Package ‘mcbette’

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**Title**  Model Comparison Using 'babette'

**Version**  1.15.1

**Maintainer**  Richèl J.C. Bilderbeek <richel@richelbilderbeek.nl>

**Description**  'BEAST2' (<https://www.beast2.org>) is a widely used Bayesian phylogenetic tool, that uses DNA/RNA/protein data and many model priors to create a posterior of jointly estimated phylogenies and parameters.

'mcbette' allows to do a Bayesian model comparison over some site and clock models, using 'babette' (<https://github.com/ropensci/babette/>).

**License**  GPL-3

**RoxygenNote**  7.2.1

**VignetteBuilder**  knitr

**URL**  https://github.com/ropensci/mcbette/

**BugReports**  https://github.com/ropensci/mcbette/issues

**Imports**  babette (>= 2.3), beautier (>= 2.6.2), beastier (>= 2.4.6), curl, devtools, mauricer (>= 2.5), Rmpfr, testit, txtplot

**Suggests**  ape, ggplot2, hunspell, knitr, lintr, markdown, nLTT, phangorn, rappdirs, rmarkdown, spelling, stringr, testthat (>= 2.1.0), tracerer

**Language**  en-US

**Encoding**  UTF-8

**SystemRequirements**  BEAST2 (https://www.beast2.org/)

**NeedsCompilation**  no

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[https://orcid.org/0000-0003-1107-7049>),
Joëlle Barido-Sottani [rev] (Joëlle reviewed the package for rOpenSci, see https://github.com/ropensci/software-review/issues/360),
Vikram Baliga [rev] (Vikram reviewed the package for rOpenSci, see https://github.com/ropensci/software-review/issues/360,
<https://orcid.org/0000-0002-9367-8974>)}

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Description

Calculate the weights for each marginal likelihood

Usage

calc_weights(marg_liks)

Arguments

marg_liks (non-log) marginal likelihood estimates

Value

the weight of each marginal likelihood estimate, which will sum up to 1.0

Author(s)

Richèl J.C. Bilderbeek
can_run_mcbette

Examples

# Evidences (aka marginal likelihoods) can be very small
evidences <- c(0.0001, 0.0002, 0.0003, 0.0004)

# Sum will be 1.0
calc_weights(evidences)

beastier::remove_beastier_folders()
beastier::check_empty_beastier_folders()

can_run_mcbette

Description

Can 'mcbette' run? Will return TRUE if:

• (1) Running on Linux or MacOS
• (2) BEAST2 is installed
• (3) The BEAST2 NS package is installed

Usage

can_run_mcbette(beast2_folder = beastier::get_default_beast2_folder())

Arguments

beast2_folder the folder where the BEAST2 is installed. Note that this is not the folder where the BEAST2 executable is installed: the BEAST2 executable is in a subfolder. Use get_default_beast2_folder to get the default BEAST2 folder. Use get_default_beast2_bin_path to get the full path to the default BEAST2 executable. Use get_default_beast2_jar_path to get the full path to the default BEAST2 jar file.

Author(s)

Richèl J.C. Bilderbeek

Examples

can_run_mcbette()

beastier::remove_beastier_folders()
beastier::check_empty_beastier_folders()
check_marg_liks

check_beast2_ns_pkg  Checks if the BEAST2 'NS' package is installed.

Description
Checks if the BEAST2 'NS' package is installed. Will stop if not.

Usage
check_beast2_ns_pkg(beast2_bin_path = beastier::get_default_beast2_bin_path())

Arguments
beast2_bin_path
path to the BEAST2 binary file

check_marg_liks  Check if the marg_liks are of the same type as returned by est_marg_liks.

Description
stop if not.

Usage
check_marg_liks(marg_liks)

Arguments
marg_liks  a table of (estimated) marginal likelihoods, as, for example, created by est_marg_liks. This data.frame has the following columns:
• site_model_name: name of the site model, must be an element of get_site_model_names
• clock_model_name: name of the clock model, must be an element of get_clock_model_names
• tree_prior_name: name of the tree prior, must be an element of get_tree_prior_names
• marg_log_lik: estimated marginal (natural) log likelihood
• marg_log_lik_sd: estimated error of marg_log_lik
• weight: relative model weight, a value from 1.0 (all evidence is in favor of this model combination) to 0.0 (no evidence in favor of this model combination)
• ess: effective sample size of the marginal likelihood estimation
Use get_test_marg_liks to get a test marg_liks. Use is_marg_liks to determine if a marg_liks is valid. Use check_marg_liks to check that a marg_liks is valid.
check_mcbette_state

Check if the mcbette_state is valid.

