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Type Package

Title Diversification Rate Estimation and Fast Simulation of Reconstructed Phylogenetic Trees under Tree-Wide Time-Heterogeneous Birth-Death Processes Including Mass-Extinction Events

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Description Simulation of reconstructed phylogenetic trees under tree-wide time-heterogeneous birth-death processes and estimation of diversification parameters under the same model. Speciation and extinction rates can be any function of time and mass-extinction events at specific times can be provided. Trees can be simulated either conditioned on the number of species, the time of the process, or both. Additionally, the likelihood equations are implemented for convenience and can be used for Maximum Likelihood (ML) estimation and Bayesian inference. Compatibility updates by Renova.

License GPL-3

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`TESS-package` *Diversification rate estimation and fast simulation of reconstructed phylogenetic trees under tree-wide time-heterogeneous birth-death processes including mass-extinction events*

Description

Simulation of reconstructed phylogenetic trees under tree-wide time-heterogeneous birth-death processes and estimation of parameters under the same model. Speciation and extinction rates can be any function of time and mass-extinction events at specific times can be provided. Trees can be simulated either conditioned on the number of species, the time of the process, or both. Additionally, the likelihood equations are implemented for convenience and can be used for Maximum Likelihood (ML) estimation and Bayesian inference.

Details

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Author(s)

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References

S. Hoehna: Fast simulation of reconstructed phylogenies under global, time-dependent birth-death processes. 2013, Bioinformatics, 29:1367-1374.

S. Hoehna: Likelihood inference of non-constant diversification rates with incomplete taxon sampling. 2014, PLoS One, 9(1), e84184.

S. Hoehna: The time-dependent reconstructed evolutionary process with a key-role for mass-extinction events. 2015, Journal of Theoretical Biology, 380, 321-331.

S. Hoehna, MR May and BR Moore: TESS: Bayesian inference of lineage diversification rates from (incompletely sampled) molecular phylogenies in R. 2015, Bioinformatics.

MR May, S. Hoehna, and BR Moore: A Bayesian approach for detecting mass-extinction events when rates of lineage diversification vary. 2015, Systematic Biology

See Also

ape coda

`cettiidae` *Cettiidae phylogeny from Alstroem et al. (2011)*

Description

This phylogeny describes the species relationship and divergence times of the bird family Cettiidae, published in Alstroem et al. (2011).

Usage

```
data(cettiidae)
```

Format

The phylogeny is stored as an object of class `"phylo"`. The structure is described in the help page of the function `read.tree` of the package `ape`.

Source

Alstroem, P., Hoehna, S., Gelang, M., Ericson, P.G.P, and Olsson, U. (2011) Non-monophyly and intricate morphological evolution within the avian family Cettiidae revealed by multilocus analysis of a taxonomically densely sampled dataset, BMC Evolutionary Biology, 11:352.

Examples

```
# load the data
data(cettiidae)

# safe the old plotting settings
op <- par()

# set the new plotting settings
par(cex = 0.3)

# plot the phylogeny
plot(cettiidae)

# restore the plotting settings
par(op)
```

---

conifers *Conifer phylogeny from Leslie et al. (2012)*

Description

This phylogeny describes the species relationships and divergence times of the plant order Conifera, published in Leslie et al. (2012).

Usage

```
data(conifers)
```

Format

The phylogeny is stored as an object of class `"phylo"`. The structure is described in the help page of the function `read.tree` of the package `ape`.

Source

Leslie, A. B., J. M. Beaulieu, H. S. Rai, P. R. Crane, M. J. Donoghue, and S. Mathews. 2012. Hemisphere-scale differences in conifer evolutionary dynamics. Proceedings of the National Academy of Sciences 109:16217-16221.

Examples

```
# load the tree
data(conifers)

# safe the settings of the plotting device
op <- par()

# set the line width for plotting the branches
par(cex = 0.3)

# plot the phylogenetic tree
plot(conifers)

# restore the settings of the device
par(op)
```

`mammalia` *Dated family level mammalian phylogeny from Meredith et al. (2011): Impacts of the cretaceous terrestrial revolution and kpg extinction on mammal diversification.*

Description

This phylogeny describes the species relationship and divergence times of the class Mammalia with 1-3 species included per family, published in Meredith et al. (2011).

Usage

```
data(mammalia)
```

Format

The phylogeny is stored as an object of class `"phylo"`. The structure is described in the help page of the function `read.tree` of the package `ape`.

Source

Meredith, R. et al. (2011): Impacts of the cretaceous terrestrial revolution and kpg extinction on mammal diversification. Science, 334:521-524

Examples

```
# load the data
data(mammalia)

# safe the current settings of the plotting device
op <- par()

# set the line width for drawing thinner lines for the branches
```

```
par(cex = 0.3)

# plot the mammalian phylogeny
plot(mammalia)

# restore the settings of the device
par(op)
```

`tess.analysis` *tess.analysis: Diversification rate estimation under an episodic birth-death process including mass-extinction events.*

Description

tess.analysis estimates diversification rates under an episodic birth-death process including mass-extinction events. The method uses a reversible-jump MCMC algorithm to estimate the number, timing and magnitude of rate-shifts and mass-extinction events. It is possible to fix either number of events and provide specific values that will be used. We assume a Poison process for the number of events and a lognormal distribution with fixed, but specified, hyper-parameters for the speciation and extinction rate; and an independent Poison process for the number of mass-extinction events where each survival probability follows a Beta distribution with fixed hyper-parameters.

The MCMC algorithm can be run either for a specified number of iterations, until a time limit in seconds has been reached, or until the effective sample size (ESS) has reached a given threshold. Once the first of these requirements are met TESS will stop the analysis. Internally we use scaling and sliding proposals to change the parameter values during the MCMC and a birth-move and death-move to add/remove events (rate-shifts or mass-extinction events).

The results of the MCMC run are stored within a directory that is specified by the user. Several files will be generated containing the sampled parameter values. To summarize the output see tess.process.output(...) and tess.plot.output(...).

Usage

```
tess.analysis( tree,
               initialSpeciationRate,
               initialExtinctionRate,
               empiricalHyperPriors = TRUE,
               empiricalHyperPriorInflation = 10.0,
               empiricalHyperPriorForm = c("lognormal","normal","gamma"),
               speciationRatePriorMean = 0.0,
               speciationRatePriorStDev = 1.0,
               extinctionRatePriorMean = 0.0,
               extinctionRatePriorStDev = 1.0,
               initialSpeciationRateChangeTime = c(),
               initialExtinctionRateChangeTime = c(),
               estimateNumberRateChanges = TRUE,
               numExpectedRateChanges = 2,
               samplingProbability = 1,
```

```
                missingSpecies = c(),
                timesMissingSpecies = c(),
                tInitialMassExtinction = c(),
                pInitialMassExtinction = c(),
                pMassExtinctionPriorShape1 = 5,
                pMassExtinctionPriorShape2 = 95,
                estimateMassExtinctionTimes = TRUE,
                numExpectedMassExtinctions = 2,
                estimateNumberMassExtinctions = TRUE,
                MRCA = TRUE,
                CONDITION = "survival",
                BURNIN = 10000,
                MAX_ITERATIONS = 200000,
                THINNING = 100,
                OPTIMIZATION_FREQUENCY = 500,
                CONVERGENCE_FREQUENCY = 1000,
                MAX_TIME = Inf, MIN_ESS = 500,
                ADAPTIVE = TRUE,
                dir = "" ,
                priorOnly = FALSE,
                verbose = TRUE)
```

Arguments

`tree`	The tree in 'phylo' format.
`initialSpeciationRate`	The initial value of the speciation rate when the MCMC is started. This can either be a single number of a vector of rates per interval.
`initialExtinctionRate`	The initial value of the extinction rate when the MCMC is started. This can either be a single number of a vector of rates per interval.
`empiricalHyperPriors`	Should we estimate the hyper-parameters empirically?
`empiricalHyperPriorInflation`	The scaling factor of the variance for the empirical hyperpriors.
`empiricalHyperPriorForm`	The possible empirical hyper prior distributions; either lognormal, normal or gamma
`speciationRatePriorMean`	The mean of the log-normal prior distribution for the speciation rate.
`speciationRatePriorStDev`	The standard deviation of the log-normal prior distribution for the speciation rate.
`extinctionRatePriorMean`	The mean of the log-normal prior distribution for the extinction rate.
`extinctionRatePriorStDev`	The standard deviation of the log-normal prior distribution for the extinction rate.

