

Package ‘PCMBaseCpp’

March 23, 2020

Type Package

Title Fast Likelihood Calculation for Phylogenetic Comparative Models

Version 0.1.9

Maintainer Venelin Mitov <vmitov@gmail.com>

Description Provides a C++ backend for multivariate phylogenetic comparative models implemented in the R-package 'PCMBase'. Can be used in combination with 'PCMBase' to enable fast and parallel likelihood calculation. Implements the pruning likelihood calculation algorithm described in Mitov et al. (2018) <arXiv:1809.09014>. Uses the 'SPLITT' C++ library for parallel tree traversal described in Mitov and Stadler (2018) <doi:10.1111/2041-210X.13136>.

Encoding UTF-8

License GPL (>= 3.0)

LazyData true

Depends R (>= 3.1.0), Rcpp, methods

Imports PCMBase, data.table, abind

Suggests testthat, knitr, rmarkdown, covr

LinkingTo Rcpp, RcppArmadillo

RoxygenNote 6.1.1

ByteCompile yes

NeedsCompilation yes

URL <https://github.com/venelin/PCMBaseCpp>, <https://venelin.github.io>

BugReports <https://github.com/venelin/PCMBaseCpp/issues>

Repository CRAN

VignetteBuilder knitr, rmarkdown

Author Venelin Mitov [aut, cre, cph] (<[a href="https://venelin.github.io">https://venelin.github.io](https://venelin.github.io)>venelin.github.io)

Date/Publication 2020-03-23 00:50:02 UTC

R topics documented:

benchmarkData	2
benchmarkResults	3
benchmarkResultsNoTransform	3
BenchmarkRvsCpp	4
MiniBenchmarkRvsCpp	5
PCListInt	6
PCMBaseCppIsADevRelease	7
PCMInfoCpp	7
PCMParmGetFullVector	8
PCMTreePreorderCpp	9
Index	10

benchmarkData	<i>Data for performing a benchmark</i>
---------------	--

Description

A dataset containing three triplets trees, trait-values and models to evaluate the likelihood calculation times for R and C++ implementations.

Usage

```
benchmarkData
```

Format

A data frame with 4 rows and 8 variables:

tree phylogenetic tree (phylo) with set edge.regimes member

model MGPM model used to simulate the data in X

X trait values

ll log-likelihood value

modelBM a random BM model

llBM log-likelihood value form modelBM

modelOU a random OU model

llOU log-likelihood value for modelOU

benchmarkResults	<i>Results from running a performance benchmark on a personal computer including the time for parameter transformation</i>
------------------	--

Description

Results from running a performance benchmark on a personal computer including the time for parameter transformation

Usage

benchmarkResults

Format

A data.table

benchmarkResultsNoTransform	<i>Results from running a performance benchmark on a personal computer excluding the time for parameter transformation</i>
-----------------------------	--

Description

Results from running a performance benchmark on a personal computer excluding the time for parameter transformation

Usage

benchmarkResultsNoTransform

Format

A data.table

BenchmarkRvsCpp	<i>A log-likelihood calculation time comparison for different numbers of traits and option-sets</i>
-----------------	---

Description

A log-likelihood calculation time comparison for different numbers of traits and option-sets

Usage

```
BenchmarkRvsCpp(ks = c(1, 2, 4, 8), includeR = TRUE,
  includeTransformationTime = TRUE, optionSets = NULL,
  includeParallelMode = TRUE, doProf = FALSE,
  RprofR.out = "RprofR.out", RprofCpp.out = "RprofCpp.out",
  verbose = FALSE)
```

Arguments

ks	a vector of positive integers, denoting different numbers of traits. Default: <code>c(1, 2, 4, 8)</code> .
includeR	logical (default TRUE) indicating if likelihood calculations in R should be included in the benchmark (can be slow).
includeTransformationTime	logical (default TRUE) indicating if the time for <code>PCMApplTransformation</code> should be included in the benchmark.
optionSets	a named list of lists of PCM-options. If NULL (the default) the option set is set to <code>DefaultBenchmarkOptions(k, includeParallelMode)</code> for each k in ks (see the code in <code>PCMBaseCpp:::DefaultBenchmarkOptions</code>).
includeParallelMode	logical (default TRUE) indicating if the default optionSet should include parallel execution modes, i.e. setting the option <code>PCMBase.Lmr.mode</code> to 21 instead of 11. This argument is taken into account only with the argument <code>optionSets</code> set to NULL (the default).
doProf	logical indicating if profiling should be activated (see <code>Rprof</code> from the <code>utils</code> R-package). Default: FALSE. Additional arguments to <code>Rprof</code> can be specified by assigning lists of arguments to the options <code>'PCMBaseCpp.ArgsRprofR'</code> and <code>'PCMBaseCpp.ArgsRprofCpp'</code> . The default values for both options is <code>list(append = TRUE, line.profiling = TRUE)</code> .
RprofR.out	character strings indicating <code>Rprof.out</code> files for the R and Cpp implementations; ignored if <code>doProf</code> is FALSE. Default values: <code>'RprofR.out'</code> and <code>'Rprofcpp.out'</code> .
RprofCpp.out	character strings indicating <code>Rprof.out</code> files for the R and Cpp implementations; ignored if <code>doProf</code> is FALSE. Default values: <code>'RprofR.out'</code> and <code>'Rprofcpp.out'</code> .
verbose	logical indicating if log-messages should be printed to the console during the benchmark. Default FALSE.

