

Package ‘MSCquartets’

September 19, 2019

Title Analyzing gene trees through quartets under the multispecies coalescent model

Version 0.4.3

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.

License MIT + file LICENSE

Imports RandomFieldsUtils,
MCMCpack,
graphics,
stats,
utils

Encoding UTF-8

LazyData true

RoxygenNote 6.1.1

NeedsCompilation no

Author Elizabeth Allman [aut],
Hector Banos [aut],
Jonathan Mitchell [aut],
John Rhodes [aut, cre]

Maintainer John Rhodes <j.rhodes@alaska.edu>

Depends R (>= 2.10),
ape (>= 5.0),
phangorn

R topics documented:

AllTaxonNames	2
DominantQuartetTable	3
HolmBonferroni	4
Jeffrey1T1	5
Jeffrey2T1	5
Jeffrey3T1	6
JprUnconsTri	6
log10Hist	7
MSCquartets	7
MultiIndepQuartetStarTest	8

MultiIndepQuartetTreeTest	9
NANUQdist	10
NANUQf	11
NexusDist	12
PlotQuartetTest	12
power.div.stat	13
QDCf	14
Qdist	15
QDS	15
QNdist	16
QuartetStarTest	17
QuartetTable	17
QuartetTreeErrorProb	18
QuartetTreeTest	19
ResolvedQuartetTable	20
SLabels	21
SPoint	22
SPrepare	22
SSegment	23
SText	24
StoP	24
T1density	25
T3density	25
WQDCAdjustLengths	26
WQDCf	27
WQdist	27
WQDS	28

Index	30
--------------	-----------

AllTaxonNames	<i>Get all taxon names from a collection of trees</i>
---------------	---

Description

Create a list of all taxa names 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

Examples

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

DominantQuartetTable	<i>Produce table of dominant quartets, with ML estimates of internal edge length under the MSC model</i>
----------------------	--

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")
```

Arguments

RQT	array as produced by ResolvedQuartetTable of size $(n \text{ choose } 4) \times (n+3)$;
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 $(n \text{ choose } 4) \times (n+1)$ 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(taxonnames[1:5],gtrees)
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 upward, to counteract the greater probability of some small values even when the null hypothesis is true.

Usage

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

Arguments

<code>pTable</code>	a table of quartets with <i>p</i> -values, as computed by <code>MultiIndepQuartetTest</code> or <code>MultiIndepStarTest</code>
<code>columnname</code>	a name of a column of <code>pTable</code> containing <i>p</i> -values
<code>alpha</code>	a critical value, for rejection of adjusted <i>p</i> -values below <code>alpha</code>

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

See Also

[MultiIndepQuartetTreeTest](#), [MultiIndepStarTreeTest](#), [PlotQuartetTest](#)

Examples

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

Jeffrey1T1	<i>Sample from Jeffreys prior for model T1 of [MAR19], with tree 1 (12 34).</i>
------------	---

Description

Sample from Jeffreys prior for model T1 of [MAR19], with tree 1 (12|34).

Usage

Jeffrey1T1(1)

Arguments

1 number of samples

Value

an lx3 array with samples in rows

Examples

Jeffrey1T1(5)

Jeffrey2T1	<i>Sample from Jeffreys prior for model T1 of [MAR19], with tree 2 (13 24).</i>
------------	---

Description

Sample from Jeffreys prior for model T1 of [MAR19], with tree 2 (13|24).

Usage

Jeffrey2T1(1)

Arguments

1 number of samples

Value

an lx3 array with samples in rows

Examples

Jeffrey2T1(5)

Jeffrey3T1	<i>Sample from Jeffreys prior for model T1 of [MAR19], with tree 3 (14 23).</i>
------------	---

Description

Sample from Jeffreys prior for model T1 of [MAR19], with tree 3 (14|23).

Usage

```
Jeffrey3T1(1)
```

Arguments

1 number of samples

Value

an lx3 array with samples in rows

Examples

```
Jeffrey3T1(5)
```

JprUnconsTri	<i>Sample from Jeffreys prior for the unconstrained trinomial model.</i>
--------------	--

Description

Sample from Jeffreys prior for the unconstrained trinomial model.

Usage

```
JprUnconsTri(1)
```

Arguments

1 number of samples

Value

an lx3 array with samples in rows

Examples

```
JprUnconsTri(5)
```

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

Examples