`initialSpeciationRateChangeTime`
: The initial value of the time points when speciation rate-shifts occur. The number of time-shifts needs to be one smaller than the number of initial speciation rates.

`initialExtinctionRateChangeTime`
: The initial value of the time points when extinction rate-shifts occur. The number of time-shifts needs to be one smaller than the number of initial extinction rates.

`estimateNumberRateChanges`
: Do we estimate the number of rate shifts? Default is true.

`numExpectedRateChanges`
: Expected number of rate changes which follow a Poisson process. The default gives 0.5 probability on 0 shifts.

`samplingProbability`
: The extant taxa sampling probability at the present time.

`missingSpecies`
: The number of species missed which originated in a given time interval (empirical taxon sampling).

`timesMissingSpecies`
: The times intervals of the missing species (empirical taxon sampling).

`tInitialMassExtinction`
: The initial value of the vector of times of the mass-extinction events. This is used as initial values for the MCMC.

`pInitialMassExtinction`
: The initial value of the vector of survival probabilities of the mass-extinction events. This is used as initial values for the MCMC.

`pMassExtinctionPriorShape1`
: The alpha (first shape) parameter of the Beta prior distribution for the survival probability of a mass-extinction event.

`pMassExtinctionPriorShape2`
: The beta (second shape) parameter of the Beta prior distribution for the survival probability of a mass-extinction event.

`estimateMassExtinctionTimes`
: Do we estimate the times of mass-extinction events? Default is true.

`numExpectedMassExtinctions`
: Expected number of mass-extinction events which follow a Poisson process. The default gives 0.5 probability on 0 events.

`estimateNumberMassExtinctions`
: Do we estimate the number of mass-extinction events? Default is true.

`MRCA`
: Does the process start with the most recent common ancestor? If not, the tree must have a root edge!

`CONDITION`
: do we condition the process on time|survival|taxa?

`BURNIN`
: The length of the burnin period.

`MAX_ITERATIONS`
: The maximum number of iteration of the MCMC. The default is 200000.

`THINNING`
: The frequency how often samples are recorded during the MCMC. The default is every 100 iterations.

OPTIMIZATION_FREQUENCY
: The frequency how often the MCMC moves are optimized. The default is every 500 iterations.

CONVERGENCE_FREQUENCY
: The frequency how often we check for convergence? The default is every 1000 iterations.

MAX_TIME
: The maximum time the MCMC is allowed to run in seconds. The default is Inf

MIN_ESS
: The minimum number of effective samples (ESS) to assume convergence. The default is 500

ADAPTIVE
: Do we use auto-tuning of the MCMC moves? The default is TRUE (recommended).

dir
: The subdirectory in which the output will be stored. The default is the present directoy ("")

priorOnly
: Do we sample from the prior only? The default is FALSE

verbose
: Do you want detailed output?

Value

There is no return value because all the results are stored into files.

Author(s)

Sebastian Hoehna

References

S. Hoehna: The time-dependent reconstructed evolutionary process with a key-role for mass-extinction events. 2015, Journal of Theoretical Biology, 380, 321-331.

S. Hoehna, MR May and BR Moore: TESS: Bayesian inference of lineage diversification rates from (incompletely sampled) molecular phylogenies in R. 2015, Bioinformatics.

MR May, S. Hoehna, and BR Moore: A Bayesian approach for detecting mass-extinction events when rates of lineage diversification vary. 2015, Systematic Biology

Examples

```
# we load the conifers as the test data set
data(conifers)

# for the conifers we know what the total number of species is
total <- 630
# thus, we can compute what the sampling fraction is
rho <- (conifers$Nnode+1)/total


# next, we specify the prior mean and standard deviation
# for the speciation and extinction rate
mu_lambda = 0.15
std_lambda = 0.02
```

```
mu_mu = 0.09
std_mu = 0.02

# now we can run the entire analysis.
# note that a full analyses should be run much longer
tess.analysis( tree=conifers,
               initialSpeciationRate=exp(mu_lambda),
               initialExtinctionRate=exp(mu_mu),
               empiricalHyperPriors = FALSE,
               speciationRatePriorMean = mu_lambda,
               speciationRatePriorStDev = std_lambda,
               extinctionRatePriorMean = mu_mu,
               extinctionRatePriorStDev = std_mu,
               numExpectedRateChanges = 2,
               samplingProbability = rho,
               numExpectedMassExtinctions = 2,
               BURNIN = 100,
               MAX_ITERATIONS = 200,
               THINNING = 10,
               dir = "analysis_conifer")

# You may want to look into the vignette for a more detailed description
# of the features for an analysis.
# also have a look at the functions tess.process.output and tess.plot.output
```

`tess.likelihood` *tess.likelihood: Probability density of a tree under a tree-wide time-dependent birth-death process*

Description

tess.likelihood computes the probability of a reconstructed phylogenetic tree under time-dependent diversification rates. The rates may be any positive function of time or a constant. Additionally, mass-extinction event can be provided and a uniform taxon sampling probability. You have several options for the start of the process (origin vs MRCA) and the condition of the process (time, survival or taxa; note that survival and taxa implicitly condition on the time too!). See equation (5) in Hoehna (2013) for more information. Note that constant rates lead to much faster computations. The likelihood can be computed for incompletely sampled trees if you give a sampling probability != 1.0. You have two options for the sampling strategy: uniform|diversified. The detailed description of these can be found in the references. More information can be obtained in the vignette about how to apply this likelihood function.

Usage

```
tess.likelihood(times,
                lambda,
```

```
                mu,
                massExtinctionTimes=c(),
                massExtinctionSurvivalProbabilities=c(),
                missingSpecies = c(),
                timesMissingSpecies = c(),
                samplingProbability=1.0,
                samplingStrategy="uniform",
                MRCA=TRUE,
                CONDITION="survival",
                log=TRUE)
```

Arguments

`times`	The branching times of the phylogeny.
`lambda`	The speciation rate function or constant.
`mu`	The extinction rate function or constant.
`massExtinctionTimes`	The set of mass-extinction times after the start of the process.
`massExtinctionSurvivalProbabilities`	The set of survival probabilities for each speciation event. The set must have the same length as the set of mass-extinction times.
`missingSpecies`	The number of species missed which originated in a given time interval (empirical taxon sampling).
`timesMissingSpecies`	The times intervals of the missing species (empirical taxon sampling).
`samplingProbability`	The probability for a species to be included in the sample.
`samplingStrategy`	The strategy how samples were obtained. Options are: uniform|diversified|age.
`MRCA`	Does the process start with the most recent common ancestor? If not, the tree must have a root edge!
`CONDITION`	do we condition the process on time|survival|taxa?
`log`	Should we log-transform the likelihood?

