Package: nodeSub (via r-universe)

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Type Package

Title Simulate DNA Alignments Using Node Substitutions

Version 1.2.9

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Description Simulate DNA sequences for the node substitution model. In the node substitution model, substitutions accumulate additionally during a speciation event, providing a potential mechanistic explanation for substitution rate variation. This package provides tools to simulate such a process, simulate a reference process with only substitutions along the branches, and provides tools to infer phylogenies from alignments. More information can be found in Janzen (2021) <doi:10.1093/sysbio/syab085>.

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URL https://github.com/thijsjanzen/nodeSub

BugReports https://github.com/thijsjanzen/nodeSub/issues

Depends ape, Rcpp

Imports beastier, beautier, DDD, geiger, lifecycle, pbapply, phangorn, phylobase, rappdirs, Rmpfr, stringr, testit, tibble, tracerer

Suggests dplyr, ggplot2, knitr, magrittr, nLTT, rmarkdown, RPANDA, testthat, tidyr, TreeSim

LinkingTo Rcpp

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`nodeSub-package` *Package providing functions to simulate sequences under different DNA evolution models*

Description

Simulate DNA sequences for the node substitution model. In the node substitution model, substitutions accumulate additionally during a speciation event, providing a potential mechanistic explanation for substitution rate variation. This package provides tools to simulate such a process, simulate a reference process with only substitutions along the branches, and provides tools to infer phylogenies from alignments. More information can be found in Janzen (2021) <doi:10.1093/sysbio/syab085>.

Version History:
Version 1.2.7 - Removed beta calculation due to apTreeshape removal from CRAN
Version 1.2.3 - Removed summary statistic tests for CRAN
Version 1.2.2 - Changed codedov links in README
Version 1.2.1 - Expanded depenency on RPANDA
Version 1.2 - Release on CRAN

Author(s)

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References

Thijs Janzen, Folmer Bokma, Rampal S Etienne, Nucleotide Substitutions during Speciation may Explain Substitution Rate Variation, Systematic Biology, 2021; syab085

`calc_expected_hidden_nodes`
Calculate the number of expected hidden nodes in a phylogenetic tree

---

Description

Calculate the number of expected hidden nodes using equation 1 in Manceau et al. 2020

Usage

```
calc_expected_hidden_nodes(phy, lambda = NULL, mu = NULL)
```

Arguments

`phy`	phylogenetic tree
`lambda`	birth rate
`mu`	death rate

Value

expected number of hidden nodes

References

Manceau, M., Marin, J., Morlon, H., & Lambert, A. (2020). Model-based inference of punctuated molecular evolution. Molecular Biology and Evolution, 37(11), 3308-3323.

`calc_fraction` *Calculate the expected fraction of substitutions at the nodes, relative to the fraction at the branches*

Description

calculates the relative contribution of substitutions at the nodes

Usage

```
calc_fraction(phy = NULL, node_time = 0, model = "unlinked")
```

Arguments

`phy`	phylogenetic tree (optional)
`node_time`	time spent at the node
`model`	node substitution model

Value

expected fraction

`calc_required_node_time` *Calculate the required node time to obtain a desired fraction of substitutions at the node*

Description

calculates the required node time to obtain a desired fraction of substitutions at the node

Usage

```
calc_required_node_time(phy = NULL, s = 0.5, model = "unlinked")
```

Arguments

`phy`	phylogenetic tree
`s`	desired fraction
`model`	node substitution model, either "linked" or "unlinked".

Value

expected fraction

`calc_sum_stats` *calculate summary statistics of a phylogenetic tree, compared with a reference tree. The following statistics are calculated: the beta statistic, gamma statistic, crown age, mean branch length, number of tips, the nLTT statistic and the laplacian difference, given by RPANDA's JSDtree. Because JSDtree can sometimes cause issues, some additional checks are performed to ensure that is possible to run this function.*

Description

calculate summary statistics of a phylogenetic tree, compared with a reference tree. The following statistics are calculated: the beta statistic, gamma statistic, crown age, mean branch length, number of tips, the nLTT statistic and the laplacian difference, given by RPANDA's JSDtree. Because JSDtree can sometimes cause issues, some additional checks are performed to ensure that is possible to run this function.

