Package ‘mcbette’

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Title Model Comparison Using 'babette'

Version 1.15

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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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**Description**

Calculate the weights for each marginal likelihood

**Usage**

```r
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
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::check_empty_beastier_folders()

---

can_run_mcbette  Can 'mcbette' run?

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::check_empty_beastier_folders()
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 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` \[ \text{the mcbette state, which is a list with the following elements:} \\
  \quad \text{• beast2_installed TRUE if BEAST2 is installed, FALSE otherwise} \\
  \quad \text{• ns_installed NA if BEAST2 is not installed. TRUE if the BEAST2 NS} \\
  \quad \text{package is installed FALSE if the BEAST2 NS package is not installed} \]

**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, \\
  ... )`
marg_liks,
mcbette_state,
mcmc,
os,
rng_seed,
site_model,
site_models,
tree_prior,
tree_priors,
verbose
)

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 folder. 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
Estimate the marginal likelihood for an inference model.

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
)

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
Arguments

<table>
<thead>
<tr>
<th>Argument</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>fasta_filename</td>
<td>name of the FASTA file</td>
</tr>
<tr>
<td>inference_model</td>
<td>an inference model, as can be created by <code>create_inference_model</code></td>
</tr>
<tr>
<td>beast2_options</td>
<td>a beast2_options structure, as can be created by <code>create_mcbette_beast2_options</code></td>
</tr>
<tr>
<td>os</td>
<td>name of the operating system, must be <code>unix</code> (Linux, Mac) or <code>win</code> (Windows)</td>
</tr>
</tbody>
</table>

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::check_empty_beaustier_folders()
}
```
**est_marg_liks**  

**Estimate the marginal likelihoods for one or more inference models**

**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**

```r
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]$mcmc$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.
est_marg_liks

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

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$mcmc <- beautier::create_test_ns_mcmc()
inference_model_2$mcmc <- 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 <- beastier::create_mcbette_beast2_options()
beast2_options_2 <- beastier::create_mcbette_beast2_options()
# Combine the two BEAST2 options sets, # use reduplicated plural
beast2_optionses <- list(beast2_options_1, beast2_options_2)

# Compare the models
marg_lik <- est_marg_lik(
  fasta_filename,
  inference_models = inference_models,
  beast2_optionses = beast2_optionses
)

# Interpret the results
interpret_marg_lik_estimates(marg_lik)

beastier::check_empty_beastier_folders()

---

**get_mcbette_state**

*Get the current state of mcbette*

**Description**

Get the current state of mcbette

**Usage**

```r
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::check_empty_beastier_folders()
```
get_test_marg_liks  Get testing marg_liks

Description
Get testing marg_liks

Usage
get_test_marg_liks()

Examples
get_test_marg_liks()
    beastier::check_empty_beastier_folders()

interpret_bayes_factor  Interpret a Bayes factor

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

Usage
interpret_bayes_factor(bayes_factor)

Arguments
bayes_factor  Bayes factor to be interpreted

Details

Value
a string with the interpretation in English

Author(s)
Richèl J.C. Bilderbeek
**Examples**

```
interpret_bayes_factor(0.5)

beastier::check_empty_beaustier_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]$input_filename` path to the the BEAST2 XML input file
- `beast2_optionses[x]$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()
mcbette_self_test

Performs a minimal mcbette run

Description

Performs a minimal mcbette run

Usage

mcbette_self_test(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.

plot_marg_liks

Plot the marg_liks

Description

Plot the marg_liks

Usage

plot_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)
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

---

**set_mcbette_state**

*Set the mcbette state.*

**Description**

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

**Usage**

```r
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

**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
Index

babette, 14
bbt_delete_temp_files, 9, 15
calc_weights, 2
can_run_mcbette, 3, 8, 10, 15
check_beast2_ns_pkg, 4
check_marg_liks, 4, 4, 7, 13, 14, 18
check_mcbette_state, 5, 19
create_clock_model, 6
create_clock_models, 6
create_inference_model, 6, 8, 9, 14
create_mcbette_beast2_options, 6, 8, 9
create_mcmc_nested_sampling, 7
create_site_model, 7
create_site_models, 7
create_tree_prior, 7
create_tree_priors, 7
data.frame, 4, 6, 10, 13, 14, 17
default_params_doc, 5
est_marg_lrk, 7
est_marg_liks, 4, 6, 8, 9, 10, 13–15, 17
FALSE, 5, 7, 11, 18
get_clock_model_names, 4, 6, 13, 14, 17
get_default_beast2_bin_path, 3, 6, 11, 16–18
get_default_beast2_folder, 3, 6, 11, 16–18
get_default_beast2_jar_path, 3, 6, 11, 16–18
get_mcbette_state, 11, 19
get_site_model_names, 4, 6, 13, 14, 17
get_test_marg_liks, 4, 7, 12, 13, 14, 18
get_tree_prior_names, 4, 6, 13, 14, 17
ggplot, 18
interpret_bayes_factor, 12
interpret_marg_lrk_estimates, 13
is_marg_liks, 4, 7, 13, 14, 14, 18
list, 5, 7, 8, 11, 18
mcbette, 5, 7, 11, 14, 16–19
mcbette_report, 16
mcbette_self_test, 17
NA, 5, 7, 18
plot_marg_liks, 17
set_mcbette_state, 18
stop, 4, 5
TRUE, 3, 5, 7, 11, 18