Value

Returns the (log) probability of the tree, i.e. the likelihood of the parameters given the tree.

Author(s)

Sebastian Hoehna

References

S. Hoehna: Fast simulation of reconstructed phylogenies under global, time-dependent birth-death processes. 2013, Bioinformatics, 29:1367-1374

S. Hoehna: Likelihood Inference of Non-Constant Diversification Rates with Incomplete Taxon Sampling. 2014, PLoS one, Public Library of Science, 9, e84184.

S. Hoehna: The time-dependent reconstructed evolutionary process with a key-role for mass-extinction events. 2015, Journal of Theoretical Biology, 380, 321-331.

Examples

```
# load a test data set
data(cettiidae)

# convert the phylogeny into the branching times
times <- as.numeric( branching.times(cettiidae) )

# construct speciation and extinction rate function that resemble the rate-shift
# any other function could be used too
l <- Vectorize(function(x) { if (x > 0.5 || x < 0.3) { return (1) } else { return (2) } })
e <- Vectorize(function(x) { if (x > 0.5 || x < 0.3) { return (0.95) } else { return (0.5) } })

# now compute the likelihood for the tree
tess.likelihood(times,l,e,MRCA=TRUE,log=TRUE)

# a second approach is the specific episodic birth-death process likelihood function
# we need to give the rates for each episode and the end time of the episodes
# you should see that both are equivalent in this setting
# the function approach is more general but also slower.
tess.likelihood.rateshift(times,
    lambda=c(2,1,2),
    mu=c(0.95,0.5,0.95),
    rateChangeTimesLambda=c(0.3,0.5),
    rateChangeTimesMu=c(0.3,0.5),
    MRCA=TRUE,
    log=TRUE)
```

`tess.likelihood.rateshift`

tess.likelihood.rateshift: Probability density of a tree under a tree-wide time-dependent birth-death-shift process

---

Description

tess.likelihood.rateshift computes the probability of a reconstructed phylogenetic tree under a rate-shift model. The rates are piecewise constant. Additionally, mass-extinction event can be provided and a uniform taxon sampling probability. You have several options for the start of the process (origin vs MRCA) and the condition of the process (time, survival or taxa; note that survival and taxa implicitly condition on the time too!). See equation (5) in the manuscript for more information. Note that constant rates lead to much faster computations. The likelihood can be computed for incompletely sampled trees. You need to give a sampling probability != 1.0. You have three options

for the sampling strategy: uniform|diversified|age. The detailed description of these can be found in the references. More information can be obtained in the vignette about how to apply this likelihood function.

Usage

```
tess.likelihood.rateshift( times,
     lambda,
     mu,
     rateChangeTimesLambda = c(),
     rateChangeTimesMu = c(),
     massExtinctionTimes = c(),
        massExtinctionSurvivalProbabilities = c(),
                 missingSpecies = c(),
                 timesMissingSpecies = c(),
     samplingStrategy = "uniform",
        samplingProbability = 1,
     MRCA = TRUE,
        CONDITION = "survival",
     log = TRUE)
```

Arguments

times	The branching times of the tree.
lambda	The speciation rate as a vector representing the rate for each time interval.
mu	The extinction rate as a vector representing the rate for each time interval.
rateChangeTimesLambda	The times of the rate-shifts for the speciation rate.
rateChangeTimesMu	The times of the rate-shifts for the extinction rate.
massExtinctionTimes	The set of mass-extinction times after the start of the process.
massExtinctionSurvivalProbabilities	The set of survival probabilities for each speciation event. The set must have the same length as the set of mass-extinction times.
missingSpecies	The number of species missed which originated in a given time interval (empirical taxon sampling).
timesMissingSpecies	The times intervals of the missing species (empirical taxon sampling).
samplingStrategy	The strategy how samples were obtained. Options are: uniform|diversified|age.
samplingProbability	The probability for a species to be included in the sample.
MRCA	Does the process start with the most recent common ancestor? If not, the tree must have a root edge!
CONDITION	do we condition the process on time|survival|taxa?
log	should the likelihood be in log-scale?

Value

Returns the (log) probability of the tree, i.e., the likelihood of the parameters given the tree.

Author(s)

Sebastian Hoehna

References

S. Hoehna: The time-dependent reconstructed evolutionary process with a key-role for mass-extinction events. 2015, Journal of Theoretical Biology, 380, 321-331.

Examples

```
# load a test data set
data(cettiidae)

# convert the phylogeny into the branching times
times <- as.numeric( branching.times(cettiidae) )

# construct speciation and extinction rate function that resemble the rate-shift
# any other function could be used too
l <- Vectorize(function(x) { if (x > 0.5 || x < 0.3) { return (1) } else { return (2) } })
e <- Vectorize(function(x) { if (x > 0.5 || x < 0.3) { return (0.95) } else { return (0.5) } })

# now compute the likelihood for the tree
tess.likelihood(times,l,e,MRCA=TRUE,log=TRUE)

# a second approach is the specific episodic birth-death process likelihood function
# we need to give the rates for each episode and the end time of the episodes
# you should see that both are equivalent in this setting
# the function approach is more general but also slower.
tess.likelihood.rateshift(times,
    lambda=c(2,1,2),
    mu=c(0.95,0.5,0.95),
    rateChangeTimesLambda=c(0.3,0.5),
    rateChangeTimesMu=c(0.3,0.5),
    MRCA=TRUE,
    log=TRUE)
```

`tess.mcmc` *tess.mcmc: Markov chain Monte Carlo simulation using a general Metropolis-Hastings algorithm.*

Description

tess.mcmc constructs a Markov chain Monte Carlo sampler (MCMC) by implementing a general Metropolis-Hastings algorithm. Any model can be used where the likelihood is known and thus can be passed in as an argument. The parameters have to be continuous. Proposals are taken from a normal distribution centered around the current value. The varaince of the new proposed values is initalized with 1 but can be automatically optimized when using the option adaptive = TRUE. The algorithm creates sampels from the posterior probility distribution and returns these a CODA mcmc object. More information can be obtained in the vignette about how to apply this method.

Usage

```
tess.mcmc(likelihoodFunction,priors,parameters,logTransforms,delta,
            iterations,burnin=round(iterations/3),thinning=1,
            adaptive=TRUE,verbose=FALSE)
```

Arguments

likelihoodFunction	The log-likelihood function which will be called internally by likelihoodFunction(parameters).
priors	A list of functions of the log-prior-densities of each parameter.
parameters	The initial parameter value list.
logTransforms	A vector of booleans telling if log-transform for the parameters should be used (e.g. for rates).
delta	The variance of new proposed values.
iterations	The number of iterations for the MCMC.
burnin	The number of iterations to burn before starting the MCMC.
thinning	The frequency of taking a sample of the parameters.
adaptive	Should we use adaptive MCMC?
verbose	Do you want detailed information during the run?

Value

Returns the posterior samples for the parameters.

Author(s)

Sebastian Hoehna

References

S. Hoehna: Fast simulation of reconstructed phylogenies under global, time-dependent birth-death processes. 2013, Bioinformatics, 29:1367-1374.

S. Hoehna, MR May and BR Moore: TESS: Bayesian inference of lineage diversification rates from (incompletely sampled) molecular phylogenies in R. 2015, Bioinformatics.