Description
Check if the mcbette_state is valid. Will stop otherwise.

Usage
check_mcbette_state(mcbette_state)

Arguments
mcbette_state   the mcbette state, which is a list with the following elements:
  • beast2_installed TRUE if BEAST2 is installed, FALSE otherwise
  • ns_installed NA if BEAST2 is not installed. TRUE if the BEAST2 NS package is installed FALSE if the BEAST2 NS package is not installed

Author(s)
Richèl J.C. Bilderbeek

default_params_doc

Documentation of general function arguments. This function does nothing. It is intended to inherit function argument documentation.

Description
Documentation of general function arguments. This function does nothing. It is intended to inherit function argument documentation.

Usage
default_params_doc(
  beast2_bin_path,
  beast2_folder,
  beast2_working_dir,
  beast2_options,
  beast2_optionses,
  clock_model,
  clock_models,
  epsilon,
  fasta_filename,
  inference_model,
  inference_models,
Arguments

beast2_bin_path
path to the the BEAST2 binary file

beast2_folder
the folder where the BEAST2 is installed. Note that this is not the folder where the BEAST2 executable is installed: the BEAST2 executable is in a subfolder. Use get_default_beast2_folder to get the default BEAST2 folder. Use get_default_beast2_bin_path to get the full path to the default BEAST2 executable. Use get_default_beast2_jar_path to get the full path to the default BEAST2 jar file.

beast2_working_dir
folder in which BEAST2 will run and produce intermediate files. By default, this is a temporary folder

beast2_options
a beast2_options structure, as can be created by create_mcbette_beast2_options.

beast2_optionses
list of one or more beast2_options structures, as can be created by create_mcbette_beast2_options. Use of reduplicated plural to achieve difference with beast2_options

clock_model
a clock model, as can be created by create_clock_model

clock_models
a list of one or more clock models, as can be created by create_clock_models

epsilon
measure of relative accuracy. Smaller values result in longer, more precise estimations

fasta_filename
name of the FASTA file

inference_model
an inference model, as can be created by create_inference_model

inference_models
a list of one or more inference models, as can be created by create_inference_model

marg_liks
a table of (estimated) marginal likelihoods, as, for example, created by est_marg_liks. This data.frame has the following columns:

• site_model_name: name of the site model, must be an element of get_site_model_names
• clock_model_name: name of the clock model, must be an element of get_clock_model_names
• tree_prior_name: name of the tree prior, must be an element of get_tree_prior_names
• marg_log_lik: estimated marginal (natural) log likelihood
est_marg_lik

- marg_log_lik_sd: estimated error of marg_log_lik
- weight: relative model weight, a value from 1.0 (all evidence is in favor of this model combination) to 0.0 (no evidence in favor of this model combination)
- ess: effective sample size of the marginal likelihood estimation

Use get_test_marg_liks to get a test marg_liks. Use is_marg_liks to determine if a marg_liks is valid. Use check_marg_liks to check that a marg_liks is valid.

mcbette_state  the mcbette state, which is a list with the following elements:
- beast2_installed TRUE if BEAST2 is installed, FALSE otherwise
- ns_installed NA if BEAST2 is not installed. TRUE if the BEAST2 NS package is installed FALSE if the BEAST2 NS package is not installed

mcmc an MCMC for the Nested Sampling run, as can be created by create_mcmc_nested_sampling

os name of the operating system, must be unix (Linux, Mac) or win (Windows)

rng_seed a random number generator seed used for the BEAST2 inference

site_model a site model, as can be created by create_site_model

site_models a list of one or more site models, as can be created by create_site_models

tree_prior a tree prior, as can be created by create_tree_prior

verbose if TRUE show debug output

Note

This is an internal function, so it should be marked with @noRd. This is not done, as this will disallow all functions to find the documentation parameters

Author(s)

Richèl J.C. Bilderbeek

est_marg_lik Estimate the marginal likelihood for an inference model.

