

Package ‘secsse’

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Type Package

Title Several Examined and Concealed States-Dependent Speciation and Extinction

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Description Simultaneously infers state-dependent diversification across two or more states of a single or multiple traits while accounting for the role of a possible concealed trait. See Herrera-Alsina et al. 2019 Systematic Biology 68: 317-328 <DOI:10.1093/sysbio/syy057>.

Depends R (>= 3.5.0)

Imports utils, DDD (>= 4.0), ape, foreach, doParallel, apTreeshape, phylobase, geiger, deSolve

Suggests diversitree, phytools, testthat, testit, knitr, rmarkdown

Enhances doMC

NeedsCompilation yes

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LazyData true

VignetteBuilder knitr

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cla_id_paramPos	<i>Parameter structure setting for cla_secsse</i>
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Description

It sets the parameters (speciation, extinction and transition) ids. Needed for ML calculation with cladogenetic options (cla_secsse_ml)

Usage

```
cla_id_paramPos(trait, num_concealed_states)
```

Arguments

traits vector with trait states, order of states must be the same as tree tips, for help, see vignette.

num_concealed_states number of concealed states, generally equivalent to number of examined states.

Value

A list that includes the ids of the parameters for ML analysis.

Examples

```
traits <- sample(c(0,1,2), 45,replace = TRUE) #get some traits
num_concealed_states <- 3
param_posit <- cla_id_paramPos(traits,num_concealed_states)
```

 cla_secsse_loglik *Likelihood for SecSSE model*

Description

Loglikelihood calculation for the cla_SecSSE model given a set of parameters and data

Usage

```
cla_secsse_loglik(parameter, phy, traits, num_concealed_states,
  use_fortran = TRUE, methode = "ode45", cond = "proper_cond",
  root_state_weight = "proper_weights", sampling_fraction,
  run_parallel = FALSE, setting_calculation = NULL,
  setting_parallel = NULL, see_ancestral_states = FALSE,
  loglik_penalty = 0)
```

Arguments

parameter	list where the first is a table where lambdas across different modes of speciation are shown, the second mus and the third transition rates.
phy	phylogenetic tree of class phylo, ultrametric, fully-resolved, rooted and with branch lengths.
traits	vector with trait states, order of states must be the same as tree tips, for help, see vignette.
num_concealed_states	number of concealed states, generally equivalent to number of examined states.
use_fortran	Should the Fortran code for numerical integration be called? Default is TRUE.
methode	Solver for the set of equations, default is "ode45".
cond	condition on the existence of a node root: "maddison_cond", "proper_cond"(default). For details, see vignette.
root_state_weight	the method to weigh the states: "maddison_weights", "proper_weights"(default) or "equal_weights". It can also be specified the root state: the vector c(1,0,0) indicates state 1 was the root state.
sampling_fraction	vector that states the sampling proportion per trait state. It must have as many elements as trait states.
run_parallel	should the routine to run in parallel be called?
setting_calculation	argument used internally to speed up calculation. It should be left blank (default : setting_calculation = NULL)
setting_parallel	argument used internally to set a parallel calculation. It should be left blank (default : setting_parallel = NULL)

see_ancestral_states

should the ancestral states be shown? Deafault FALSE

loglik_penalty the size of the penalty for all parameters; default is 0 (no penalty)

Value

The loglikelihood of the data given the parameters

Note

To run in parallel it is needed to load the following libraries when windows: apTreeshape, doparallel and foreach. When unix, it requires: apTreeshape, doparallel, foreach and doMC