Examples

```
# load in a test data set
data(cettiidae)

# convert the phylogeny into the branching times
times <- as.numeric( branching.times(cettiidae) )

# specify a likelihood function that takes in a vector of parameters
likelihood <- function(params) {
  # We use the parameters as diversification rate and turnover rate.
  # Thus we need to transform first
  b <- params[1] + params[2]
  d <- params[2]

  lnl <- tess.likelihood(times,b,d,samplingProbability=1.0,log=TRUE)
  return (lnl)
}

# specify a the prior functions
prior.diversification <- function(x) { dexp(x,rate=0.1,log=TRUE) }
prior.turnover <- function(x) { dexp(x,rate=0.1,log=TRUE) }
priors <- c(prior.diversification,prior.turnover)

# Note, the number of iterations and the burnin is too small here
# and should be adapted for real analyses
samples <- tess.mcmc( likelihood,
        priors,
        runif(2,0,1),
        logTransforms=c(TRUE,TRUE),
        delta=c(0.1,0.1),
        iterations=100,
        burnin=20)

# now summarize and visualize the results
#plot(samples)
summary(samples)
colMeans(samples)
```

`tess.nTaxa.expected` *tess.nTaxa.expected: The expected number of taxa at present of a tree under a global, time-dependent birth-death process (E[N(T)])*

Description

tess.nTaxa.expected computes the expected number of taxa at the present time T (the process start at time s and times increases until the present) under time-dependent. The rates may be any positive function of time or a constant. Additionally, mass-extinction event can be provided and a uniform

taxon sampling probability. You have several options for the start of the process (origin vs MRCA). One important feature is that you can compute the expected number of taxa under the reconstructed process, that is, only lineages that survive until the present.

Usage

```
tess.nTaxa.expected( begin,
      t,
      end,
      lambda,
      mu,
      massExtinctionTimes=c(),
      massExtinctionSurvivalProbabilities=c(),
      samplingProbability=1.0,
      MRCA=TRUE,
      reconstructed=FALSE)
```

Arguments

`begin`	The time when the process starts.
`t`	The time at which we want to know the expected number of lineages (could be equal to end).
`end`	The time when the process end (e.g. the present).
`lambda`	The speciation rate function or constant.
`mu`	The extinction rate function or constant.
`massExtinctionTimes`	The set of mass-extinction times after the start of the process.
`massExtinctionSurvivalProbabilities`	The set of survival probabilities for each speciation event. The set must have the same length as the set of mass-extinction times.
`samplingProbability`	The probability for a species to be included in the sample.
`MRCA`	Does the process start with the most recent common ancestor? If not, the tree must have a root edge!
`reconstructed`	Are we computing the expected number of lineage at time t in the reconstructed process?

Value

Returns the expected number of taxa.

Author(s)

Sebastian Hoehna

References

S. Hoehna: Fast simulation of reconstructed phylogenies under global, time-dependent birth-death processes. 2013, Bioinformatics, 29:1367-1374

Examples

```
# create the time-dependent speciation and extinction rate functions
# here we use episodic functions
l <- Vectorize(function(x) { if (x > 0.5 || x < 0.3) { return (1) } else { return (2) } })
e <- Vectorize(function(x) { if (x > 0.5 || x < 0.3) { return (0.95) } else { return (0.5) } })

# now we can compute the expected number of taxa at time t
# note that we compute here the actual diversity at time t
# if you set reconstructed=TRUE, then you get the expected
# number of lineages that will survive until the present
tess.nTaxa.expected(begin=0,t=2,end=5,l,e,MRCA=TRUE)
```

`tess.pathSampling` *tess.pathSampling: Marginal likelihood estimation via Path-Sampling.*

Description

tess.pathSampling uses a power posterior series and path-sampling to estimate the marginal likelihood of a model. This is a very general implementation of this algorithm which can be applied basically to any model. More information can be obtained in the vignette about how to apply this method.

Usage

```
tess.pathSampling(likelihoodFunction,priorFunction,parameters,logTransforms,
                          iterations,burnin=round(iterations/3),K=50)
```

Arguments

`likelihoodFunction`	The log-likelihood function which will be called internally by likelihoodFunction(parameters).
`priorFunction`	A list of functions of the log-prior-densities of each parameter.
`parameters`	The initial parameter value list.
`logTransforms`	A vector of booleans telling if log-transform for the parameters should be used (e.g. for rates).
`iterations`	The number of iterations for the MCMC.
`burnin`	The number of iterations to burn before starting the MCMC.
`K`	The number of stepping stones.

Value

Returns the posterior samples for the parameters.

Author(s)

Sebastian Hoehna

References

Lartillot, N. and Philippe, H., 2006: Computing Bayes factors using thermodynamic integration. Systematic Biology, 55, 195

Baele et al., 2012: Improving the accuracy of demographic and molecular clock model comparison while accommodating phylogenetic uncertainty

Baele et al., 2013: Accurate Model Selection of Relaxed Molecular Clocks in Bayesian Phylogenetics

Examples

```
# load a test data set
data(cettiidae)
# convert the phylogeny into the branching times
times <- as.numeric( branching.times(cettiidae) )

# construct a likelihood function taking in a vector of parameters
likelihood <- function(params) {
  # We use the parameters as diversification rate and turnover rate.
  # Thus we need to transform first
  b <- params[1] + params[2]
  d <- params[2]

  lnl <- tess.likelihood(times,b,d,samplingProbability=1.0,log=TRUE)
  return (lnl)
}

# next, create the prior density functions
prior_diversification <- function(x) { dexp(x,rate=0.1,log=TRUE) }
prior_turnover <- function(x) { dexp(x,rate=0.1,log=TRUE) }
priors <- c(prior_diversification,prior_turnover)

# Note, the number of iterations, the burnin
# and the number of stepping stones is too small here
# and should be adapted for real analyses
marginalLikelihood <- tess.pathSampling( likelihood,
        priors,
        runif(2,0,1),
        c(TRUE,TRUE),
        10,
        10,
        K=4)
```

`tess.plot.multichain.diagnostics` *tess.plot.multichain.diagnostics: Plotting the mcmc diagnostics of a episodic diversification rate analysis with mass-extinction events.*

Description

tess.plot.multichain.diagnostics plots MCMC diagnostics for the output generated by a tess.process.output(...) command. Fore more examples see the vignette.

Usage

```
tess.plot.multichain.diagnostics(outputs,
                                 parameters=c("speciation rates",
                                              "speciation shift times",
                                              "extinction rates",
                                              "extinction shift times",
                                              "net-diversification rates",
                                              "relative-extinction rates",
                                              "mass extinction times"),
                                 diagnostics="Gelman-Rubin",
                                 gelman.crit=1.05,
                                 xlab="million years ago",
                                 col=NULL,
                                 xaxt="n",
                                 yaxt="s",
                                 pch=19,
                                 ...)
```

Arguments

`outputs`	The processed output for plotting.
`parameters`	Which parameters to diagnose. See details for a complete description.
`diagnostics`	Which diagnostics to use. Currently the only option is "Rubin-Gelman".
`gelman.crit`	The critical value above which a Rubin-Gelman statistic is considered a failure.
`xlab`	The label of the x-axis. By default, millions of years.
`col`	Colors used for printing. Must be of same length as fig.types.
`xaxt`	The type of x-axis to plot. By default, no x-axis is plotted (recommended).
`yaxt`	The type of y-axis to plot.
`pch`	The type of points to draw (if points are drawn).
`...`	Arguments delegated to plot()

Details

This function generates visual summaries of multi-chain MCMC diagnostics for the CoMET analysis in the output object. The argument parameters specifies the aspects of the model to summarize. Valid options are:

- speciation rates: Plots the interval-specific speciation rates.
- speciation shift times: Plots the posterior probability of at least one speciation-rate shift for each interval.
- extinction rates: Plots the interval-specific extinction rates.
- extinction shift times: Plots the posterior probability of at least one extinction-rate shift for each interval.
- net-diversification rates: Plots the interval-specific net-diversification rates.
- relative-extinction rates: Plots the interval-specific relative-extinction rates.
- mass extinction times: Plots the posterior probability of at least one mass-extinction event for each interval.