Description

Estimate the marginal likelihood for an inference model.

Usage

est_marg_lik(
  fasta_filename,
  inference_model = beautier::create_ns_inference_model(),
  beast2_options = beastier::create_mcbette_beast2_options(),
  os = rappdirs::app_dir()$os
)
est_marg_lik

Arguments

- `fasta_filename`: name of the FASTA file
- `inference_model`: an inference model, as can be created by `create_inference_model`
- `beast2_options`: a `beast2_options` structure, as can be created by `create_mcbette_beast2_options`
- `os`: name of the operating system, must be `unix` (Linux, Mac) or `win` (Windows)

Value

A list showing the estimated marginal likelihoods (and its estimated error), its items are:

- `marg_log_lik`: estimated marginal (natural) log likelihood
- `marg_log_lik_sd`: estimated error of `marg_log_lik`
- `esses`: the Effective Sample Size

Author(s)

Richèl J.C. Bilderbeek

See Also

- `can_run_mcbette`: see if `mcbette` can run
- `est_marg_liks`: estimate multiple marginal likelihoods

Examples

```r
if (can_run_mcbette()) {

  # An example FASTA file
  fasta_filename <- system.file("extdata", "simple.fas", package = "mcbette")

  # A testing inference model with inaccurate (thus fast) marginal
  # likelihood estimation
  inference_model <- beautier::create_ns_inference_model()

  # Shorten the run, by doing a short (dirty, unreliable) MCMC
  inference_model$mcmc <- beautier::create_test_ns_mcmc()

  # Setup the options for BEAST2 to be able to call BEAST2 packages
  beast2_options <- beautier::create_mcbette_beast2_options()

  # Estimate the marginal likelihood
  est_marg_lik(
    fasta_filename = fasta_filename,
    inference_model = inference_model,
    beast2_options = beast2_options
  )

  beastier::remove_beaustier_folders()
}
```
est_marg_liks

Description

Estimate the marginal likelihoods (aka evidence) for one or more inference models, based on a single alignment. Also, the marginal likelihoods are compared, resulting in a relative weight for each model, where a relative weight of a model close to 1.0 means that that model is way likelier than the others.

Usage

est_marg_liks(
  fasta_filename,
  inference_models = list(beautier::create_inference_model(mcmc =
    beautier::create_ns_mcmc())),
  beast2_optionses = rep(list(beastier::create_mcbette_beast2_options()), times =
    length(inference_models)),
  verbose = FALSE,
  os = rappdirs::app_dir()$os
)

Arguments

fasta_filename  name of the FASTA file
inference_models  a list of one or more inference models, as can be created by create_inference_model
beast2_optionses  list of one or more beast2_options structures, as can be created by create_mcbette_beast2_options. Use of reduplicated plural to achieve difference with beast2_options
verbose  if TRUE show debug output
os  name of the operating system, must be unix (Linux, Mac) or win (Windows)

Details

In the process, multiple (temporary) files are created (where [x] denotes the index in a list)

- beast2_optionses[x]$input_filename path to the the BEAST2 XML input file
- beast2_optionses[x]$output_state_filename path to the BEAST2 XML state file
- inference_models[x]$mcmc$tracer$filename path to the BEAST2 trace file with parameter estimates
- inference_models[x]$mcmc$trees$filename path to the BEAST2 trees file with the posterior trees
- inference_models[x]$mcmc$screen$filename path to the BEAST2 screen output file

These file can be deleted manually by bbt_delete_temp_files, else these will be deleted automatically by the operating system.
Value

a `data.frame` showing the estimated marginal likelihoods (and its estimated error) per combination of models. Columns are:

- `site_model_name`: name of the site model
- `clock_model_name`: name of the clock model
- `tree_prior_name`: name of the tree prior
- `marg_log_lik`: estimated marginal (natural) log likelihood
- `marg_log_lik_sd`: estimated error of `marg_log_lik`
- `weight`: relative model weight, a value from 1.0 (all evidence is in favor of this model combination) to 0.0 (no evidence in favor of this model combination)
- `ess`: effective sample size of the marginal likelihood estimation