Examples

```
rm(list=ls(all=TRUE))
library(secsse)
library(DDD)
library(deSolve)
#library(diversitree)
library(apTreeshape)
library(foreach)
set.seed(13)
phyloree <- ape::rcoal(12, tip.label = 1:12)
traits <- sample(c(0,1,2),ape::Ntip(phyloree),replace=TRUE)
num_concealed_states <- 3
sampling_fraction <- c(1,1,1)
methode <- "ode45"
phy <- phyloree
# the idparlist for a ETD model (dual state inheritance model of evolution)
# would be set like this:
idparlist <- cla_id_paramPos(traits,num_concealed_states)
lambd_and_modeSpe <- idparlist$lambda
lambd_and_modeSpe[1,] <- c(1,1,1,2,2,2,3,3,3)
idparlist[[1]] <- lambd_and_modeSpe
idparlist[[2]][,] <- 0
masterBlock <- matrix(4,ncol=3,nrow=3,byrow=TRUE)
diag(masterBlock) <- NA
idparlist [[3]] <- q_doubletrans(traits,masterBlock,diff.conceal = FALSE)
# Now, internally, clsecsse sorts the lambda matrices, so they look like:
prepare_full_lambdas(traits,num_concealed_states,idparlist[[1]])
# which is a list with 9 matrices, corresponding to the 9 states (0A,1A,2A,0B,etc)
# if we want to calculate a single likelihood:
parameter <- idparlist
lambd_and_modeSpe <- parameter$lambda
lambd_and_modeSpe[1,] <- c(0.2,0.2,0.2,0.4,0.4,0.4,0.01,0.01,0.01)
parameter[[1]] <- prepare_full_lambdas(traits,num_concealed_states,lambd_and_modeSpe)
parameter[[2]] <- rep(0,9)
masterBlock <- matrix(0.07,ncol=3,nrow=3,byrow=TRUE)
diag(masterBlock) <- NA
parameter [[3]] <- q_doubletrans(traits,masterBlock,diff.conceal = FALSE)
cla_secsse_loglik(parameter, phy, traits, num_concealed_states,
```

```

use_fortran = FALSE, methode = "ode45", cond = "maddison_cond",
root_state_weight = "maddison_weights", sampling_fraction,
run_parallel = FALSE, setting_calculation = NULL,
setting_parallel = NULL, see_ancestral_states = FALSE,
loglik_penalty = 0)
# LL = -37.8741

```

cla_secsse_ml

*Maximum likelihood estimation for (SecSSE)***Description**

Maximum likelihood estimation under Several examined and concealed States-dependent Speciation and Extinction (SecSSE) with cladogenetic option

Usage

```

cla_secsse_ml(phy, traits, num_concealed_states, idparslist, idparsopt,
  initparsopt, idparsfix, parsfix, cond = "proper_cond",
  root_state_weight = "proper_weights", sampling_fraction,
  tol = c(1e-04, 1e-05, 1e-07), maxiter = 1000 *
  round((1.25)^length(idparsopt)), use_fortran = TRUE,
  methode = "ode45", optimmethod = "simplex", num_cycles = 1,
  run_parallel = FALSE, loglik_penalty = 0)

```

Arguments

phy	phylogenetic tree of class phylo, ultrametric, rooted and with branch lengths.
traits	a vector with trait states for each tip in the phylogeny.
num_concealed_states	number of concealed states, generally equivalent to the number of examined states in the dataset.
idparslist	overview of parameters and their values.
idparsopt	id of parameters to be estimated.
initparsopt	initial guess of the parameters to be estimated.
idparsfix	id of the fixed parameters.
parsfix	value of the fixed parameters.
cond	condition on the existence of a node root: "maddison_cond", "proper_cond"(default). For details, see vignette.
root_state_weight	the method to weigh the states: "maddison_weights", "proper_weights"(default) or "equal_weights". It can also be specified the root state: the vector c(1,0,0) indicates state 1 was the root state.
sampling_fraction	vector that states the sampling proportion per trait state. It must have as many elements as there are trait states.

tol maximum tolerance. Default is "c(1e-04, 1e-05, 1e-05)".
 maxiter max number of iterations. Default is "1000 *round((1.25)^length(idparsopt))".
 use_fortran Should the Fortran code for numerical integration be called? Default is TRUE.
 methode method used for integration calculation. Default is "ode45".
 optimmethod method used for optimization. Default is "simplex".
 num_cycles number of cycles of the optimization (default is 1).
 run_parallel should the routine to run in parallel be called?
 loglik_penalty the size of the penalty for all parameters; default is 0 (no penalty)

Value

Parameter estimated and maximum likelihood

Note

To run in parallel it is needed to load the following libraries when windows: apTreeshape, doparallel and foreach. When unix, it requires: apTreeshape, doparallel, foreach and doMC

