babette: BEAUti 2, BEAST2 and Tracer for R

- Richèl J.C. Bilderbeek¹ and Rampal S. Etienne¹
- ¹Groningen Institute for Evolutionary Life Sciences, University of
- Groningen, Groningen, The Netherlands

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Summary

- 1. In the field of phylogenetics, BEAST2 is one of the most widely used software tools. It comes with the graphical user interfaces BEAUti 2, DensiTree and Tracer, to create BEAST2 configuration files and to interpret BEAST2's output files. However, when many different alignments or model setups are required, a workflow of graphical user interfaces is cumbersome.
- 2. Here, we present a free, libre and open-source package, babette: 'BEAUti 2, BEAST2 and Tracer for R', for the R programming language. babette creates BEAST2 input files, runs BEAST2 and parses its results, all from an R function call.
 - 3. We describe babette's usage and the novel functionality it provides compared to the original tools and we give some examples.
 - 4. As babette is designed to be of high quality and extendable, we conclude by describing the further development of the package.

Samenvatting

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- 23 1. In de fylogenetica is BEAST2 een van de meest gebruikte hulpprogramma's. Het is gebundeld met de grafische gebruiksinterface BEAUti
 25 2, DensiTree en Tracer, om BEAST2-configuratiebestanden te maken en
 26 om BEAST2-outputbestanden te interpreteren. Echter, als veel verschil27 lende aligneringen of modelopzetten nodig zijn, is een werkvolgorde van
 28 meerdere grafische gebruiksinterfaces onhandig.
- 29 2. Hier presenteren we een gratis, vrij en open-source package, babette:

 'BEAUti 2, BEAST2 en Tracer voor R', voor de programmeertaal R.

 babette schrijft BEAST2-configuratiebestanden, start BEAST2 and verwerkt de resultaten, alles met een enkele R functie-aanroep.
- 33. We beschrijven hoe babette te gebruiken is en de nieuwe mogelijkheden die het biedt vergeleken met de originele programma's, aan de hand van enkele voorbeelden.
 - 4. Omdat babette ontworpen is voor uitbreidbaarheid en hoge kwaliteit, sluiten we af met het beschrijven van de verdere ontwikkeling van dit package.

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Keywords: computational biology, evolution, phylogenetics, BEAST2, R

$_{\scriptscriptstyle 41}$ 1 Introduction

- Phylogenies are commonly used to explore evolutionary hypotheses. Not only
- can phylogenies show us how species (or other evolutionary units) are related
- 44 to each other, but we can also estimate relevant parameters such as extinction
- 45 and speciation rates from them. There are many phylogenetics tools available
- to obtain an estimate of the phylogeny of a given set of species. BEAST2
- 47 (Bouckaert et al. 2014) is one of the most widely used ones. It uses a Bayesian
- 48 statistical framework to estimate the joint posterior distribution of phylogenies
- and model parameters, from one or more DNA, RNA or amino acid alignments

(see figure 1 for an overview of the workflow).

BEAST2 has a graphical and a command-line interface, that both need a configuration file containing alignments and model parameters. BEAST2 is bundled with BEAUti 2 (Drummond *et al.* 2012) ('BEAUti' from now on), a desktop application to create a BEAST2 configuration file. BEAUti has a user-friendly graphical user interface, with helpful default settings. As such, BEAUti is an attractive alternative to manual and error-prone editing of BEAST2 configuration files.

However, BEAUti cannot be called from a command-line script. This implies that when the user wants to explore the consequences of various settings, this must be done manually. This is the managable workflow when using a few alignments and doing a superficial analysis of sensitivity of the reconstructed tree to model settings. For exploring many trees (for instance from simulations), for a sliding-window analysis on a genomic alignment, or for a more thorough sensitivity analysis, one would like to loop through multiple (simulated or shortened) alignments, nucleotide substitution models, clock models and tree priors. One such tool to replace BEAUti is BEASTmasteR (Matzke 2015), which focuses on morphological traits and tip-dating, but also supports DNA data. BEASTmasteR, however, requires hundreds of lines of R code to setup the BEAST2 model configuration and a Microsoft Excel file to specify alignment files.