```
pTable=NANUQf(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)
```

MSCquartets

*Multispecies Coalescent Model Quartet Package***Description**

A package for analyzing quartets displayed on gene trees, under the multispecies coalescent (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] *Topological 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 boundaries*, 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

Multiple 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

T	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

[QuartetStarTest](#), [QuartetTreeTest](#), [MultiIndepQuartetTreeTest](#), [ResolvedQuartetTable](#), [PlotQuartetTest](#)

Examples

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

MultiIndepQuartetTreeTest

Multiple independent hypothesis tests for quartet counts fitting multi-species 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].

Usage

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

Arguments

T	table of resolved quartet counts, as produced by <code>ResolvedQuartetTable</code> , or <code>MultiIndepQuartetStarTest</code>
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	if non-zero, number of samples for bootstrapping
method	"MLest" or "conservative"
speciestree	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 abcd on species tree, 2 if aclbd, 3 if adlbc

See Also

[QuartetTreeTest](#), [PlotQuartetTest](#), [MultiIndepQuartetStarTest](#), [ResolvedQuartetTable](#)

Examples

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

NANUQdist	<i>Compute NANUQ distance and write to file</i>
-----------	---

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 NANUQf, or by MultiIndepQuartetTreeTest and MultiIndepQuartetStarTest, with columns "p_T3" and "p_star"
outfile	an output file name stub, to which will be appended alpha and beta values and ".nex", for saving distance matrix
alpha	significance level for judging p_T3 indicating hybridization on quartet; smaller values mean fewer calls of hybridization
beta	significance level for judging p_star indicating star quartet tree; smaller values result in fewer calls of resolved tree
plot	TRUE produces simplex plots of hypothesis tests, FALSE omits plots

Details

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

If alpha and beta are vectors, they must be of same length k, in which case k distance tables/plots are produced.

Value

None

See Also

[NANUQf](#), [MultiIndepQuartetTreeTest](#), [MultiIndepQuartetStarTest](#)

Examples

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

NANUQf	<i>Apply NANUQ network inference algorithm to Newick gene trees in a file</i>
--------	---

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 tables under the level-1 network quartet distance, writing it to a file. This 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 split graph. The split graph should be interpreted 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

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

Arguments

genetreesfile	an input file containing gene trees in Newick format
outfile	an output file name stub, to which will be appended an alpha value and ".nex", for saving the NANUQ distance matrix
alpha	a 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 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	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 used
plot	TRUE produces simplex plots of hypothesis test results, FALSE omits plots

Details

In most instances of NANUQ, an initial call to NANUQf 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 NANUQf will allow for the time-consuming computation of quartet counts and p-values to be saved, for input to NANUQdist along with new choices of alpha and beta

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 MSC on tree; this table can be used as input to 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

[NANUQdist](#), [MultiIndepQuartetTreeTest](#), [MultiIndepQuartetStarTest](#)

Examples

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

NexusDist	<i>Write a distance table to a file in nexus format</i>
-----------	---

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

PlotQuartetTest	<i>Produce simplex plot of results of MultiIndepQuartetTreeTest, Multi-IndepQuartetStarTest, or NANUQ</i>
-----------------	---

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 column 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. 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

[MultiIndepQuartetTreeTest](#), [MultiIndepQuartetStarTest](#), [NANUQf](#), [NANUQdist](#)

Examples

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

power.div.stat

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

QDCf	<i>Compute QDC tree from file of trees</i>
------	--

Description

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

Usage

```
QDCf(treefile, taxanames = NULL, omit = FALSE)
```

Arguments

- | | |
|-----------|---|
| treefile | 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 distance between taxa, and building a tree which consistently estimates the species tree topology under the multispecies coalescent model.

Value

an unrooted tree

See Also

[QuartetTable](#), [ResolvedQuartetTable](#), [DominantQuartetTable](#), [Qdist](#), [QDS](#), [WQDCf](#)

Examples

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

Qdist	<i>Compute Quartet Distance between taxa</i>
-------	--

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 <code>DominantQuartetTable</code> (Note: n+1th column of DQT is ignored)
-----	---

Value

A pairwise distance matrix on n taxa

See Also

[DominantQuartetTable](#), [QDS](#), [QDCf](#), [QDCf](#), [WQdist](#)

Examples

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

QDS	<i>Compute Quartet Distance Supertree</i>
-----	---

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 <code>DominantQuartetTable</code> (Note: n+1th column of DQT is ignored)
method	tree building method function (<code>fastme.bal</code> , <code>nj</code> , 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](#), [QDCf](#), [WQDS](#)

Examples

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

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

Description

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

Usage

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

Arguments

- | | |
|--------|---|
| pTable | a table of quartets and p-values, as computed by NANUQf, 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

[NANUQf](#), [NANUQdist](#)

QuartetStarTest	<i>Hypothesis tests for fit of quartet counts to star tree multispecies coalescent model</i>
-----------------	--

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)
```