Examples

```
# Example of how to set the arguments for a ML search.
library(secsse)
library(DDD)
set.seed(13)
# Check the vignette for a better working exercise.
# lambdas for 0A and 1A and 2A are the same but need to be estimated (CTD model, see Syst Biol
# paper)
# mus are fixed to zero,
# the transition rates are constrained to be equal and fixed 0.01
phyloree <- ape::rcoal(31, tip.label = 1:31)
traits <- sample(c(0,1,2), ape::Ntip(phyloree),replace=TRUE) #get some traits
num_concealed_states <- 3
idparslist <- cla_id_paramPos(traits,num_concealed_states)
idparslist$lambda[1,] <- c(1,1,1,2,2,2,3,3,3)
idparslist[[2]][,] <- 4
masterBlock <- matrix(5,ncol = 3,nrow = 3,byrow = TRUE)
diag(masterBlock) <- NA
diff.conceal <- FALSE
idparslist[[3]] <- q_doubletrans(traits,masterBlock,diff.conceal)
startingpoint <- bd_ML(brts = ape::branching.times(phyloree))
intGuessLamba <- startingpoint$lambda0
intGuessMu <- startingpoint$mu0
idparsopt <- c(1,2,3)
initparsopt <- c(rep(intGuessLamba,3))
idparsfix <- c(0,4,5)
parsfix <- c(0,0,0.01)
tol <- c(1e-04, 1e-05, 1e-07)
maxiter <- 1000 * round((1.25) ^ length(idparsopt))
use_fortran <- FALSE
methode <- "ode45"
```

```

optimmethod <- "simplex"
run_parallel <- FALSE
cond <- "proper_cond"
root_state_weight <- "proper_weights"
sampling_fraction <- c(1,1,1)
#model <- cla_secsse_ml(
# phylotree,
# traits,
# num_concealed_states,
# idparslist,
# idparsopt,
# initparsopt,
# idparsfix,
# parsfix,
# cond,
# root_state_weight,
# sampling_fraction,
# tol,
# maxiter,
# use_fortran,
# methode,
# optimmethod,
# num_cycles = 1,
# run_parallel)
# [1] -90.97626

```

cla_secsse_ml_func_def_pars

Maximum likelihood estimation for (SecSSE) with parameter as complex functions. Cladogenetic version

Description

Maximum likelihood estimation under cla Several examined and concealed States-dependent Speciation and Extinction (SecSSE) where some paramaters are functions of other parameters and/or factors. Offers the option of cladogenesis

Usage

```

cla_secsse_ml_func_def_pars(phy, traits, num_concealed_states, idparslist,
  idparsopt, initparsopt, idfactorsopt, initfactors, idparsfix, parsfix,
  idparsfuncdefpar, functions_defining_params, cond = "proper_cond",
  root_state_weight = "proper_weights", sampling_fraction,
  tol = c(1e-04, 1e-05, 1e-07), maxiter = 1000 *
  round((1.25)^length(idparsopt)), use_fortran = TRUE,
  methode = "ode45", optimmethod = "simplex", num_cycles = 1,
  run_parallel = FALSE, loglik_penalty = 0)

```

Arguments

phy	phylogenetic tree of class phylo, ultrametric, rooted and with branch lengths.
traits	a vector with trait states for each tip in the phylogeny.
num_concealed_states	number of concealed states, generally equivalent to the number of examined states in the dataset.
idparslist	overview of parameters and their values.
idparsopt	id of parameters to be estimated.
initparsopt	initial guess of the parameters to be estimated.
idfactorsopt	id of the factors that will be optimized. There are not fixed factors, so use a constant within 'functions_defining_params'.
initfactors	the initial guess for a factor (it should be set to NULL when no factors).
idparsfix	id of the fixed parameters (it should be set to NULL when no factors).
parsfix	value of the fixed parameters.
idparsfuncdefpar	id of the parameters which will be a function of optimized and/or fixed parameters. The order of id should match functions_defining_params
functions_defining_params	a list of functions. Each element will be a function which defines a parameter e.g. <code>id_3 <- (id_1+id_2)/2</code> . See example and vignette
cond	condition on the existence of a node root: "maddison_cond", "proper_cond"(default). For details, see vignette.
root_state_weight	the method to weigh the states: "maddison_weights", "proper_weights"(default) or "equal_weights". It can also be specified the root state: the vector <code>c(1,0,0)</code> indicates state 1 was the root state.
sampling_fraction	vector that states the sampling proportion per trait state. It must have as many elements as there are trait states.
tol	maximum tolerance. Default is "c(1e-04, 1e-05, 1e-05)".
maxiter	max number of iterations. Default is "1000 *round((1.25)^length(idparsopt))".
use_fortran	Should the Fortran code for numerical integration be called? Default is TRUE.
methode	method used for integration calculation. Default is "ode45".
optimmethod	method used for optimization. Default is "simplex".
num_cycles	number of cycles of the optimization (default is 1).
run_parallel	should the routine to run in parallel be called? Read note below
loglik_penalty	the size of the penalty for all parameters; default is 0 (no penalty)