Author(s)

Michael R. May

Examples

```
# Load the data, compute the sampling fraction rho
data(conifers)
totalConiferSpecies <- 630
sampledConiferSpecies <- conifers$Nnode+1
rho <- sampledConiferSpecies / totalConiferSpecies

# Run a tess analysis
tess.analysis(tree = conifers,
              initialSpeciationRate=c(1.0),
              initialExtinctionRate=c(0.5),
              empiricalHyperPriors = FALSE,
              numExpectedRateChanges = 2,
              numExpectedMassExtinctions = 2,
              samplingProbability = rho,
              MAX_ITERATIONS = 200,
              BURNIN = 100,
              dir = "./run_1")

tess.analysis(tree = conifers,
              initialSpeciationRate=c(1.0),
              initialExtinctionRate=c(0.5),
              empiricalHyperPriors = FALSE,
              numExpectedRateChanges = 2,
              numExpectedMassExtinctions = 2,
              samplingProbability = rho,
              MAX_ITERATIONS = 200,
              BURNIN = 100,
```

```
              dir = "./run_2")

# Process the output
coniferOutput_1 <- tess.process.output(dir="./run_1",
                                       numExpectedRateChanges=2,
                                       numExpectedMassExtinctions=2)

coniferOutput_2 <- tess.process.output(dir="./run_2",
                                       numExpectedRateChanges=2,
                                       numExpectedMassExtinctions=2)

# Plot the output
outputs <- list(coniferOutput_1,coniferOutput_2)
tess.plot.multichain.diagnostics(outputs)
```

`tess.plot.output` *tess.plot.output: Plotting the output of a diversification rate estimation including mass-extinction events.*

Description

tess.output.summary plots the output generated by a tess.process.output(...) command. More specifically, you can plot the speciation, extinction, diversification and relative extinction rate over time, as well as the probability and Bayes factor for the timing of rate shifts and mass-extinction events. For more examples see the vignette.

Usage

```
tess.plot.output(output,
                 fig.types=c("speciation rates",
                             "speciation shift times",
                             "speciation Bayes factors",
                             "extinction rates",
                             "extinction shift times",
                             "extinction Bayes factors",
                             "net-diversification rates",
                             "relative-extinction rates",
                             "mass extinction times",
                             "mass extinction Bayes factors"),
                 xlab="million years ago",
                 col=NULL,
                 col.alpha=50,
                 xaxt="n",
                 yaxt="s",
                 pch=19,
                 plot.tree=FALSE,
                           ...)
```

Arguments

output	The processed output for plotting.
fig.types	Which aspects of the model to visualize. See details for a complete description.
xlab	The label of the x-axis. By default, millions of years.
col	Colors used for printing. Must be of same length as fig.types.
col.alpha	Alpha channel parameter for credible intervals.
xaxt	The type of x-axis to plot. By default, no x-axis is plotted (recommended).
yaxt	The type of y-axis to plot.
pch	The type of points to draw (if points are drawn).
plot.tree	Are we plotting the tree too?
...	Arguments delegated to plot()

Details

This function generates visual summaries of the CoMET analysis in the output object. The argument fig.types specifies the aspects of the model to summarize. Valid options are:

- speciation rates: Plots the interval-specific speciation rates.
- speciation shift times: Plots the posterior probability of at least one speciation-rate shift for each interval.
- speciation Bayes factors: Plots the Bayes factor support for at least one speciation-rate shift for each interval (as 2 ln BF).
- extinction rates: Plots the interval-specific extinction rates.
- extinction shift times: Plots the posterior probability of at least one extinction-rate shift for each interval.
- extinction Bayes factors: Plots the Bayes factor support for at least one extinction-rate shift for each interval (as 2 ln BF).
- net-diversification rates: Plots the interval-specific net-diversification rates.
- relative-extinction rates: Plots the interval-specific relative-extinction rates.
- mass extinction times: Plots the posterior probability of at least one mass-extinction event for each interval.
- mass extinction Bayes factors: Plots the Bayes factor support for at least one mass-extinction event for each interval (as 2 ln BF).

Author(s)

Michael R. May

Examples

```
# Load the data, compute the sampling fraction rho
data(conifers)
totalConiferSpecies <- 630
sampledConiferSpecies <- conifers$Nnode+1
rho <- sampledConiferSpecies / totalConiferSpecies

# Run a tess analysis
tess.analysis(tree = conifers,
              initialSpeciationRate=c(1.0),
              initialExtinctionRate=c(0.5),
              empiricalHyperPriors = FALSE,
              numExpectedRateChanges = 2,
              numExpectedMassExtinctions = 2,
              samplingProbability = rho,
              MAX_ITERATIONS = 200,
              BURNIN = 100)

# Process the output
coniferOutput <- tess.process.output(dir=getwd(),
                                     numExpectedRateChanges=2,
                                     numExpectedMassExtinctions=2)

# Plot the output
tess.plot.output(coniferOutput)
```

---

tess.plot.singlechain.diagnostics

tess.plot.mcmc.diagnostics: Plotting the single chain mcmc diagnostics of a episodic diversification rate analysis with mass-extinction events.

Description

tess.plot.singlechain.diagnostics plots MCMC diagnostics for the output generated by a tess.process.output(...) command. Fore more examples see the vignette.

Usage

```
tess.plot.singlechain.diagnostics(output,
                                  parameters=c("speciation rates",
                                               "speciation shift times",
                                               "extinction rates",
                                               "extinction shift times",
                                               "net-diversification rates",
                                               "relative-extinction rates",
                                               "mass extinction times"),
                                  diagnostics=c("ESS","geweke"),
                                  ess.crit=c(100,200),
```

```
                                    geweke.crit=0.05,
                                    correction="bonferroni",
                                    xlab="million years ago",
                                    col=NULL,
                                    xaxt="n",
                                    yaxt="s",
                                    pch=19,
                                    ...)
```

Arguments

output	The processed output for plotting.
parameters	Which parameters to diagnose. See details for a complete description.
diagnostics	Which diagnostics to use. Options are "ESS" and "geweke".
ess.crit	Two values which correspond to low ESS threshold and acceptable ESS threshold. Default values are 100 and 200.
geweke.crit	The p-value cutoff for Geweke's diagnostic. Default is the canonical 0.05.
correction	What type of multiple-correction method to use. Options are "bonferroni" and "sidak".
xlab	The label of the x-axis. By default, millions of years.
col	Colors used for printing. Must be of same length as fig.types.
xaxt	The type of x-axis to plot. By default, no x-axis is plotted (recommended).
yaxt	The type of y-axis to plot.
pch	The type of points to draw (if points are drawn).
...	Arguments delegated to plot()

Details

This function generates visual summaries of single-chain MCMC diagnostics for the CoMET analysis in the output object. The argument parameters specifies the aspects of the model to summarize. Valid options are:

- speciation rates: Plots the interval-specific speciation rates.
- speciation shift times: Plots the posterior probability of at least one speciation-rate shift for each interval.
- extinction rates: Plots the interval-specific extinction rates.
- extinction shift times: Plots the posterior probability of at least one extinction-rate shift for each interval.
- net-diversification rates: Plots the interval-specific net-diversification rates.
- relative-extinction rates: Plots the interval-specific relative-extinction rates.
- mass extinction times: Plots the posterior probability of at least one mass-extinction event for each interval.