QuartetTable	<i>Produce table of counts of quartets displayed on trees</i>
--------------	---

Description

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

Usage

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

Arguments

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

trees multiphylo object containing un/rooted metric/topological trees

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

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 than 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(taxonnames[1:5],gtrees)
RQT=ResolvedQuartetTable(QT)
DQT=DominantQuartetTable(RQT)
```

QuartetTreeErrorProb	<i>Bayesian posterior probability of correctness of 4-taxon species tree estimate</i>
----------------------	---

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. Result is approximate, as it depends on simulation.

Usage

```
QuartetTreeErrorProb(obs, samples = 10^4, prior1 = Jeffrey1T1,
  prior2 = Jeffrey2T1, prior3 = Jeffrey3T1, treepriors = (1/3) * c(1,
  1, 1))
```

Arguments

obs	vector of 3 counts
samples	number of samples from each tree topology to be used for approximating value
prior1	function to sample from prior for 12 34 tree (default is Jeffreys)
prior2	function to sample from prior for 13 24 tree (default is Jeffreys)
prior3	function to sample from prior for 14 23 tree (default is Jeffreys)
treepriors	vector of 3 prior probabilities of tree topologies (default is uniform)

Value

posterior probability

QuartetTreeTest	<i>Hypothesis test for fit of a quartet counts to multispecies coalescent model.</i>
-----------------	--

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], 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 this is a more accurate test than, say, a chi-squared with one degree of freedom.

Usage

```
QuartetTreeTest(obs, model = "T3", lambda = 0,
  smallcounts = "approximate", bootstraps = 0, method = "MLtest")
```

Arguments

obs	vector of 3 counts of resolved quartet frequencies,
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	if non-zero, number of samples for bootstrapping
method	"MLtest" or "conservative"

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 χ^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.

If `bootstraps=0`, the test is as just described. If `bootstraps` is positive, a parametric bootstrap test is applied instead. When some expected topology counts are small, the parameter `smallcounts` determines whether bootstrapping or an approximate method that uses precomputed p-values is used. The expected topology counts are based on parameter 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.

Value

(p-value, `t`) where `t` is the ML estimate of internal edge length in coalescent units

See Also

[MultiIndepQuartetTreeTest](#)

Examples

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

ResolvedQuartetTable *Modify table of counts of quartets to only show resolved ones*

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

<code>QT</code>	table as produced by <code>QuartetTable</code> of size $(n \text{ choose } 4) \times (n+4)$
<code>omit</code>	TRUE deletes unresolved quartets column; FALSE redistributes unresolved counts as $(1/3, 1/3, 1/3)$ to resolved counts

Value

A table of size $(n \text{ choose } 4) \times (n+3)$, similar to `QuartetTable`

See Also

[QuartetTable](#), [DominantQuartetTable](#)

Examples

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

SLabels	<i>2-d simplex plotting routine to label vertices of simplex</i>
---------	--

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](#)

Examples

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

SPoint	<i>Plot point in 2-d simplex</i>
--------	----------------------------------

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](#), [SPPrepare](#), [SSegment](#), [SText](#), [StoP](#)

Examples

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

SPrepare	<i>Draw 2-d probability simplex, with model lines for T3 or T1 model</i>
----------	--

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", titletext = NULL)
```

Arguments

model	"T1" or "T3", for 1-tree or 3-tree model
titletext	additional text for title

Value

None

See Also

[SLabels](#), [SPoint](#), [SSegment](#), [SText](#), [StoP](#)

Examples

```
SPrepare("T3", "Example Plot")
```

SSegment	<i>Plot line segment in 2-d simplex</i>
----------	---

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](#)

Examples

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

SText	<i>Add text at a point in 2-d simplex</i>
-------	---

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	<i>Convert 3-d coordinates to planar 2-d simplex coordinates, for plotting</i>
------	--