Value

Parameter estimated and maximum likelihood

Note

To run in parallel the following libraries must be loaded under windows: apTreeshape, doparallel and foreach. Under unix/linux, apTreeshape, doparallel, foreach and doMC must be loaded.

Examples

```
# Example of how to set the arguments for a ML search.
rm(list=ls(all=TRUE))
library(secsse)
library(DDD)
set.seed(16)
phyloTree <- ape::rbdTree(0.07,0.001,Tmax=50)
startingpoint <- bd_ML(brts = ape::branching.times(phyloTree))
intGuessLamba <- startingpoint$lambda0
intGuessMu <- startingpoint$mu0
traits <- sample(c(0,1,2), ape::Ntip(phyloTree),replace=TRUE) #get some traits
num_concealed_states <- 3
idparslist <- cla_id_paramPos(traits,num_concealed_states)
idparslist$lambda0[1,] <- c(1,2,3,1,2,3,1,2,3)
idparslist[[2]][,] <- 4
masterBlock <- matrix(c(5,6),ncol=3,nrow=3,byrow=TRUE)
diag(masterBlock) <- NA
diff.conceal <- FALSE
idparslist[[3]] <- q_doubletrans(traits,masterBlock,diff.conceal)
idparsfuncdefpar <- c(3,5,6)
idparsopt <- c(1,2)
idparsfix <- c(0,4)
initparsopt <- c(rep(intGuessLamba,2))
parsfix <- c(0,0)
idfactorsopt <- 1
initfactors <- 4
# functions_defining_params is a list of functions. Each function has no arguments and to refer
# to parameters ids should be indicated as "par_" i.e. par_3 refers to parameter 3. When a
# function is defined, be sure that all the parameters involved are either estimated, fixed or
# defined by previous functions (i.e. a function that defines parameter in
# 'functions_defining_params'). The user is responsible for this. In this example, par_3
# (i.e., parameter 3) is needed to calculate par_6. This is correct because par_3 is defined
# in the first function of 'functions_defining_params'. Notice that factor_1 indicates a value
# that will be estimated to satisfy the equation. The same factor can be shared to define
# several parameters.
functions_defining_params <- list()
functions_defining_params[[1]] <- function(){
  par_3 <- par_1 + par_2
}
functions_defining_params[[2]] <- function(){
  par_5 <- par_1 * factor_1
}
functions_defining_params[[3]] <- function(){
  par_6 <- par_3 * factor_1
}

tol = c(1e-04, 1e-05, 1e-07)
```

```

maxiter = 1000 * round((1.25)^length(idparsopt))
use_fortran = TRUE
methode = "ode45"
optimmethod = "simplex"
run_parallel = FALSE
cond <- "proper_cond"
root_state_weight <- "proper_weights"
sampling_fraction <- c(1,1,1)
#model <- cla_secsse_ml_func_def_pars(phyloree, traits, num_concealed_states, idparslist,
#                                     idparsopt, initparsopt, idfactorsopt, initfactors,
#                                     idparsfix, parsfix, idparsfuncdefpar,
#                                     functions_defining_params, cond, root_state_weight,
#                                     sampling_fraction, tol, maxiter, use_fortran,
#                                     methode, optimmethod, num_cycles = 1,run_parallel)

# ML -136.5796

```

example_phy_GeoSSE *A phylogeny with traits at the tips*

Description

An example phylogeny for testing purposes

Usage

phy

Format

A phylogeny as created by GeoSSE (diversitree)

id_paramPos *Parameter structure setting*

Description

It sets the parameters (speciation, extinction and transition) ids. Needed for ML calculation (secsse_ml)

Usage

id_paramPos(traits, num_concealed_states)

Arguments

`traits` vector with trait states, order of states must be the same as tree tips, for help, see vignette.

`num_concealed_states` number of concealed states, generally equivalent to number of examined states.