Author(s)

Michael R. May

Examples

```
# Load the data, compute the sampling fraction rho
data(conifers)
totalConiferSpecies <- 630
sampledConiferSpecies <- conifers$Nnode+1
rho <- sampledConiferSpecies / totalConiferSpecies

# Run a tess analysis
tess.analysis(tree = conifers,
              initialSpeciationRate=c(1.0),
              initialExtinctionRate=c(0.5),
              empiricalHyperPriors = FALSE,
              numExpectedRateChanges = 2,
              numExpectedMassExtinctions = 2,
              samplingProbability = rho,
              MAX_ITERATIONS = 200,
              BURNIN = 100)

# Process the output
coniferOutput <- tess.process.output(dir=getwd(),
                                     numExpectedRateChanges=2,
                                     numExpectedMassExtinctions=2)

# Plot the output
tess.plot.singlechain.diagnostics(coniferOutput)
```

---

tess.PosteriorPrediction

tess.PosteriorPrediction: Approximation of the posterior predictive distribution.

Description

tess.PosteriorPrediction calls the simulation function exactly once for each sampled parameter combination. In that way, posterior predictive simulations can be obtained which then in turn can be used to compute summary statistics based on these posterior predictive simulations. Fore more information see the vignette.

Usage

```
tess.PosteriorPrediction(simulationFunction,parameters,burnin)
```

Arguments

simulationFunction	The simulation function which will be called internally by simulationFunction(parameters).
parameters	A matrix of parameters where the rows represent samples of parameters and the column the different parameters.
burnin	The fraction of samples to be discarded as burnin. This is 0.25 by default

Value

Returns samples simulated from the posterior predictive distribution.

Author(s)

Sebastian Hoehna

References

S. Hoehna: Fast simulation of reconstructed phylogenies under global, time-dependent birth-death processes. 2013, Bioinformatics, 29:1367-1374

Examples

```
# We first run an MCMC to obtain samples from the posterior distribution
# and then simulate the posterior predictive distribution.

# The bird phylogeny as the test data set
data(cettiidae)
times <- as.numeric( branching.times(cettiidae) )

# The log-likelihood function
likelihood <- function(params) {
  # We use the parameters as diversification rate and turnover rate.
  # Thus we need to transform first
  b <- params[1] + params[2]
  d <- params[2]

  lnl <- tess.likelihood(times,b,d,samplingProbability=1.0,log=TRUE)
  return (lnl)
}

prior_diversification <- function(x) { dexp(x,rate=0.1,log=TRUE) }
prior_turnover <- function(x) { dexp(x,rate=0.1,log=TRUE) }
priors <- c(prior_diversification,prior_turnover)

# Note, the number of iterations and the burnin is too small here
# and should be adapted for real analyses
samples <- tess.mcmc(likelihood,priors,c(1,0.1),c(TRUE,TRUE),c(0.1,0.1),10,10)

tmrca <- max(branching.times(cettiidae))
# The simulation function
sim <- function(params) {
```

```
  # We use the parameters as diversification rate and turnover rate.
  # Thus we need to transform first
  b <- params[1] + params[2]
  d <- params[2]

  tree <- tess.sim.age(n=1,age=tmrca,b,d,samplingProbability=1.0)[[1]]
  return (tree)
}

trees <- tess.PosteriorPrediction(sim,samples)

# compute the posterior predictive test statistic
ppt <- tess.PosteriorPredictiveTest(trees,cettiidae,gammaStat)
# get the p-value of the observed test-statistic
ppt[[2]]
```

`tess.PosteriorPredictiveTest` *tess.PosteriorPredictiveTest: Approximation of the posterior predictive distribution.*

Description

tess.PosteriorPredictiveTest computes the values of the statistic for the posterior predictive simulations and computes the p-value for the observed statistic.

Usage

```
tess.PosteriorPredictiveTest(samples,observation,statistic)
```

Arguments

`samples`	Samples from the posterior predictive distribution.
`observation`	The observed value.
`statistic`	The function that computes the statistic.

Value

Returns a list of the statistic for each sample.

Author(s)

Sebastian Hoehna

References

S. Hoehna: Fast simulation of reconstructed phylogenies under global, time-dependent birth-death processes. 2013, Bioinformatics, 29:1367-1374

Examples

```
# We first run an MCMC to obtain samples from the posterior distribution
# and then simulate the posterior predictive distribution.

# The bird phylogeny as the test data set
data(cettiidae)
times <- as.numeric( branching.times(cettiidae) )

# The log-likelihood function
likelihood <- function(params) {
  # We use the parameters as diversification rate and turnover rate.
  # Thus we need to transform first
  b <- params[1] + params[2]
  d <- params[2]

  lnl <- tess.likelihood(times,b,d,samplingProbability=1.0,log=TRUE)
  return (lnl)
}

prior_diversification <- function(x) { dexp(x,rate=0.1,log=TRUE) }
prior_turnover <- function(x) { dexp(x,rate=0.1,log=TRUE) }
priors <- c(prior_diversification,prior_turnover)

# Note, the number of iterations and the burnin is too small here
# and should be adapted for real analyses
samples <- tess.mcmc(likelihood,priors,c(1,0.1),c(TRUE,TRUE),c(0.1,0.1),10,10)

tmrca <- max(branching.times(cettiidae))
# The simulation function
sim <- function(params) {
  # We use the parameters as diversification rate and turnover rate.
  # Thus we need to transform first
  b <- params[1] + params[2]
  d <- params[2]

  # We need trees with at least three tips for the gamma-statistics
  repeat {
    tree <- tess.sim.age(n=1,age=tmrca,b,d,samplingProbability=1.0,MRCA=TRUE)[[1]]
    if (tree$Nnode > 1) break
  }
  return (tree)
}

# simulate trees from the posterior predictive distribution
trees <- tess.PosteriorPrediction(sim,samples)

# compute the posterior predictive test statistic
ppt <- tess.PosteriorPredictiveTest(trees,cettiidae,gammaStat)
# get the p-value of the observed test-statistic
ppt[[2]]
```

tess.process.output	*tess.process.output: Summarizing the output of a diversification rate estimation including mass-extinction events. See the tess.analysis function for more information on how such output is generated and the tess.plot.output how the output can be visualized. Also have a look at the vignette for more in detail description and examples.*

Description

tess.process.output summarizes the output generated by a tess.analysis(...) run.

Usage

```
tess.process.output(dir,
                    tree=NULL,
                    numExpectedRateChanges=2,
                    numExpectedMassExtinctions=2,
                    burnin=0.25,
                    numIntervals=100,
                    criticalBayesFactors=c(2,6,10))
```

Arguments

dir	The directory from which the CoMET output will be read.
tree	The tree analyzed with CoMET in phylo format. By default, looks for a tree in the target directory.
numExpectedRateChanges	The number of expected diversification-rate changes.
numExpectedMassExtinctions	The number of expected mass-extinction events.
burnin	The fraction of samples that will be discarded as burnin.
numIntervals	The number of discrete intervals in which to break the tree.
criticalBayesFactors	The Bayes factor thresholds to use to assess significance of events.