Author(s)

Richèl J.C. Bilderbeek

See Also

- `can_run_mcbette`: see if ’mcbette’ can run
- `est_marg_liks`: estimate multiple marginal likelihood of a single inference mode

Examples

```r
if (can_run_mcbette()) {

  # Use an example FASTA file
  fasta_filename <- system.file("extdata", "simple.fas", package = "mcbette")

  # Create two inference models
  inference_model_1 <- beautier::create_ns_inference_model(
    site_model = beautier::create_jc69_site_model()
  )
  inference_model_2 <- beautier::create_ns_inference_model(
    site_model = beautier::create_hky_site_model()
  )

  # Shorten the run, by doing a short (dirty, unreliable) MCMC
  inference_model_1$pmcmc <- beautier::create_test_ns_mcmc()
  inference_model_2$pmcmc <- beautier::create_test_ns_mcmc()

  # Combine the inference models
  inference_models <- list(inference_model_1, inference_model_2)

  # Create the BEAST2 options, that will write the output
  # to different (temporary) filenames
  beast2_options_1 <- beautier::create_mcbette_beast2_options()
  beast2_options_2 <- beautier::create_mcbette_beast2_options()
}
```
get_mcbette_state

# Combine the two BEAST2 options sets,
# use reduplicated plural
beast2_optionses <- list(beast2_options_1, beast2_options_2)

# Compare the models
marg_liks <- est_marg_liks(
  fasta_filename,
  inference_models = inference_models,
  beast2_optionses = beast2_optionses
)

# Interpret the results
interpret_marg_lik_estimates(marg_liks)

beastier::remove_beaustier_folders()
beastier::check_empty_beaustier_folders()

---

get_mcbette_state  
*Get the current state of mcbette*

**Description**

Get the current state of mcbette

**Usage**

get_mcbette_state(beast2_folder = beastier::get_default_beast2_folder())

**Arguments**

beast2_folder  the folder where the BEAST2 is installed. Note that this is not the folder where the BEAST2 executable is installed: the BEAST2 executable is in a subfolder. Use get_default_beast2_folder to get the default BEAST2 folder. Use get_default_beast2_bin_path to get the full path to the default BEAST2 executable. Use get_default_beast2_jar_path to get the full path to the default BEAST2 jar file.

**Value**

a list with the following elements:

- beast2_installed  TRUE if BEAST2 is installed, FALSE otherwise
- ns_installed  TRUE if the BEAST2 NS package is installed FALSE if the BEAST2 or the BEAST2 NS package is not installed
**Examples**

```r
get_mcbette_state()

beastier::remove_beastier_folders()
beastier::check_empty_beastier_folders()
```

**Description**

Get testing marg_liks

**Usage**

```r
get_test_marg_liks()
```

**Examples**

```r
get_test_marg_liks()

beastier::remove_beastier_folders()
beastier::check_empty_beastier_folders()
```

**interpret_bayes_factor**

*Interpret a Bayes factor*

**Description**

Interpret a Bayes factor, using the interpretation from [1].

**Usage**

```r
interpret_bayes_factor(bayes_factor)
```

**Arguments**

- `bayes_factor` Bayes factor to be interpreted

**Details**


**Value**

a string with the interpretation in English
interpret_marg_lik_estimates

Author(s)

Richèl J.C. Bilderbeek

Examples

interpret_bayes_factor(0.5)

beastier::remove_beastier_folders()
beastier::check_empty_beastier_folders()

interpret_marg_lik_estimates

Interpret the marginal likelihood estimates

Description

Interpret the marginal likelihood estimates as created by est_marg_liks.

Usage

interpret_marg_lik_estimates(marg_liks)

Arguments

marg_liks

a table of (estimated) marginal likelihoods, as, for example, created by est_marg_liks.

This data.frame has the following columns:

- site_model_name: name of the site model, must be an element of get_site_model_names
- clock_model_name: name of the clock model, must be an element of get_clock_model_names
- tree_prior_name: name of the tree prior, must be an element of get_tree_prior_names
- marg_log_lik: estimated marginal (natural) log likelihood
- marg_log_lik_sd: estimated error of marg_log_lik
- weight: relative model weight, a value from 1.0 (all evidence is in favor of this model combination) to 0.0 (no evidence in favor of this model combination)
- ess: effective sample size of the marginal likelihood estimation

Use get_test_marg_liks to get a test marg_liks. Use is_marg_liks to determine if a marg_liks is valid. Use check_marg_liks to check that a marg_liks is valid.