BEAST2 is also associated with Tracer (Rambaut & Drummond 2007) and
DensiTree (Bouckaert & Heled 2014). Both are desktop applications to analyze the output of BEAST2, each with a user-friendly graphical user interface. Tracer's purpose is to analyze the parameter estimates generated from
a (BEAST1 and) BEAST2 run. It shows, among others, the effective sample
size (ESS) and time series ('the trace', hence the name) of each variable in the
MCMC run. Both ESS and trace are needed to assess the strength of the infer-

ence. DensiTree visualizes the phylogenies of a BEAST2 posterior, with many options to improve the simultaneous display of many phylogenies.

However, for exploring the output of many BEAST2 runs, one would like a script to collect all parameters' ESSes, parameter traces and posterior phylogenies. There is no single package that offers a complete solution, but examples of R packages that offer a partial solution are rBEAST (Ratmann 2015) and RBeast (Faria & Suchard 2015). RBeast provides some plotting options and parsing of BEAST2 output files, but the plotting functions are too specific for general use. rBEAST was developed to test a particular biological hypothesis (Ratmann et al. 2016), and hence was not designed for general use.

Here, we present babette: BEAUti 2, BEAST2 and Tracer for R, which
creates BEAST2 (v.2.4.7) configuration files, runs BEAST2, and analyzes its
results, all from an R function call. This will save time, tedious mouse clicking
and reduces the chances of errors in such repetitive actions. The interface of
babette mimics the tools it is based on. This familiarity helps both beginner
and experienced BEAST2 users to make the step from those tools to babette.
babette enables the creation of a single-script pipeline from sequence alignments

95 2 Description

to posterior analysis in R.

babette is written in the R programming language (R Core Team 2013) and enables the full BEAST2 workflow from a single R function call, in a similar way to what subsequent usage of BEAUti, DensiTree and Tracer would produce. babette's main function is bbt_run, which configures BEAST2, runs it and parses its output. bbt_run needs at least the name of a FASTA file containing a DNA alignment. The default settings for the other arguments of bbt_run are identical to BEAUti's and BEAST2's default settings. Per alignment, a site

model, clock model and tree prior can be chosen. Multiple alignments can be used, each with its own (unlinked) site model, clock model and tree prior.

babette currently has 108 exported functions to set up a BEAST2 config-105 uration file. babette can currently handle the majority of BEAUti use cases. 106 Because of BEAUti's high number of plugins, babette uses a software architec-107 ture that is designed to be extended. Furthermore, babette has 13 exported 108 functions to run and help run BEAST2. One function is used to run BEAST2, 109 another one installs BEAST2 to a default location. Finally, babette has 21 110 exported function to parse the BEAST2 output files and analyze the created 111 posterior. babette gives the same ESSes and summary statistics as Tracer. 112 The data is formatted such that it can easily be visualized using ggplot2 (for a trace, similar to Tracer) or phangorn (Schliep 2011) (for the phylogenies in a 114 posterior, similar to DensiTree). 115

Currently, babette does not contain all functionality in BEAUti, BEAST2 and their many plug-ins, because these tools themselves also change in time.

babette currently works only on DNA data, because this is the most common use case. Nevertheless, babette provides the majority of default tree priors and supports the most important command-line arguments of BEAST2, provides the core Tracer analysis options, and has the most basic subset of plotting options of DensiTree. Up till now, the babette features implemented are those requested by users. Further extension of babette will be based on future user requests.