Details

The output of a CoMET analysis is stored in a directory with different files containing the MCMC samples from the posterior distribution. For example, the tess.analysis function stores the times and survival probabilities of the mass-extinction events in a file. This function, converts the output by counting the number of events that fall into a given time-bin. This pre-processing of the output simplifies the plotting.

Value

This function returns a list with the following elements:

`posterior` An object of class 'mcmc' that contains the trace of the model's posterior probability.

`numSpeciationCategories`
An object of class 'mcmc' that contains samples from the posterior distribution of the number of speciation categories (minimum 1, since this includes the initial speciation rate).

`numExtinctionCategories`
An object of class 'mcmc' that contains samples from the posterior distribution of the number of extinction categories (minimum 1, since this includes the initial extinction rate).

`numMassExtinctions`
An object of class 'mcmc' that contains samples from the posterior distribution of the number of mass-extinction events.

`speciation rates`
An object of class 'mcmc' that contains speciation rates sampled from the posterior distribution for each of numIntervals discrete time intervals. Rows correspond to samples from the posterior distribution, columns correspond to intervals.

`speciation change times`
An object of class 'mcmc' that contains speciation-rate-change events sampled from the posterior distribution for each of numIntervals discrete time intervals. A value of 1 indicates an event was contained in the interval, 0 that no event was contained in the interval. Rows correspond to samples from the posterior distribution, columns correspond to intervals.

`speciation Bayes factors`
A vector of class 'numeric' that contains the Bayes factor support for there being a speciation-rate-change event for each of numIntervals discrete time intervals. The ith element corresponds to the Bayes factor support for an event in the ith interval.

`speciationRateChangeCriticalPosteriorProbabilities`
A vector of posterior probabilities that correspond to critical Bayes factor thresholds (specified by the argument criticalBayesFactors). Element i is the posterior probability of a speciation-rate-change event in an interval needed to produce Bayes factor support of criticalBayesFactors[i].

`extinction rates`
An object of class 'mcmc' that contains extinction rates sampled from the posterior distribution for each of numIntervals discrete time intervals. Rows correspond to samples from the posterior distribution, columns correspond to intervals.

`extinction change times`
An object of class 'mcmc' that contains extinction-rate-change events sampled from the posterior distribution for each of numIntervals discrete time intervals. A value of 1 indicates an event was contained in the interval, 0 that no event was contained in the interval. Rows correspond to samples from the posterior distribution, columns correspond to intervals.

`extinction Bayes factors`
: A vector of class 'numeric' that contains the Bayes factor support for there being a extinction-rate-change event for each of numIntervals discrete time intervals. The ith element corresponds to the Bayes factor support for an event in the ith interval.

`extinctionRateChangeCriticalPosteriorProbabilities`
: A vector of posterior probabilities that correspond to critical Bayes factor thresholds (specified by the argument criticalBayesFactors). Element i is the posterior probability of a extinction-rate-change event in an interval needed to produce Bayes factor support of criticalBayesFactors[i].

`net-diversification rates`
: An object of class 'mcmc' that contains net-diversification (speciation - extinction) rates sampled from the posterior distribution for each of numIntervals discrete time intervals. Rows correspond to samples from the posterior distribution, columns correspond to intervals.

`relative-extinction rates`
: An object of class 'mcmc' that contains relative-extinction (extinction / speciation) rates sampled from the posterior distribution for each of numIntervals discrete time intervals. Rows correspond to samples from the posterior distribution, columns correspond to intervals.

`mass extinction times`
: An object of class 'mcmc' that contains mass-extinction events sampled from the posterior distribution for each of numIntervals discrete time intervals. A value of 1 indicates an event was contained in the interval, 0 that no event was contained in the interval. Rows correspond to samples from the posterior distribution, columns correspond to intervals.

`mass extinction Bayes factors`
: A vector of class 'numeric' that contains the Bayes factor support for there being a mass-extinction event for each of numIntervals discrete time intervals. The ith element corresponds to the Bayes factor support for an event in the ith interval.

`massExtinctionCriticalPosteriorProbabilities`
: A vector of posterior probabilities that correspond to critical Bayes factor thresholds (specified by the argument criticalBayesFactors). Element i is the posterior probability of a mass-extinction event in an interval needed to produce Bayes factor support of criticalBayesFactors[i].

`criticalBayesFactors`
: The critical Bayes factor values used for the Bayes factor tests (default 2 ln BF = {2,6,10}).

`tree`
: The tree analyzed with CoMET (just in case).

`intervals`
: The discrete intervals used to compute the interval-specific parameters.

Author(s)

Michael R. May

Examples

```
# Load the data, compute the sampling fraction rho
```

```
data(conifers)
totalConiferSpecies <- 630
sampledConiferSpecies <- conifers$Nnode+1
rho <- sampledConiferSpecies / totalConiferSpecies

# Run a tess analysis
tess.analysis(tree = conifers,
              initialSpeciationRate=c(1.0),
              initialExtinctionRate=c(0.5),
              empiricalHyperPriors = FALSE,
              numExpectedRateChanges = 2,
              numExpectedMassExtinctions = 2,
              samplingProbability = rho,
              MAX_ITERATIONS = 200,
              BURNIN=100)

# Process the output
coniferOutput <- tess.process.output(dir=getwd(),
                                     numExpectedRateChanges=2,
                                     numExpectedMassExtinctions=2)

# Plot the output
tess.plot.output(coniferOutput)
```

`tess.sim.age` *tess.sim.age: Simulate a reconstructed tree for a given age under a global, time-dependent birth-death process.*

Description

tess.sim.age simulates a reconstructed phylogenetic tree under a global, time-dependent birth-death process conditioned on the age of the tree. The rates may be any positive function of time or a constant. The process starts at time 0 and goes forward in time, hence the rates and events should be interpreted in the time after the origin. Additionally, mass-extinction event can be provided and a uniform taxon sampling probability. It is possible to start either with the origin (1 species) or with the most recent common ancestor (2 species).

Usage

```
tess.sim.age(n, age, lambda, mu, massExtinctionTimes = c(),
   massExtinctionSurvivalProbabilities = c(), samplingProbability = 1,
   samplingStrategy = "uniform", maxTaxa = Inf, MRCA = TRUE)
```

Arguments

n	Number of simulations.
age	The age of the tree, i.e. the time to simulate.

`lambda` The speciation rate function or constant.

`mu` The extinction rate function or constant.

`massExtinctionTimes`
The set of mass-extinction times after the start of the process.

`massExtinctionSurvivalProbabilities`
The set of survival probabilities for each speciation event. The set must have the same length as the set of mass-extinction times.

`samplingProbability`
The probability for a species to be included in the sample.

`samplingStrategy`
The strategy how samples were obtained. Options are: uniform|diversified.

`maxTaxa` The maximum number of possible taxa. If by chance a higher number is simulated, than simply ntaxa=maxTaxa. This is useful when too large trees should be simulated because this takes too much time and memory.

`MRCA` Does the process start with the most recent common ancestor?

Value

Returns a set of trees in 'phylo' format.

