrees=read.tree(file=system.file("genetreeSample",package="MSCquartets"))
taxanames=AllTaxonNames(gtrees)
QT=QuartetTable(gtrees,taxanames[1:5])
RQT=ResolvedQuartetTable(QT)
DQT=DominantQuartetTable(RQT,bigweights="finite")
D=WQdist(DQT)
tree=NJ(D)
stree=WQDSAdjustLengths(tree)
```

WQDS

Compute the Weighted Quartet Distance Supertree

### Description

Apply the Weighted Quartet Distance Supertree method of [YR19] to a collection of quartets onn taxa together with internal quartet branch lengths, specified by a table

### Usage

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

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#### **Arguments**

DQT an (n choose 4) x n+1) matrix of form output by DominantQuartetTable

method tree building method function (fastme.bal, NJ, etc.)

#### **Details**

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

### Value

an unrooted metric tree (type phylo)

#### See Also

DominantQuartetTable, WQdist, WQDSAdjustLengths, WQDC, WQDCrec, QDS

#### **Examples**

```
gtrees=read.tree(file=system.file("genetreeSample",package="MSCquartets"))
taxanames=AllTaxonNames(gtrees)
QT=QuartetTable(gtrees,taxanames[1:5])
RQT=ResolvedQuartetTable(QT)
DQT=DominantQuartetTable(RQT,bigweights= "finite")
tree=WQDS(DQT)
```

WQDSAdjustLengths

Adjust edge lengths on tree produced by weighted quartet distance supertree algorithm to estimate metric tree

### Description

Modify edge lengths of WQDC tree to remove scaling factors related to the topology, giving an estimate of the metric tree.

### Usage

```
WQDSAdjustLengths(tree)
```

### Arguments

tree

an unrooted metric tree, such as output from WQDS

### Details

As explained in [YR19], the metric tree produced by the weighted quartet supertree algorithm has edge lengths inflated by a factor dependent on the associated split size. Dividing by these factors yields a consistent estimate of the metric species tree when WQDC is applied to a collection of gene trees under the multispecies coalescent model.

This function should not be used on trees output from WQDS, WQDC, or WQDCrec, as their edges are already adjusted.

### Value

An unrooted metric tree (type phylo)

### See Also

WQDS, WQDC

```
gtrees=read.tree(file=system.file("genetreeSample",package="MSCquartets"))
taxanames=AllTaxonNames(gtrees)
QT=QuartetTable(gtrees,taxanames[1:5])
RQT=ResolvedQuartetTable(QT)
DQT=DominantQuartetTable(RQT,bigweights="finite")
D=WQdist(DQT)
tree=NJ(D)
stree=WQDSAdjustLengths(tree)
```

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