$_{24}$ 3 Usage

babette can be installed easily from CRAN:

install.packages("babette")

For the most up-to-date version, one can download and install the package from

```
babette's GitHub repository:
    devtools::install_github("richelbilderbeek/babette")
129
   To start using babette, load its functions in the global namespace first:
130
    library(babette)
    Because babette calls BEAST2, BEAST2 must be installed. This can be done
132
   from R, using:
133
    install_beast2()
134
    This will install BEAST2 to the default user data folder, but a different path
135
    can be specified as well. BEAUti, and likewise babette, needs at least a FASTA
136
   filename to produce a BEAST2 configuration file. In BEAUti, this is achieved
137
   by loading a FASTA file, then saving an output file using a common save file
138
    dialog. After this, BEAST2 needs to be applied to the created configuration
   file. It creates multiple files storing the posterior. These output files must be
140
   parsed by either Tracer or DensiTree. In babette, all this is achieved by:
    out <- bbt_run(fasta_filenames = "anthus_aco.fas")</pre>
    This code will create a (temporary) BEAST2 configuration file, from the FASTA
143
   file with name anthus_aco.fas (which is supplied with the package, from
144
    Van Els & Norambuena 2018), using the same default settings as BEAUti, which
145
    are, among others, a Jukes-Cantor site model, a strict clock, and a Yule birth
146
   tree prior. babette will then execute BEAST2 using that file, and parses the
    output. The returned data structure, named out, is a list of parameter estimates
148
    (called estimates), posterior phylogenies (called anthus_aco_trees, named af-
    ter the alignment's name) and MCMC operator performance (operators). An
150
   example of using a different site model, clock model and tree prior is:
151
    out <- bbt_run(
      fasta_filenames = "anthus_aco.fas",
153
```

```
site_models = create_hky_site_model(),
154
     clock_models = create_rln_clock_model(),
155
     tree_priors = create_bd_tree_prior()
156
   )
157
```

This code uses an HKY site model, a relaxed log-normal clock model and a birthdeath tree prior, each with their default settings in BEAUti. Table 1 shows an 159 overview of all functions to create site models, clock models and tree priors. Note 160 that the arguments' names site_models, clock_models and tree_priors are 161 plural, as each of these can be (a list of) one or more elements. Each of these 162 arguments must have the same number of elements, so that each alignment has 163 its own site model, clock model and tree prior. An example of two alignments, 164 each with its own site model, is: 165

```
out <- bbt_run(
166
      fasta_filenames = c(
        "anthus_aco.fas",
168
        "anthus_nd2.fas"
169
      ),
170
      site_models = list(
171
        create_tn93_site_model(),
172
        create_gtr_site_model()
173
      )
174
   )
175
```