Usage

```
calc_sum_stats(trees, true_tree, verbose = FALSE)
```

Arguments

`trees`	a phyloList object containing multiple trees
`true_tree`	a phylo object containing the reference tree, preferably without extinct lineages. If extinct lineages are found, these are dropped.
`verbose`	verbose output if true (e.g. progressbars)

Value

list with two tibbles 1) containing the summary statistics of all trees and 2) containing the difference with the true tree

`count_hidden` *Function to calculate the number of hidden speciation events, e.g. speciation events that have lead to an extinct species. Thus, these hidden speciation events can only be detected in complete trees (as opposed to reconstructed trees).*

Description

Function to calculate the number of hidden speciation events, e.g. speciation events that have lead to an extinct species. Thus, these hidden speciation events can only be detected in complete trees (as opposed to reconstructed trees).

Usage

```
count_hidden(tree)
```

Arguments

tree	phylo object

Value

number of hidden speciation events

---

create_balanced_tree *create a balanced tree out of branching times*

Description

create a balanced tree out of branching times

Usage

```
create_balanced_tree(brts)
```

Arguments

brts	vector of branching times

Value

phylo phylo object

---

create_equal_alignment *function create an alignment with identical information content*

Description

function create an alignment with identical information content

Usage

```
create_equal_alignment(
  input_tree,
  sub_rate,
  alignment_result,
  sim_function = NULL,
  verbose = FALSE,
  node_time = NULL,
  input_alignment_type = "nodesub"
)
```

Arguments

input_tree	phylogeny for which to generate alignment
sub_rate	substitution rate used in the original phylogeny
alignment_result	result of sim_normal, sim_linked or sim_unlinked
sim_function	function that accepts a tree, sequence length, rootsequence and substitution rate (in that order). Default is sim_normal
verbose	provide intermediate output
node_time	node time
input_alignment_type	was the input alignment simulated with a node substitution model or a normal substitution model? Used to calculate the twin mutation rate. Options are "nodesub" and "normal".

Value

list with four properties: 1) alignment: the alignment itself, 2) adjusted rate: the substitution rate used to obtain identical information content 3) total_accumulated_substitutions: the total number of substitutions accumulated. 4) total_node_substitutions: total number of substitutions accumulated on the nodes 5) total_branch_substitutions: total number of substitutions accumulated on the branches.

---

create_equal_alignment_explicit

function create an alignment with identical information content, using the explicit method to simulate substitutions

---

Description

function create an alignment with identical information content, using the explicit method to simulate substitutions

Usage

```
create_equal_alignment_explicit(
  input_tree,
  sub_rate,
  alignment_result,
  verbose = FALSE
)
```

Arguments

input_tree	phylogeny for which to generate alignment
sub_rate	substitution rate used in the original phylogeny
alignment_result	result of sim_normal, sim_linked or sim_unlinked
verbose	provide intermediate output

Value

list with four properties: 1) alignment: the alignment itself, 2) adjusted rate: the substitution rate used to obtain identical information content 3) total_accumulated_substitutions: the total number of substitutions accumulated. 4) total_node_substitutions: total number of substitutions accumulated on the nodes 5) total_branch_substitutions: total number of substitutions accumulated on the branches.

---

create_unbalanced_tree

create an unbalanced tree out of branching times

Description

create an unbalanced tree out of branching times

Usage

```
create_unbalanced_tree(brts)
```

Arguments

brts	vector of branching times

Value

phylo phylo object

`estimate_marginal_models` *estimate the marginal likelihood of the relaxed and strict clock model for a provided alignment*

Description

estimate_marginal_models estimates the marginal likelihood of both the strict and the relaxed clock model, given the JC69 substitution model, using the NS package in BEAST, made available via the babette R package. The NS package performs nested sampling, and uses an MCMC approach to estimate the marginal likelihood. Sampling is performed until convergence of the MCMC chain. Unfortunately, currently the babette package is unavailable on CRAN, requiring installation through GitHub to enjoy the full functionality of this function.

Usage

```
estimate_marginal_models(
  fasta_filename,
  use_yule_prior = FALSE,
  rng_seed = 42,
  sub_rate = 1,
  verbose = FALSE
)
```

Arguments

`fasta_filename`	file name of fasta file holding alignment for which the marginal likelihood is to be estimated
`use_yule_prior`	by default, a birth-death prior is used as tree prior, but if use_yule_prior is set to TRUE, a pure-birth prior will be used.
`rng_seed`	seed of pseudo-random number generator
`sub_rate`	substitution rate
`verbose`	boolean indicating if verbose intermediate output is to be generated

Value

data frame with marginal likelihoods and relative weights per clock model.