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

See Also

[SLabels](#), [SPoint](#), [SPrepate](#), [SSegment](#), [SText](#)

Examples

StoP(c(15,65,20))

T1density	<i>Probability density function for Model T1 of [MAR19], Proposition 5.2</i>
-----------	--

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	<i>Probability density function for Model T3 of [MAR19], Proposition 4.2</i>
-----------	--

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

Value

value of density function

See Also

[T1density](#)

WQDCAdjustLengths	<i>Adjust edge lengths on tree produced by WQDC/WQDS to estimate metric tree</i>
-------------------	--

Description

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

Usage

```
WQDCAdjustLengths(tree)
```

Arguments

tree an unrooted metric tree, such as output from WQDS

Details

As explained in [YR19], the metric tree produced by WQDC/WQDS 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.

Value

An unrooted metric tree (type phylo)

See Also

[WQDS](#), [WQDCf](#)

Examples

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

WQDCf

Compute WQDC (edge length adjusted) tree from file of trees

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

```
WQDCf(treefile, taxanames = NULL, omit = FALSE)
```

Arguments

treefile	a file containing gene trees in Newick
taxanames	list of taxa to construct tree on; may be subset of those on gene trees
omit	TRUE leaves out 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, 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 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](#), [WQDS](#), [QDCf](#)

Examples

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

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 $(n \text{ choose } 4) \times n+1$ matrix of form output by `DominantQuartetTable`

Value

A pairwise distance matrix on n taxa

See Also

[DominantQuartetTable](#), [WQDCAdjustLengths](#), [WQDS](#), [WQDCf](#), [Qdist](#)

Examples

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

WQDS

Compute the Weighted Quartet Distance Supertree tree

Description

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

Usage

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

Arguments

DQT an $(n \text{ choose } 4) \times n+1$ 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 `WQDCAdjustLengths`.

Value

An unrooted metric tree (type `phylo`)

See Also

[DominantQuartetTable](#), [WQdist](#), [WQDCAdjustLengths](#), [WQDCf](#), [QDS](#)

Examples

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

Index

AllTaxonNames, [2](#)

DominantQuartetTable, [3](#), [14–16](#), [18](#), [20](#), [27](#), [28](#)

HolmBonferroni, [4](#)

Jeffrey1T1, [5](#)

Jeffrey2T1, [5](#)

Jeffrey3T1, [6](#)

JprUnconsTri, [6](#)

log10Hist, [7](#)

MSCQuartets, [7](#)

MSCQuartets-package (MSCQuartets), [7](#)

MultiIndepQuartetStarTest, [8](#), [9](#), [10](#), [12](#), [13](#)

MultiIndepQuartetTreeTest, [4](#), [8](#), [9](#), [10](#), [12](#), [13](#), [20](#)

MultiIndepStarTreeTest, [4](#)

NANUQdist, [10](#), [12](#), [13](#), [16](#)

NANUQf, [10](#), [11](#), [13](#), [16](#)

NexusDist, [12](#)

PlotQuartetTest, [4](#), [8](#), [9](#), [12](#)

power.div.stat, [13](#)

QDCf, [14](#), [15](#), [16](#), [27](#)

Qdist, [14](#), [15](#), [16](#), [28](#)

QDS, [14](#), [15](#), [15](#), [28](#)

QNdist, [16](#)

QuartetStarTest, [8](#), [17](#)

QuartetTable, [3](#), [14](#), [17](#), [20](#), [27](#)

QuartetTreeErrorProb, [18](#)

QuartetTreeTest, [8](#), [9](#), [19](#)

ResolvedQuartetTable, [3](#), [8](#), [9](#), [14](#), [18](#), [20](#), [27](#)

SLabels, [21](#), [22–25](#)

SPoint, [21](#), [22](#), [23–25](#)

SPrepare, [21](#), [22](#), [22](#), [23–25](#)

SSegment, [21–23](#), [23](#), [24](#), [25](#)

SText, [21–23](#), [24](#), [25](#)

StoP, [21–24](#), [24](#)

T1density, [25](#), [26](#)

T3density, [25](#), [25](#)

WQDCAdjustLengths, [26](#), [28](#)

WQDCf, [14](#), [26](#), [27](#), [28](#)

WQdist, [15](#), [27](#), [27](#), [28](#)

WQDS, [16](#), [26–28](#), [28](#)