

Package ‘mcbette’

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Title Model Comparison Using 'babette'

Version 1.13

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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

LazyData true

RoxygenNote 7.1.1

VignetteBuilder knitr

URL <https://github.com/ropensci/mcbette/>

BugReports <https://github.com/ropensci/mcbette/issues>

Imports babette (>= 2.1.5), beautier (>= 2.4), beastier (>= 2.2.1), curl, devtools, mauricer (>= 2.3), Rmpfr, testit, txtplot

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

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SystemRequirements BEAST2 (<https://www.beast2.org/>)

NeedsCompilation no

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calc_weights	<i>Calculate the weights for each marginal likelihood</i>
--------------	---

Description

Calculate the weights for each marginal likelihood

Usage

```
calc_weights(marg_lik)
```

Arguments

marg_lik (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)
```

can_run_mcbette	<i>Can 'mcbette' run?</i>
-----------------	---------------------------

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

check_beast2_ns_pkg	<i>Checks if the BEAST2 'NS' package is installed.</i>
---------------------	--

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_lik *Check if the marg_lik are of the same type as returned by [est_marg_lik](#).*

Description

[stop](#) if not.

Usage

```
check_marg_lik(marg_lik)
```

Arguments

marg_lik a table of (estimated) marginal likelihoods, as, for example, created by [est_marg_lik](#). 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_lik](#) to get a test marg_lik. Use [is_marg_lik](#) to determine if a marg_lik is valid. Use [check_marg_lik](#) to check that a marg_lik 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,  
  marg_lik,  
  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 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 <code>beast2_options</code> structure, as can be created by create_mcbette_beast2_options .
beast2_optionses	list of one or more <code>beast2_options</code> structures, as can be created by create_mcbette_beast2_options . Use of reduplicated plural to achieve difference with <code>beast2_options</code>
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_lik	a table of (estimated) marginal likelihoods, as, for example, created by est_marg_lik . This <code>data.frame</code> has the following columns: <ul style="list-style-type: none"> • <code>site_model_name</code>: name of the site model, must be an element of get_site_model_names • <code>clock_model_name</code>: name of the clock model, must be an element of get_clock_model_names • <code>tree_prior_name</code>: name of the tree prior, must be an element of get_tree_prior_names • <code>marg_log_lik</code>: estimated marginal (natural) log likelihood • <code>marg_log_lik_sd</code>: estimated error of <code>marg_log_lik</code> • <code>weight</code>: 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) • <code>ess</code>: effective sample size of the marginal likelihood estimation Use get_test_marg_lik to get a test <code>marg_lik</code> . Use is_marg_lik to determine if a <code>marg_lik</code> is valid. Use check_marg_lik to check that a <code>marg_lik</code> is valid.
mcbette_state	the <code>mcbette</code> state, which is a <code>list</code> with the following elements: <ul style="list-style-type: none"> • <code>beast2_installed</code> <code>TRUE</code> if BEAST2 is installed, <code>FALSE</code> otherwise

	<ul style="list-style-type: none"> • 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
tree_priors	a list of one or more tree priors, as can be created by create_tree_priors
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	<i>Estimate the marginal likelihood for an inference model.</i>
--------------	---

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
)
```

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_lik](#): estimate multiple marginal likelihoods

Examples

```
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
  )
}
```

est_marg_lik

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

```
est_marg_lik(
  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 [bvt_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_lik](#): 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)
}
```

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

```
get_mcbette_state()
```

get_test_marg_lik *Get testing marg_lik*

Description

Get testing `marg_lik`

Usage

```
get_test_marg_lik()
```

`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

- [1] H. Jeffreys (1961). The Theory of Probability (3rd ed.). Oxford. p. 432

Value

a string with the interpretation in English

Author(s)

Richèl J.C. Bilderbeek

Examples

```
interpret_bayes_factor(0.5)
```

`interpret_marg_lik_estimates`*Interpret the marginal likelihood estimates*

Description

Interpret the marginal likelihood estimates as created by [est_marg_lik](#).

Usage

```
interpret_marg_lik_estimates(marg_lik)
```

Arguments

`marg_lik` a table of (estimated) marginal likelihoods, as, for example, created by `est_marg_lik`. 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_lik` to get a test `marg_lik`s. Use `is_marg_lik` to determine if a `marg_lik`s is valid. Use `check_marg_lik` to check that a `marg_lik`s is valid.

Author(s)

Richèl J.C. Bilderbeek

<code>is_marg_lik</code>	<i>Determine if the <code>marg_lik</code>s is valid</i>
--------------------------	---

Description

Determine if the `marg_lik`s is valid

Usage

```
is_marg_lik(marg_lik, verbose = FALSE)
```

Arguments

`marg_lik` a table of (estimated) marginal likelihoods, as, for example, created by `est_marg_lik`. 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_lik](#)s to get a test `marg_lik`s. Use [is_marg_lik](#) to determine if a `marg_lik`s is valid. Use [check_marg_lik](#) to check that a `marg_lik`s is valid.

`verbose` if TRUE show debug output

Value

TRUE if the argument is a valid `marg_lik`s, 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_lik](#)s, 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

```

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,
    inference_models = inference_models
  )

  # Interpret the results
  interpret_marg_lik_estimates(marg_liks)
}

```

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 = beautier::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_lik      Plot the marg_lik
```

Description

Plot the `marg_lik`

Usage

```
plot_marg_lik(marg_lik)
```


Arguments

- `marg_lik` a table of (estimated) marginal likelihoods, as, for example, created by `est_marg_lik`. 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_lik` to get a test `marg_lik`s. Use `is_marg_lik` to determine if a `marg_lik`s is valid. Use `check_marg_lik` to check that a `marg_lik`s 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

```
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

Examples

```
mcbette_state <- get_mcbette_state()
mcbette_state$beast2_installed <- TRUE
mcbette_state$ns_installed <- TRUE

set_mcbette_state(mcbette_state)
```

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