Value

A list that includes the ids of the parameters for ML analysis.

Examples

```
traits <- sample(c(0,1,2), 45,replace = TRUE) #get some traits
num_concealed_states <- 3
param_posit <- id_paramPos(traits,num_concealed_states)
```

phylo_Vign *A phylogenetic reconstruction to run the vignette*

Description

An example phylogeny in the right format for secsse

Format

Phylogenetic tree in format nexus, rooted, including branch lengths

prepare_full_lambdas *Prepares the entire set of lambda matrices for cla_secsse.*

Description

It provides the set of matrices containing all the speciation rates

Usage

```
prepare_full_lambdas(traits, num_concealed_states, lambd_and_modeSpe)
```

Arguments

`traits` vector with trait states, order of states must be the same as tree tips, for help, see vignette.

`num_concealed_states` number of concealed states, generally equivalent to number of examined states.

`lambd_and_modeSpe` a matrix with the 4 models of speciation possible.

Value

A list of lambdas, its length would be the same than the number of trait states * num_concealed_states..

q_doubletrans	<i>Basic Qmatrix</i>
---------------	----------------------

Description

Sets a Q matrix where double transitions are not allowed

Usage

```
q_doubletrans(traits, masterBlock, diff.conceal)
```

Arguments

traits	vector with trait states, order of states must be the same as tree tips, for help, see vignette.
masterBlock	matrix of transitions among only examined states, NA in the main diagonal, used to build the full transition rates matrix.
diff.conceal	should the concealed states be different? Normally it should be FALSE.

Value

Q matrix that includes both examined and concealed states, it should be declared as the third element of idparslist.

Examples

```
traits <- sample(c(0,1,2), 45,replace = TRUE) #get some traits
masterBlock <- matrix(99,ncol = 3,nrow = 3,byrow = TRUE) #For a three-state trait
diag(masterBlock) <- NA
masterBlock[1,2] <- 6
masterBlock[1,3] <- 7
masterBlock[2,1] <- 8
masterBlock[2,3] <- 9
masterBlock[3,1] <- 10
masterBlock[3,2] <- 11
myQ <- q_doubletrans(traits,masterBlock,diff.conceal = FALSE)
# now, it can replace the Q matrix from id_paramPos
num_concealed_states <- 3
param_posit <- id_paramPos(traits,num_concealed_states)
param_posit[[3]] <- myQ
```

secsse_loglik

Likelihood for SecSSE model

Description

Loglikelihood calculation for the SecSSE model given a set of parameters and data

Usage

```
secsse_loglik(parameter, phy, traits, num_concealed_states,
  use_fortran = TRUE, methode = "ode45", cond = "proper_cond",
  root_state_weight = "proper_weights", sampling_fraction,
  run_parallel = FALSE, setting_calculation = NULL,
  setting_parallel = NULL, see_ancestral_states = FALSE,
  loglik_penalty = 0)
```

Arguments

parameter	list where first vector represents lambdas, the second mus and the third transition rates.
phy	phylogenetic tree of class phylo, ultrametric, fully-resolved, rooted and with branch lengths.
traits	vector with trait states, order of states must be the same as tree tips, for help, see vignette.
num_concealed_states	number of concealed states, generally equivalent to number of examined states.
use_fortran	Should the Fortran code for numerical integration be called? Default is TRUE.
methode	Solver for the set of equations, default is "ode45".
cond	condition on the existence of a node root: "maddison_cond", "proper_cond"(default). For details, see vignette.
root_state_weight	the method to weigh the states: "maddison_weights", "proper_weights"(default) or "equal_weights". It can also be specified the root state: the vector c(1,0,0) indicates state 1 was the root state.
sampling_fraction	vector that states the sampling proportion per trait state. It must have as many elements as trait states.
run_parallel	should the routine to run in parallel be called?
setting_calculation	argument used internally to speed up calculation. It should be leave blank (default : setting_calculation = NULL)
setting_parallel	argument used internally to set a parallel calculation. It should be left blank (default : setting_parallel = NULL)

`see_ancestral_states`
 should the ancestral states be shown? Deafault FALSE

`loglik_penalty` the size of the penalty for all parameters; default is 0 (no penalty)