Value

a `data.table` for results similar to the `data.table` returned from `MiniBenchmarkRvsCpp` with additional columns for `k`, option-set and the type of model.

MiniBenchmarkRvsCpp *Evaluate the likelihood calculation times for example trees and data*

Description

Evaluate the likelihood calculation times for example trees and data

Usage

```
MiniBenchmarkRvsCpp(data = PCMBaseCpp::benchmarkData, includeR = TRUE,
  includeTransformationTime = TRUE, nRepsCpp = 10L,
  listOptions = list(PCMBase.Lmr.mode = 11, PCMBase.Threshold.EV = 0,
    PCMBase.Threshold.SV = 0), doProf = FALSE, RprofR.out = "RprofR.out",
  RprofCpp.out = "RprofCpp.out")
```

Arguments

<code>data</code>	a ‘ <code>data.frame</code> ’ with at least the following columns: <ul style="list-style-type: none"> • <code>tree</code>: a list column of phylo objects with an <code>edge.part</code> member set. • <code>X</code>: a list column of <code>k x N</code> numerical matrices. • <code>model</code>: a list column of PCM objects. Defaults: to ‘ <code>benchmarkData</code> ’, which is small <code>data.table</code> included with the <code>PCMBaseCpp</code> package.
<code>includeR</code>	logical (default <code>TRUE</code>) indicating if likelihood calculations in R should be included in the benchmark (can be slow).
<code>includeTransformationTime</code>	logical (default <code>TRUE</code>) indicating if the time for <code>PCMAApplyTransformation</code> should be included in the benchmark.
<code>nRepsCpp</code>	: number of repetitions for the <code>cpp</code> likelihood calculation calls: a bigger value increases the precision of time estimation at the expense of longer running time for the benchmark. Defaults to 10.
<code>listOptions</code>	options to set before measuring the calculation times. Defaults to ‘ <code>list(PCMBase.Lmr.mode = 11, PCMBase.Threshold.EV = 0, PCMBase.Threshold.SV = 0)</code> ’. ‘ <code>PCMBase.Lmr.mode</code> ’ corresponds to the parallel traversal mode for the tree traversal algorithm (see this page for possible values).
<code>doProf</code>	logical indicating if profiling should be activated (see <code>Rprof</code> from the <code>utils</code> R-package). Default: <code>FALSE</code> . Additional arguments to <code>Rprof</code> can be specified by assigning lists of arguments to the options ‘ <code>PCMBaseCpp.ArgsRprofR</code> ’ and ‘ <code>PCMBaseCpp.ArgsRprofCpp</code> ’. The default values for both options is <code>list(append = TRUE, line.profiling = TRUE)</code> .
<code>RprofR.out</code> , <code>RprofCpp.out</code>	character strings indicating <code>Rprof.out</code> files for the R and Cpp implementations; ignored if <code>doProf</code> is <code>FALSE</code> . Default values: ‘ <code>RprofR.out</code> ’ and ‘ <code>Rprofcpp.out</code> ’.

Value

a data.frame.

Examples

```
library(PCMBase)
library(PCMBaseCpp)
library(data.table)

testData <- PCMBaseCpp::benchmarkData[1]
# original MGPM model
MiniBenchmarkRvsCpp(data = testData)

# original MGPM model and parallel mode
MiniBenchmarkRvsCpp(
  data = testData,
  listOptions = list(PCMBase.Lmr.mode = 21, PCMBase.Threshold.EV = 1e-9,
    PCMBase.Threshold.SV = 1e-9))

# single-trait data, original MGPM model and single mode and enabled option
# PCMBase.Use1DClasses
MiniBenchmarkRvsCpp(
  data = PCMBaseCpp::benchmarkData[1, list(
    tree,
    X = lapply(X, function(x) x[1,, drop=FALSE]),
    model = lapply(model, function(m) PCMExtractDimensions(m, dims = 1)))]),
  listOptions = list(
    PCMBase.Lmr.mode = 11,
    PCMBase.Threshold.EV = 1e-9,
    PCMBase.Threshold.SV = 1e-9,
    PCMBase.Use1DClasses = FALSE))
```

PCListInt

Converts the logical matrix pc into a list of vectors denoting the (0-based) TRUE-indices in each column

Description

Converts the logical matrix pc into a list of vectors denoting the (0-based) TRUE-indices in each column

Usage

```
PCListInt(pc)
```

Arguments

pc a logical matrix.