`get_p_matrix` *calculate p matrix*

Description

calculates the p matrix

Usage

```
get_p_matrix(branch_length, eig = phangorn::edQt(), rate = 1)
```

Arguments

`branch_length`	branch length
`eig`	eigen object
`rate`	rate

Value

p matrix

`infer_phylogeny` *infer the time calibrated phylogeny associated with the provided alignment. This function uses the R package babette to infer the phylogeny using BEAST2.*

Description

infer the time calibrated phylogeny associated with the provided alignment. This function uses the R package babette to infer the phylogeny using BEAST2.

Usage

```
infer_phylogeny(
  alignment,
  treatment_name,
  tree_prior = beautier::create_bd_tree_prior(),
  clock_prior = beautier::create_strict_clock_model(),
  mcmc_seed = NULL,
  chain_length = 1e+07,
  sample_interval = 5000,
  burnin = 0.1,
  working_dir = NULL,
  sub_rate = 1
)
```

Arguments

alignment	Phydat object containing the focal alignment
treatment_name	string to be appended to BEAST files
tree_prior	tree prior used, default = birth-death prior
clock_prior	clock prior used, default = strict clock
mcmc_seed	seed of the mcmc chain, default is the system time
chain_length	length of the mcmc chain, default is 1e7.
sample_interval	interval of sampling, default is 5000
burnin	burnin of posterior distribution
working_dir	beast2 working dir
sub_rate	substitution rate used to generate the original alignment (if available), default is 1

Value

list with all trees, and the consensus tree

---

reduce_tree *Function to remove speciation events occuring after an extinction event. Extinct species are pruned randomly, such that only a single extinct species per branching event (if any extinct species) remains.*

Description

Function to remove speciation events occuring after an extinction event. Extinct species are pruned randomly, such that only a single extinct species per branching event (if any extinct species) remains.

Usage

```
reduce_tree(tree)
```

Arguments

tree	phylo object

Value

pruned tree

`sim_linked` *simulate a sequence assuming conditional substitutions on the node.*

Description

simulate a sequence assuming conditional substitutions on the node.

Usage

```
sim_linked(
  phy,
  Q = rep(1, 6),
  rate = 0.1,
  node_mut_rate_double = 1e-09,
  l = 1000,
  bf = rep(0.25, 4),
  rootseq = NULL,
  node_time = 0.01
)
```

Arguments

`phy`	tree for which to simulate sequences
`Q`	substitution matrix along the branches, default = JC
`rate`	mutation rate , default = 1
`node_mut_rate_double`	mutation rate on the node, default = 1e-9
`l`	number of base pairs to simulate
`bf`	base frequencies, default = c(0.25, 0.25, 0.25, 0.25)
`rootseq`	sequence at the root, simulated by default
`node_time`	time spent at the node

Value

list with four items

1. alignment Phydat object with the resulting alignment
2. rootseq the rootsequence used
3. total_branch_substitutions total number of substitutions accumulated on the branches
4. total_node_substitutions total number of substitutions accumulated at the nodes

`sim_normal` *Simulate sequences for a given evolutionary tree, using a standard model of sequence evolution along the branches. Code for this function was heavily inspired by the function* `simSeq` *from the phangorn package.*

Description

Simulate sequences for a given evolutionary tree, using a standard model of sequence evolution along the branches. Code for this function was heavily inspired by the function `simSeq` from the phangorn package.

Usage

```
sim_normal(x, l = 1000, Q = NULL, bf = NULL, rootseq = NULL, rate = 1)
```

Arguments

`x`	a phylogenetic tree `tree`, i.e. an object of class `phylo`
`l`	length of the sequence to simulate.
`Q`	the rate matrix.
`bf`	base frequencies.
`rootseq`	a vector of length l containing the root sequence, other root sequence is randomly generated.
`rate`	mutation rate

Value

list with four items

1. alignment Phydat object with the resulting alignment
2. rootseq the rootsequence used
3. total_branch_substitutions total number of substitutions accumulated on the branches
4. total_node_substitutions total number of substitutions accumulated at the nodes