Author(s)

Richèl J.C. Bilderbeek
is_marg_liks  
*Determine if the marg_liks is valid*

**Description**

Determine if the marg_liks is valid

**Usage**

```r
is_marg_liks(marg_liks, verbose = FALSE)
```

**Arguments**

- `marg_liks`: a table of (estimated) marginal likelihoods, as, for example, created by `est_marg_liks`. This data.frame has the following columns:
  - `site_model_name`: name of the site model, must be an element of `get_site_model_names`
  - `clock_model_name`: name of the clock model, must be an element of `get_clock_model_names`
  - `tree_prior_name`: name of the tree prior, must be an element of `get_tree_prior_names`
  - `marg_log_lik`: estimated marginal (natural) log likelihood
  - `marg_log_lik_sd`: estimated error of `marg_log_lik`
  - `weight`: relative model weight, a value from 1.0 (all evidence is in favor of this model combination) to 0.0 (no evidence in favor of this model combination)
  - `ess`: effective sample size of the marginal likelihood estimation

Use `get_test_marg_liks` to get a test marg_liks. Use `is_marg_liks` to determine if a marg_liks is valid. Use `check_marg_liks` to check that a marg_liks is valid.

- `verbose`: if TRUE show debug output

**Value**

TRUE if the argument is a valid marg_liks, FALSE otherwise

**mcbette**  
*mcbette: Model Comparison Using Babette*

**Description**

'mcbette' does a model comparing using babette, where the models are Bayesian phylogenetic models, as created by `create_inference_model`. 
Details

The main function is `est_marg_liks`, which estimate the marginal likelihoods (aka evidence) for one or more inference models, based on a single alignment. Also, the marginal likelihoods are compared, resulting in a relative weight for each model, where a relative weight of a model close to 1.0 means that that model is way likelier than the others.

In the process, multiple (temporary) files are created (where [x] denotes the index in a list)

- `beast2_optionses[x]$input_filename` path to the BEAST2 XML input file
- `beast2_optionses[x]$output_state_filename` path to the BEAST2 XML state file
- `inference_models[x]$mcmc$tracelog$filename` path to the BEAST2 trace file with parameter estimates
- `inference_models[x]$mcmc$treelog$filename` path to the BEAST2 trees file with the posterior trees
- `inference_models[x]$mcmc$screenlog$filename` path to the BEAST2 screen output file

These file can be deleted manually by `bbt_delete_temp_files`, else these will be deleted automatically by the operating system.

Author(s)

Richèl J.C. Bilderbeek

See Also

Use `can_run_mcbette` to see if `mcbette` can run.

Examples

```r
if (can_run_mcbette()) {

  # An example FASTA file
  fasta_filename <- system.file("extdata", "simple.fas", package = "mcbette")

  inference_model_1 <- beautier::create_ns_inference_model(
    site_model = beautier::create_jc69_site_model()
  )
  inference_model_2 <- beautier::create_ns_inference_model(
    site_model = beautier::create_gtr_site_model()
  )

  # Shorten the run, by doing a short (dirty, unreliable) MCMC
  inference_model_1$mcmc <- beautier::create_test_ns_mcmc()
  inference_model_2$mcmc <- beautier::create_test_ns_mcmc()

  inference_models <- c(list(inference_model_1), list(inference_model_2))

  # Estimate the marginal log-likelihoods of the two models
  marg_liks <- est_marg_liks(
    fasta_filename = fasta_filename,
```
mcbette_report

Create a mcbette report, to be used when reporting bugs

Description

Create a mcbette report, to be used when reporting bugs

Usage

mcbette_report(beast2_folder = beastier::get_default_beast2_folder())

Arguments

beast2_folder the folder where the BEAST2 is installed. Note that this is not the folder where the BEAST2 executable is installed: the BEAST2 executable is in a subfolder. Use get_default_beast2_folder to get the default BEAST2 folder. Use get_default_beast2_bin_path to get the full path to the default BEAST2 executable. Use get_default_beast2_jar_path to get the full path to the default BEAST2 jar file.