babette also uses the same default prior distributions as BEAUti for each of 176 the site models, clock models and tree priors. For example, by default, a Yule 177 tree prior assumes that the birth rate follows a uniform distribution, from minus 178 infinity to plus infinity. One may prefer a different ddistribution instead. Here 179 is an example how to specify an exponential distribution for the birth rate in a 180 Yule tree prior in babette: 181

```
out <- bbt_run(
182
      fasta_filenames = "anthus_aco.fas",
183
      tree_priors = create_yule_tree_prior(
184
        birth_rate_distr = create_exp_distr()
185
      )
186
   )
187
   In this same example, one may specify the initial shape parameters of the expo-
   nential distribution. In BEAST2's implementation, an exponential distribution
189
   has one shape parameter: its mean, which can be set to any value with BEAUti.
    To set the mean value of the exponential distribution to a fixed (non-estimated)
191
   value, do:
    out <- bbt_run(
193
      fasta_filenames = "anthus_aco.fas",
194
      tree_priors = create_yule_tree_prior(
        birth_rate_distr = create_exp_distr(
196
           mean = create_mean_param(
197
              value = 1.0,
198
              estimate = FALSE
199
           )
200
         )
201
      )
202
   )
203
   babette also supports node dating. Like BEAUti, one can specify Most Recent
204
    Common Ancestor ('MRCA') priors. An MRCA prior allows to specify taxa
   having a common ancestor, including a distribution for the date of that ancestor.
206
   With babette, this is achieved as follows:
207
    out <- bbt_run(
208
      fasta_filenames = "anthus_aco.fas",
```

```
mrca_priors = create_mrca_prior(
210
         taxa_names = sample(get_taxa_names("anthus_aco.fas"),
211
             size = 2),
212
         alignment_id = get_alignment_id("anthus_aco.fas"),
213
         is_monophyletic = TRUE,
214
        mrca_distr = create_normal_distr(
           mean = create_mean_param(value = 15.0, estimate =
               FALSE),
217
           sigma = create_sigma_param(value = 0.025, estimate =
218
               FALSE)
219
         )
220
      )
221
    )
222
    Instead of dating the ancestor of two random taxa, any subset of taxa can
223
    be selected, and multiple sets are allowed. babette allows for the same core
    functionality as Tracer to show the values of the parameter estimates sampled
225
    in the BEAST2 run. This is called the "trace" (hence the name). The start
    of the trace, called the "burn-in", is usually discarded, as an MCMC algorithm
227
    (such as used by BEAST2) first has to converge to its equilibrium and hence
    the parameter estimates are not representative. By default, Tracer discards the
229
    first 10% of all the parameter estimates. To remove a 20% burn-in from all
230
    parameter estimates in babette, the following code can be used:
231
    traces <- remove_burn_ins(</pre>
232
      traces = out$estimates,
233
      burn_in_fraction = 0.2
234
    )
235
    Tracer shows the ESSes of each posterior's variables. These ESSes are important
236
```

to determine the strength of the inference. As a rule of thumb, an ESS of 200 is

```
acceptable for any parameter estimate. To calculate the effective sample sizes
    (of all estimated variables) in babette:
    esses <- calc_esses(
      traces = traces,
241
242
      sample_interval = 1000
    )
243
    Tracer displays multiple summary statistics for each estimated variable: the
244
    mean and its standard error, standard deviation, variance, median, mode, geo-
    metric mean, 95% highest posterior density interval, auto-correlation time and
246
    effective sample size. It displays these statistics per variable. In babette, these
    summary statistics are collected for all estimated parameters at once:
248
    sum_stats <- calc_summary_stats(</pre>
249
      traces = traces,
250
      sample_interval = 1000
251
252
    babette allows for the same functionality as DensiTree. DensiTree displays the
253
    phylogenies in a posterior at the same time scale, drawn one over one another,
254
    allowing to see the uncertainty in topology and branch lengths. The posterior
255
    phylogenies are stored as anthus_aco_trees in the object out, and can be
256
    plotted as follows:
257
    plot_densitree(phylos = out$anthus_aco_trees)
258
    Instead of running the full pipeline, babette also allows to only create a BEAST2
    configuration file. To create a BEAST2 configuration file, with all settings to
260
    default, use:
261
    create_beast2_input_file(
262
      input_filenames = babette::get_babette_path("anthus_aco.
```

fas"),

```
output_filename = "beast2.xml"
   )
266
   This file can then be loaded and edited by BEAUti, run by BEAST2, or run by
   babette:
268
   run_beast2(
      input_filename = "beast2.xml",
      output_log_filename = "run.log",
271
      output_trees_filenames = "posterior.trees",
272
      output_state_filename = "final.xml.state"
273
   )
274
   run_beast2 is a function that only runs BEAST2, and does not parse the output
   files (unlike bbt_run). In the example above, we specify the names of the desired
276
   BEAST2 output files explicitly, and these will be created in the R working
    directory, after which they can be inspected with other tools, or used to continue
278
    a BEAST2 run. When the names of these files are not specified, both bbt_run
279
   and run_beast2 put these files in the default temporary folder (as obtained
280
   from temp.dir()) to keep the working directory clean of intermediate files.
```