Author(s)

Sebastian Hoehna

References

S. Hoehna: Fast simulation of reconstructed phylogenies under global, time-dependent birth-death processes. 2013, Bioinformatics, 29:1367-1374

Examples

```
l <- Vectorize(function(x) { if (x > 0.5 || x < 0.3) { return (1) } else { return (2) } })
e <- Vectorize(function(x) { if (x > 0.5 || x < 0.3) { return (0.95) } else { return (0.5) } })

tess.sim.age(n=1,age=1,l,e,MRCA=TRUE)

# simulation under constant rates
tess.sim.age(n=1,age=1,2.0,1.0,MRCA=TRUE)
```

`tess.sim.taxa` *tess.sim.taxa.taxa: Simulate a reconstructed tree for a given number of taxa under a global, time-dependent birth-death process.*

Description

tess.sim.taxa simulates a reconstructed phylogenetic tree under a global, time-dependent birth-death process conditioned on the number of taxa sampled. The rates may be any positive function of time or a constant. The process starts at time 0 and goes forward in time, hence the rates and events should be interpreted in the time after the origin. Additionally, mass-extinction event can be provided and a uniform taxon sampling probability. It is possible to start either with the origin (1 species) or with the most recent common ancestor (2 species).

Usage

```
tess.sim.taxa(n, nTaxa, max, lambda, mu, massExtinctionTimes = c(),
   massExtinctionSurvivalProbabilities = c(), samplingProbability = 1,
   samplingStrategy = "uniform", SURVIVAL = TRUE, MRCA = TRUE, t_crit = c())
```

Arguments

`n`	Number of simulations.
`nTaxa`	Number of species sampled.
`max`	Maximum time/height of the tree.
`lambda`	The speciation rate function or constant.
`mu`	The extinction rate function or constant.
`massExtinctionTimes`	The set of mass-extinction times after the start of the process.
`massExtinctionSurvivalProbabilities`	The set of survival probabilities for each speciation event. The set must have the same length as the set of mass-extinction times.
`samplingProbability`	The probability for a species to be included in the sample.
`samplingStrategy`	The strategy how samples were obtained. Options are: uniform|diversified.
`SURVIVAL`	Do you want to condition on survival of the process?
`MRCA`	Does the process start with the most recent common ancestor?
`t_crit`	The critical time points when a jump in the rate function occurs. Only a help for the numerical integration routine.

Value

Returns a tree in 'phylo' format.

Author(s)

Sebastian Hoehna

References

S. Hoehna: Fast simulation of reconstructed phylogenies under global, time-dependent birth-death processes. 2013, Bioinformatics, 29:1367-1374

Examples

```
l <- Vectorize(function(x) { if (x > 0.5 || x < 0.3) { return (1) } else { return (2) } })
e <- Vectorize(function(x) { if (x > 0.5 || x < 0.3) { return (0.95) } else { return (0.5) } })

tess.sim.taxa(n=1,nTaxa=10,max=10,l,e,MRCA=TRUE)

# simulation under constant rates
tess.sim.taxa(n=1,nTaxa=10,max=10,2.0,1.0,MRCA=TRUE)
```

---

tess.sim.taxa.age — *tess.sim.taxa.taxa.age: Simulate a reconstructed tree for a given age and number of taxa under a global, time-dependent birth-death process.*

Description

tess.sim.taxa.age simulates a reconstructed phylogenetic tree under a global, time-dependent birth-death process conditioned on the age of the tree and number of taxa sampled. The rates may be any positive function of time or a constant. The process starts at time 0 and goes forward in time, hence the rates and events should be interpreted in the time after the origin. Additionally, mass-extinction event can be provided and a uniform taxon sampling probability. It is possible to start either with the origin (1 species) or with the most recent common ancestor (2 species).

Usage

```
tess.sim.taxa.age(n, nTaxa, age, lambda, mu, massExtinctionTimes = c(),
   massExtinctionSurvivalProbabilities = c(), samplingProbability = 1,
   samplingStrategy = "uniform", MRCA = TRUE)
```

Arguments

n	Number of simulations.
nTaxa	Number of species sampled.
age	The age of the tree, i.e. the time to simulate.
lambda	The speciation rate function or constant.
mu	The extinction rate function or constant.

massExtinctionTimes
: The set of mass-extinction times after the start of the process.

massExtinctionSurvivalProbabilities
: The set of survival probabilities for each speciation event. The set must have the same length as the set of mass-extinction times.

samplingProbability
: The probability for a species to be included in the sample.

samplingStrategy
: The strategy how samples were obtained. Options are: uniform|diversified.

MRCA
: Does the process start with the most recent common ancestor?

Value

Returns a tree in 'phylo' format.

Author(s)

Sebastian Hoehna

References

S. Hoehna: Fast simulation of reconstructed phylogenies under global, time-dependent birth-death processes. 2013, Bioinformatics, 29:1367-1374

Examples

```
l <- Vectorize(function(x) { if (x > 0.5 || x < 0.3) { return (1) } else { return (2) } })
e <- Vectorize(function(x) { if (x > 0.5 || x < 0.3) { return (0.95) } else { return (0.5) } })

tess.sim.taxa.age(n=1,l,e,nTaxa=10,age=1,MRCA=TRUE)

# simulation under constant rates
tess.sim.taxa.age(n=1,2.0,1.0,nTaxa=10,age=1,MRCA=TRUE)
```

---

tess.steppingStoneSampling

tess.steppingStoneSampling: Marginal likelihood estimation via Stepping-Stone-Sampling.

Description

tess.steppingStoneSampling uses a power posterior series and stepping-stone-sampling to estimate the marginal likelihood of a model.

Usage

```
tess.steppingStoneSampling(likelihoodFunction,priors,parameters,logTransforms,
                           iterations,burnin=round(iterations/3),K=50)
```

Arguments

likelihoodFunction	The log-likelihood function which will be called internally by likelihoodFunction(parameters).
priors	A list of functions of the log-prior-densities of each parameter.
parameters	The initial parameter value list.
logTransforms	A vector of booleans telling if log-transform for the parameters should be used (e.g. for rates).
iterations	The number of iterations for the MCMC.
burnin	The number of iterations to burn before starting the MCMC.
K	The number of stepping stones.

Value

Returns the posterior samples for the parameters.

Author(s)

Sebastian Hoehna

References

Xie et al., 2011: Improving marginal likelihood estimation for Bayesian phylogenetic model selection Baele et al., 2012: Improving the accuracy of demographic and molecular clock model comparison while accommodating phylogenetic uncertainty Baele et al., 2013: Accurate Model Selection of Relaxed Molecular Clocks in Bayesian Phylogenetics

Examples

```
data(cettiidae)
times <- as.numeric( branching.times(cettiidae) )

likelihood <- function(params) {
  # We use the parameters as diversification rate and turnover rate.
  # Thus we need to transform first
  b <- params[1] + params[2]
  d <- params[2]

  lnl <- tess.likelihood(times,b,d,samplingProbability=1.0,log=TRUE)
  return (lnl)
}

prior_diversification <- function(x) { dexp(x,rate=0.1,log=TRUE) }
prior_turnover <- function(x) { dexp(x,rate=0.1,log=TRUE) }
priors <- c(prior_diversification,prior_turnover)

# Note, the number of iterations, the burnin
# and the number of stepping stones is too small here
# and should be adapted for real analyses
```

```
marginalLikelihood <- tess.steppingStoneSampling( likelihood,
        priors,
        runif(2,0,1),
        c(TRUE,TRUE),
        10,
        10,
        K=4)
```

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