Value

nothing. It is intended that the output (not the return value) is copy-pasted from screen.

Author(s)

Richèl J.C. Bilderbeek

Examples

mcbette_report()
\textit{mcbette\_self\_test} \quad \textit{Performs a minimal \textit{mcbette} run}

\section*{mcbette\_self\_test}

\textbf{Description}

Performs a minimal \textit{mcbette} run

\textbf{Usage}

\texttt{mcbette\_self\_test(beast2\_folder = beastier::get\_default\_beast2\_folder())}

\textbf{Arguments}

\begin{description}
\item[beast2\_folder] the folder where the BEAST2 is installed. Note that this is not the folder where the BEAST2 executable is installed: the BEAST2 executable is in a subfolder. Use \texttt{get\_default\_beast2\_folder} to get the default BEAST2 folder. Use \texttt{get\_default\_beast2\_bin\_path} to get the full path to the default BEAST2 executable. Use \texttt{get\_default\_beast2\_jar\_path} to get the full path to the default BEAST2 jar file.
\end{description}

\section*{plot\_marg\_liks}

\textbf{Plot the marg\_liks}

\textbf{Description}

Plot the marg\_liks

\textbf{Usage}

\texttt{plot\_marg\_liks(marg\_liks)}

\textbf{Arguments}

\begin{description}
\item[marg\_liks] a table of (estimated) marginal likelihoods, as, for example, created by \texttt{est\_marg\_liks}. This \texttt{data\_frame} has the following columns:
\begin{itemize}
\item site\_model\_name: name of the site model, must be an element of \texttt{get\_site\_model\_names}
\item clock\_model\_name: name of the clock model, must be an element of \texttt{get\_clock\_model\_names}
\item tree\_prior\_name: name of the tree prior, must be an element of \texttt{get\_tree\_prior\_names}
\item marg\_log\_lik: estimated marginal (natural) log likelihood
\item marg\_log\_lik\_sd: estimated error of marg\_log\_lik
\item weight: relative model weight, a value from 1.0 (all evidence is in favor of this model combination) to 0.0 (no evidence in favor of this model combination)
\end{itemize}
\end{description}
set_mcbette_state

- ess: effective sample size of the marginal likelihood estimation

Use get_test_marg_liks to get a test marg_liks. Use is_marg_liks to determine if a marg_liks is valid. Use check_marg_liks to check that a marg_liks is valid.

Value

a ggplot

Examples

plot_marg_liks(get_test_marg_liks())

beastier::remove_beaustier_folders()
beastier::check_empty_beaustier_folders()

Description

Set the mcbette state to having BEAST2 installed with or without installing the BEAST2 NS package.

Usage

set_mcbette_state(
  mcbette_state,
  beast2_folder = beastier::get_default_beast2_folder(),
  verbose = FALSE
)

Arguments

mcbette_state the mcbette state, which is a list with the following elements:
  • beast2_installed TRUE if BEAST2 is installed, FALSE otherwise
  • ns_installed NA if BEAST2 is not installed. TRUE if the BEAST2 NS package is installed FALSE if the BEAST2 NS package is not installed

beast2_folder the folder where the BEAST2 is installed. Note that this is not the folder where the BEAST2 executable is installed: the BEAST2 executable is in a subfolder. Use get_default_beast2_folder to get the default BEAST2 folder. Use get_default_beast2_bin_path to get the full path to the default BEAST2 executable. Use get_default_beast2_jar_path to get the full path to the default BEAST2 jar file.

verbose if TRUE show debug output
**set_mcbette_state**

**Note**

In newer versions of BEAST2, BEAST2 comes pre-installed with the BEAST2 NS package. For such a version, one cannot install BEAST2 without NS. A warning will be issues if one intends to only install BEAST2 (i.e. without the BEAST2 NS package) and gets the BEAST2 NS package installed as a side effect as well.

Also, installing or uninstalling a BEAST2 package from a BEAST2 installation will affect all installations.

**See Also**

- Use `get_mcbette_state` to get the current mcbette state
- Use `check_mcbette_state` to check the current mcbette state
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