Value

a list

PCMBaseCppIsADevRelease

Check if the PCMBaseCpp version corresponds to a dev release

Description

This function is used during unit-testing, to disable some unit- tests which run extremely long or are consistently failing on some systems.

Usage

```
PCMBaseCppIsADevRelease()
```

Value

a logical

PCMInfoCpp

A S3 generic for creating C++ backend objects given a model, data and a tree.

Description

Replace calls to PCMInfo() with this method in order to use C++ for likelihood calculation.

Usage

```
PCMInfoCpp(X, tree, model, SE = matrix(0, PCMNumTraits(model),
  PCMTreeNumTips(tree)), metaI = PCMInfo(X = X, tree = tree, model =
  model, SE = SE, verbose = verbose, preorder = PCMTreePreorderCpp(tree)),
  verbose = FALSE, ...)
```

Arguments

X	a k x N numerical matrix with possible NA and NaN entries. Each column of X contains the measured trait values for one species (tip in tree). Missing values can be either not-available (NA) or not existing (NaN). These two values have are treated differently when calculating likelihoods: see PCMPresentCoordinates .
tree	a phylo object with N tips.
model	an S3 object specifying both, the model type (class, e.g. "OU") as well as the concrete model parameter values at which the likelihood is to be calculated (see also Details).

SE	a $k \times N$ matrix specifying the standard error for each measurement in X . Alternatively, a $k \times k \times N$ cube specifying an upper triangular $k \times k$ Choleski factor of the variance covariance matrix for the measurement error for each node $i=1, \dots, N$. Default: <code>matrix(0.0, PCMNumTraits(model), PCMTreeNumTips(tree))</code> .
metaI	a list returned from a call to <code>PCMInfo(X, tree, model, SE)</code> , containing meta-data such as N , M and k . Default: <code>PCMInfo(X, tree, model, verbose, preorder=PCMTreePreorderCpp(tree))</code> .
verbose	logical indicating if some debug-messages should be printed. Default: FALSE
...	passed to methods.

Value

a list to be passed to `PCMLik` as argument `metaI`.

Examples

```
metaICpp <- PCMInfoCpp(
  PCMBase::PCMBaseTestObjects$traits.a.123,
  PCMBase::PCMBaseTestObjects$tree.a,
  PCMBase::PCMBaseTestObjects$model.a.123)
PCMBase::PCMLik(
  PCMBase::PCMBaseTestObjects$traits.a.123,
  PCMBase::PCMBaseTestObjects$tree.a,
  PCMBase::PCMBaseTestObjects$model.a.123,
  metaI = metaICpp)
```

`PCMParmGetFullVector` *Get a vector with all model parameters unrolled*

Description

Get a vector with all model parameters unrolled

Usage

```
PCMParmGetFullVector(model, ...)
```

Arguments

model	a PCM model object
...	passed to methods

Value

a numerical vector

Examples

```
PCMParmGetFullVector(PCMBase::PCMBaseTestObjects$model.a.123)
```

PCMTreePreorderCpp *Fast preorder of the edges in a tree*

Description

Fast preorder of the edges in a tree

Usage

```
PCMTreePreorderCpp(tree)
```

Arguments

tree a phylo object

Value

an integer vector containing indices of rows in tree\$edge in their preorder order.

Examples

```
PCMTreePreorderCpp(PCMBase::PCMBaseTestObjects$tree.a)
```

Index

*Topic **datasets**

- benchmarkData, [2](#)
- benchmarkResults, [3](#)
- benchmarkResultsNoTransform, [3](#)

- benchmarkData, [2](#)
- benchmarkResults, [3](#)
- benchmarkResultsNoTransform, [3](#)
- BenchmarkRvsCpp, [4](#)

- MiniBenchmarkRvsCpp, [5](#), [5](#)

- PCListInt, [6](#)
- PCMAppliedTransformation, [4](#), [5](#)
- PCMBaseCppIsADevRelease, [7](#)
- PCMInfoCpp, [7](#)
- PCMParmGetFullVector, [8](#)
- PCMPresentCoordinates, [7](#)
- PCMTreePreorderCpp, [9](#)