$_{\scriptscriptstyle 282}$ 4 babette resources

babette is free, libre and open source software available at http://github.
com/richelbilderbeek/babette and is licensed under the GNU General Public License v3.0. babette uses the Travis CI (https://travis-ci.org) continuous integration service, which is known to significantly increase the number
of bugs exposed (Vasilescu et al. 2015) and increases the speed at which new
features are added (Vasilescu et al. 2015). babette has a 100% code coverage, which correlates with code quality (Horgan et al. 1994; Del Frate et al.
1995). babette follows Hadley Wickham's style guide (Wickham 2015), which

```
improves software quality (Fang 2001). babette depends on multiple packages,
    which are ape (Paradis et al. 2004), beautier (Bilderbeek 2018b), beastier
292
    (Bilderbeek 2018a), devtools (Wickham & Chang 2016), geiger (Harmon et al.
293
    2008), ggplot2 (Wickham 2009), knitr (Xie 2017), phangorn (Schliep 2011),
294
    rmarkdown (Allaire et al. 2017), seqinr (Charif & Lobry 2007), stringr (Wick-
295
    ham 2017), testit (Xie 2014) and tracerer (Bilderbeek 2018c). We tested
296
    babette to give a clean error message for incorrect input, by calling babette
    one million times with random or random sensible inputs, using a high perfor-
298
    mance computer cluster. The test scripts are supplied with babette.
       babette's development takes place on GitHub, https://github.com/richelbilderbeek/
300
    babette, which accommodates collaboration (Perez-Riverol et al. 2016) and im-
    proves transparency (Gorgolewski & Poldrack 2016). babette's GitHub facili-
302
    tates feature requests and has guidelines how to do so.
       babette's documentation is extensive. All functions are documented in the
304
    package's internal documentation. For quick use, each exported function shows
305
    a minimal example. For easy exploration, each exported function's documen-
    tation links to related functions. Additionally, babette has a vignette that
307
    demonstrates extensively how to use it. There is documentation on the GitHub
308
    to get started, with a dozen examples of BEAUti screenshots with equivalent
309
    babette code. Finally, babette has tutorial videos that can be downloaded or
310
    viewed on YouTube, https://goo.gl/weKaaU.
311
```

5 Citation of babette

Scientists using babette in a published paper can cite this article, and/or cite
the babette package directly. To obtain this citation from within an R script,
use:

> citation("babette")

$_{\scriptscriptstyle 7}$ 6 Acknowledgements

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7 Authors' contributions

RJCB and RSE conceived the idea for the package. RJCB created and tested
the package, and wrote the first draft of the manuscript. RSE contributed
substantially to revisions.

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- tion in R. R package version 1.17.

Name	Description
bbt_run	Run BEAST2
create_gtr_site_model	Create a GTR site model
create_hky_site_model	Create an HKY site model
create_jc69_site_model	Create a Jukes-Cantor site model
create_tn93_site_model	Create a TN93 site model
create_rln_clock_model	Create a relaxed log-normal clock model
create_strict_clock_model	Create a strict clock model
create_bd_tree_prior	Create a birth-death tree prior
create_cbs_tree_prior	Create a coalescent Bayesian skyline tree prior
create_ccp_tree_prior	Create a coalescent constant-population tree prior
create_cep_tree_prior	Create a coalescent exponential-population tree prior
create_yule_tree_prior	Create a Yule tree prior
create_beta_distr	Create a beta distribution
create_exp_distr	Create an exponential distribution
create_gamma_distr	Create a gamma distribution
create_inv_gamma_distr	Create an inverse gamma distribution
create_laplace_distr	Create a Laplace distribution
create_log_normal_distr	Create a log-normal distribution
create_normal_distr	Create a normal distribution
create_one_div_x_distr	Create a 1/X distribution
create_poisson_distr	Create a Poisson distribution
create_uniform_distr	Create a uniform distribution

Table 1: babette's main functions