Value

The loglikelihood of the data given the parameters

Note

To run in parallel it is needed to load the following libraries when windows: apTreeshape, doparallel and foreach. When unix, it requires: apTreeshape, doparallel, foreach and doMC

Examples

```
rm(list = ls(all = TRUE))
library(secsse)
library(DDD)
library(deSolve)
library(apTreeshape)
library(foreach)
set.seed(13)
phylotree <- ape::rcoal(31, tip.label = 1:31)
traits <- sample(c(0,1,2),ape::Ntip(phylotree),replace = TRUE)
num_concealed_states <- 2
use_fortran <- TRUE
cond <- "proper_cond"
methode <- "ode45"
root_state_weight <- "proper_weights"
sampling_fraction <- c(1,1,1)
run_parallel <- FALSE
drill <- id_paramPos(traits,num_concealed_states)
drill[[1]][,] <- c(0.12,0.01,0.2,0.21,0.31,0.23)
drill[[2]][,] <- 0
drill[[3]][,] <- 0.1
diag(drill[[3]]) <- NA
secsse_loglik(parameter=drill,phylotree,traits,num_concealed_states,
  use_fortran,methode,cond,root_state_weight,sampling_fraction,see_ancestral_states = FALSE)

#[1] -113.1018
```

secsse_ml

Maximum likelihood estimation for (SecSSE)

Description

Maximum likelihood estimation under Several examined and concealed States-dependent Speciation and Extinction (SecSSE)

Usage

```
secsse_ml(phy, traits, num_concealed_states, idparslist, idparsopt,
  initparsopt, idparsfix, parsfix, cond = "proper_cond",
  root_state_weight = "proper_weights", sampling_fraction,
  tol = c(1e-04, 1e-05, 1e-07), maxiter = 1000 *
  round((1.25)^length(idparsopt)), use_fortran = TRUE,
  methode = "ode45", optimmethod = "simplex", num_cycles = 1,
  run_parallel = FALSE, loglik_penalty = 0)
```

Arguments

phy	phylogenetic tree of class phylo, ultrametric, rooted and with branch lengths.
traits	a vector with trait states for each tip in the phylogeny.
num_concealed_states	number of concealed states, generally equivalent to the number of examined states in the dataset.
idparslist	overview of parameters and their values.
idparsopt	id of parameters to be estimated.
initparsopt	initial guess of the parameters to be estimated.
idparsfix	id of the fixed parameters.
parsfix	value of the fixed parameters.
cond	condition on the existence of a node root: "maddison_cond", "proper_cond"(default). For details, see vignette.
root_state_weight	the method to weigh the states: "maddison_weights", "proper_weights"(default) or "equal_weights". It can also be specified the root state: the vector c(1,0,0) indicates state 1 was the root state.
sampling_fraction	vector that states the sampling proportion per trait state. It must have as many elements as there are trait states.
tol	maximum tolerance. Default is "c(1e-04, 1e-05, 1e-05)".
maxiter	max number of iterations. Default is "1000 *round((1.25)^length(idparsopt))".
use_fortran	Should the Fortran code for numerical integration be called? Default is TRUE.
methode	method used for integration calculation. Default is "ode45".
optimmethod	method used for optimization. Default is "simplex".
num_cycles	number of cycles of the optimization (default is 1).
run_parallel	should the routine to run in parallel be called?
loglik_penalty	the size of the penalty for all parameters; default is 0 (no penalty)

Value

Parameter estimated and maximum likelihood

Note

To run in parallel it is needed to load the following libraries when windows: apTreeshape, doparallel and foreach. When unix, it requires: apTreeshape, doparallel, foreach and doMC