Author(s)

Klaus Schliep <klaus.schliep@gmail.com>

sim_normal_explicit *simulate a sequence assuming substitutions are only accumulated along the branches, using the explicit simulation method (e.g. reverse substitutions are modeled explicitly)*

Description

simulate a sequence assuming substitutions are only accumulated along the branches, using the explicit simulation method (e.g. reverse substitutions are modeled explicitly)

Usage

```
sim_normal_explicit(x, l = 1000, Q = NULL, bf = NULL, rootseq = NULL, rate = 1)
```

Arguments

x	a phylogenetic tree tree, i.e. an object of class phylo or and object of class pml.
l	length of the sequence to simulate.
Q	the rate matrix.
bf	base frequencies.
rootseq	a vector of length l containing the root sequence, other root sequence is randomly generated.
rate	mutation rate or scaler for the edge length, a numerical value greater than zero.

Value

list with four items

1. alignment Phydat object with the resulting alignment
2. rootseq the rootsequence used
3. total_branch_substitutions total number of substitutions accumulated on the branches
4. total_node_substitutions total number of substitutions accumulated at the nodes

sim_unlinked *Simulate a sequence assuming node substitutions are not shared amongst offspring, given two substitution matrices: one for substitutions occuring on the nodes, and one for substitutions occuring along the branches.*

Description

Simulate a sequence assuming node substitutions are not shared amongst offspring, given two substitution matrices: one for substitutions occuring on the nodes, and one for substitutions occuring along the branches.

Usage

```
sim_unlinked(
  phy,
  Q1 = rep(1, 6),
  Q2 = rep(1, 6),
  rate1 = 0.1,
  rate2 = 0.1,
  l = 1000,
  bf = rep(0.25, 4),
  rootseq = NULL,
  node_time = 0.001
)
```

Arguments

phy	tree for which to simulate sequences
Q1	substitution matrix along the branches, default = JC
Q2	substitution matrix on the nodes, default = JC
rate1	mutation rate along the branch, default = 0.1
rate2	mutation rate on the node, default = 0.1
l	number of base pairs to simulate
bf	base frequencies, default = c(0.25, 0.25, 0.25, 0.25)
rootseq	sequence at the root, simulated by default
node_time	amount of time spent at the nodes

Value

list with four items

1. alignment Phydat object with the resulting alignment
2. rootseq the rootsequence used
3. total_branch_substitutions total number of substitutions accumulated on the branches
4. total_node_substitutions total number of substitutions accumulated at the nodes

---

sim_unlinked_explicit *Simulate a sequence assuming node substitutions are not shared amongst offspring, using the explicit simulation method (e.g. reverse substitutions are modeled explicitly)*

Description

Simulate a sequence assuming node substitutions are not shared amongst offspring, using the explicit simulation method (e.g. reverse substitutions are modeled explicitly)

Usage

```
sim_unlinked_explicit(
  phy,
  Q1 = rep(1, 6),
  Q2 = rep(1, 6),
  rate1 = 0.1,
  rate2 = 0.1,
  l = 1000,
  bf = rep(0.25, 4),
  rootseq = NULL,
  node_time = 0.001
)
```

Arguments

phy	phylogenetic tree for which to simulate sequences
Q1	substitution matrix along the branches, default = JC
Q2	substitution matrix on the nodes, default = JC
rate1	mutation rate along the branch, default = 0.1
rate2	mutation rate on the node, default = 0.1
l	number of base pairs to simulate
bf	base frequencies, default = c(0.25, 0.25, 0.25, 0.25)
rootseq	sequence at the root, simulated by default
node_time	amount of time spent at the nodes

Value

list with four items

1. alignment Phydat object with the resulting alignment
2. rootseq the rootsequence used
3. total_branch_substitutions total number of substitutions accumulated on the branches
4. total_node_substitutions total number of substitutions accumulated at the nodes

---

slow_matrix *this function calculates the p matrix within R this is slower than the C++ implementation in* get_p_matrix *but provides a way to debug and verify*

Description

this function calculates the p matrix within R this is slower than the C++ implementation in `get_p_matrix` but provides a way to debug and verify

Usage

```
slow_matrix(eig, branch_length, rate)
```

Arguments

`eig`	eigen object
`branch_length`	branch length
`rate`	substitution rate

Value

p matrix

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