Examples

```
# Example of how to set the arguments for a ML search.
library(secsse)
library(DDD)
set.seed(13)
# Check the vignette for a better working exercise.
# lambdas for 0A and 1A and 2A are the same but need to be estimated
# mus are fixed to
# the transition rates are constrained to be equal and fixed 0.01
phyloree <- ape::rcoal(31, tip.label = 1:31)
traits <- sample(c(0,1,2), ape::Ntip(phyloree),replace=TRUE) #get some traits
num_concealed_states<-3
idparslist<-id_paramPos(traits, num_concealed_states)
idparslist[[1]][c(1,4,7)]<-1
idparslist[[1]][c(2,5,8)]<-2
idparslist[[1]][c(3,6,9)]<-3
idparslist[[2]][ ]<-4
masterBlock<-matrix(5,ncol=3,nrow=3,byrow=TRUE)
diag(masterBlock)<-NA
diff.conceal<-FALSE
idparslist[[3]]<-q_doubletrans(traits,masterBlock,diff.conceal)
startingpoint<-bd_ML(brts = ape::branching.times(phyloree))
intGuessLamba <- startingpoint$lambda0
intGuessMu <- startingpoint$mu0
idparsopt<-c(1,2,3,5)
initparsopt<-c(rep(intGuessLamba,3),rep((intGuessLamba/5),1))
idparsfix<-c(0,4)
parsfix<-c(0,0)
tol = c(1e-04, 1e-05, 1e-07)
maxiter = 1000 * round((1.25)^length(idparsopt))
use_fortran = TRUE
methode = "ode45"
optimmethod = "simplex"
run_parallel = FALSE
cond<-"proper_cond"
root_state_weight <- "proper_weights"
sampling_fraction<-c(1,1,1)
#model<-secsse_ml(
#phyloree,
#traits,
#num_concealed_states,
#idparslist,
#idparsopt,
#initparsopt,
#idparsfix,
#parsfix,
#cond,
```



```

#root_state_weight,
#sampling_fraction,
#tol,
#maxiter,
#use_fortran,
#methode,
#optimmethod,
#num_cycles = 1,
#run_parallel
#)
# $ML
# [1] -16.43162

```

secsse_ml_func_def_pars

Maximum likelihood estimation for (SecSSE) with parameter as complex functions.

Description

Maximum likelihood estimation under Several examined and concealed States-dependent Speciation and Extinction (SecSSE) where some parameters are functions of other parameters and/or factors.

Usage

```

secsse_ml_func_def_pars(phy, traits, num_concealed_states, idparslist,
  idparsopt, initparsopt, idfactorsopt, initfactors, idparsfix, parsfix,
  idparsfuncdefpar, functions_defining_params, cond = "proper_cond",
  root_state_weight = "proper_weights", sampling_fraction,
  tol = c(1e-04, 1e-05, 1e-07), maxiter = 1000 *
  round((1.25)^length(idparsopt)), use_fortran = TRUE,
  methode = "ode45", optimmethod = "simplex", num_cycles = 1,
  run_parallel = FALSE, loglik_penalty = 0)

```

Arguments

phy	phylogenetic tree of class phylo, ultrametric, rooted and with branch lengths.
traits	a vector with trait states for each tip in the phylogeny.
num_concealed_states	number of concealed states, generally equivalent to the number of examined states in the dataset.
idparslist	overview of parameters and their values.
idparsopt	id of parameters to be estimated.
initparsopt	initial guess of the parameters to be estimated.
idfactorsopt	id of the factors that will be optimized. There are not fixed factors, so use a constant within 'functions_defining_params'.

<code>initfactors</code>	the initial guess for a factor (it should be set to NULL when no factors).
<code>idparsfix</code>	id of the fixed parameters (it should be set to NULL when there are no factors).
<code>parsfix</code>	value of the fixed parameters.
<code>idparsfuncdefpar</code>	id of the parameters which will be a function of optimized and/or fixed parameters. The order of id should match <code>functions_defining_params</code>
<code>functions_defining_params</code>	a list of functions. Each element will be a function which defines a parameter e.g. <code>id_3 <- (id_1+id_2)/2</code> . See example and vignette
<code>cond</code>	condition on the existence of a node root: "maddison_cond", "proper_cond"(default). For details, see vignette.
<code>root_state_weight</code>	the method to weigh the states: "maddison_weights", "proper_weights"(default) or "equal_weights". It can also be specified the root state: the vector <code>c(1,0,0)</code> indicates state 1 was the root state.
<code>sampling_fraction</code>	vector that states the sampling proportion per trait state. It must have as many elements as there are trait states.
<code>tol</code>	maximum tolerance. Default is "c(1e-04, 1e-05, 1e-05)".
<code>maxiter</code>	max number of iterations. Default is "1000 *round((1.25)^length(idparsopt))".
<code>use_fortran</code>	Should the Fortran code for numerical integration be called? Default is TRUE.
<code>methode</code>	method used for integration calculation. Default is "ode45".
<code>optimmethod</code>	method used for optimization. Default is "simplex".
<code>num_cycles</code>	number of cycles of the optimization (default is 1).
<code>run_parallel</code>	should the routine to run in parallel be called? Read note below
<code>loglik_penalty</code>	the size of the penalty for all parameters; default is 0 (no penalty)

Value

Parameter estimated and maximum likelihood

Note

To run in parallel it is needed to load the following libraries when windows: `apTreeshape`, `doparallel` and `foreach`. When unix, it requires: `apTreeshape`, `doparallel`, `foreach` and `doMC`

Examples

```
# Example of how to set the arguments for a ML search.
rm(list=ls(all=TRUE))
library(secsse)
library(DDD)
set.seed(16)
phylotree <- ape::rbdtree(0.07, 0.001, Tmax=50)
startingpoint<-bd_ML(brts = ape::branching.times(phylotree))
intGuessLamba <- startingpoint$lambda0
```

```

intGuessMu <- startingpoint$mu0
traits <- sample(c(0,1,2), ape::Ntip(phyloree),replace=TRUE) #get some traits
num_concealed_states<-3
idparslist<-id_paramPos(traits, num_concealed_states)
idparslist[[1]][c(1,4,7)] <- 1
idparslist[[1]][c(2,5,8)] <- 2
idparslist[[1]][c(3,6,9)] <- 3
idparslist[[2]][c(1,4,7)] <- 4
masterBlock <- matrix(c(5,6),ncol = 3,nrow = 3,byrow = TRUE)
diag(masterBlock) <- NA
diff.conceal <- FALSE
idparslist[[3]] <- q_doubletrans(traits,masterBlock,diff.conceal)
idparsfuncdefpar <- c(3,5,6)
idparsopt <- c(1,2)
idparsfix <- c(0,4)
initparsopt <- c(rep(intGuessLamba,2))
parsfix <- c(0,0)
idfactorsopt <- 1
initfactors <- 4
# functions_defining_params is a list of functions. Each function has no arguments and to refer
# to parameters ids should be indicated as "par_" i.e. par_3 refers to parameter 3. When a
# function is defined, be sure that all the parameters involved are either estimated, fixed or
# defined by previous functions (i.e. a function that defines parameter in
# 'functions_defining_params'). The user is responsible for this. In this example, par_3
# (i.e., parameter 3) is needed to calculate par_6. This is correct because par_3 is defined in
# the first function of 'functions_defining_params'. Notice that factor_1 indicates a value
# that will be estimated to satisfy the equation. The same factor can be shared to define
# several parameters.
functions_defining_params <- list()
functions_defining_params[[1]] <- function(){
  par_3 <- par_1 + par_2
}
functions_defining_params[[2]] <- function(){
  par_5 <- par_1 * factor_1
}
functions_defining_params[[3]] <- function(){
  par_6 <- par_3 * factor_1
}

tol = c(1e-04, 1e-05, 1e-07)
maxiter = 1000 * round((1.25)^length(idparsopt))
use_fortran = TRUE
methode = "ode45"
optimmethod = "simplex"
run_parallel = FALSE
cond<-"proper_cond"
root_state_weight <- "proper_weights"
sampling_fraction <- c(1,1,1)
#model <- secsse_ml_func_def_pars(phyloree, traits, num_concealed_states, idparslist, idparsopt,
#                               initparsopt, idfactorsopt, initfactors, idparsfix, parsfix,
#                               idparsfuncdefpar, functions_defining_params, cond,
#                               root_state_weight, sampling_fraction, tol, maxiter, use_fortran,
#                               methode, optimmethod, num_cycles = 1,run_parallel)

```

```
# ML -136.5796
```

```
sortingtraits      Data checking and trait sorting
```

Description

In preparation for likelihood calculation, it orders trait data according to the tree tips

Usage

```
sortingtraits(traitinfo, phy)
```

Arguments

traitinfo	data frame where first column has species ids and the second one is the trait associated information.
phy	phy phylogenetic tree of class phylo, ultrametric, fully-resolved, rooted and with branch lengths.

Value

Vector of traits

Examples

```
# Some data we have prepared
data(traitinfo)
data("phylo_Vign")
traits <- sortingtraits(traitinfo, phylo_Vign)
```

```
traitinfo      A table with trait info to run the vignette
```

Description

An example of trait information in the right format for secsse

Format

A data frame where each species has a trait state associated

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