

1 babette: BEAUti 2, BEAST2 and Tracer for R

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6 Summary

7 **1.** In the field of phylogenetics, BEAST2 is one of the most widely
8 used software tools. It comes with the graphical user interfaces BEAUti
9 2, DensiTree and Tracer, to create BEAST2 configuration files and to in-
10 terpret BEAST2's output files. However, when many different alignments
11 or model setups are required, a workflow of graphical user interfaces is
12 cumbersome.

13 **2.** Here, we present a free, libre and open-source package, **babette**:
14 'BEAUti 2, BEAST2 and Tracer for R', for the R programming language.
15 **babette** creates BEAST2 input files, runs BEAST2 and parses its results,
16 all from an R function call.

17 **3.** We describe **babette**'s usage and the novel functionality it provides
18 compared to the original tools and we give some examples.

19 **4.** As **babette** is designed to be of high quality and extendable, we
20 conclude by describing the further development of the package.

21
22 **Keywords:** computational biology, evolution, phylogenetics, BEAST2, R

1 Introduction

Phylogenies are commonly used to explore evolutionary hypotheses. Not only can phylogenies show us how species (or other evolutionary units) are related to each other, but we also estimate relevant parameters such as extinction and speciation rates. There are many phylogenetics tools available to obtain an estimate of the phylogeny of a given set of species. BEAST2 (Bouckaert *et al.* 2014) is one of the most widely used ones. It uses a Bayesian statistical framework to estimate the joint posterior distribution of estimated phylogenies and model parameters, from one or more DNA, RNA or amino acid alignments (see figure 1 for an overview of the workflow).

It 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) and for more thorough sensitivity analysis, one would like to loop through multiple (simulated) alignments, nucleotide substitution models, clock models and tree priors. One such tool to replace BEAUti is BEASTmasterR (Matzke 2015), which focuses on morphological traits and tip-dating, but also supports DNA data. BEASTmasterR, however, requires hundreds of lines of R code to setup the

50 BEAST2 model configuration and a Microsoft Excel file to specify alignment
51 files.

52 BEAST2 is also associated with Tracer (Rambaut & Drummond 2007) and
53 DensiTree (Bouckaert & Heled 2014). Both are desktop applications to an-
54alyze the output of BEAST2, each with a user-friendly graphical user inter-
55face. Tracer’s purpose is to analyze the parameter estimates generated from a
56BEAST2 run. It shows, among others, the effective sample size (ESS) and time
57series (‘the trace’, hence the name) of each variable in the MCMC run. Both
58ESS and trace are needed to assess the strength of the inference. DensiTree vi-
59sualizes the phylogenies of a BEAST2 posterior, with many options to improve
60the simultaneous display of many phylogenies.

61 However, for exploring the output of many BEAST2 runs, one would like a
62script to collect all parameters’ ESSes, parameter traces and posterior phyloge-
63nies. There is no single package that offers a complete solution, but examples
64of R packages that offer a partial solution are rBEAST (Ratmann 2015) and
65RBeast (Faria & Suchard 2015). RBeast provides some plotting options and
66parsing of BEAST2 output files, but the plotting functions are too specific for
67general use, whilst the functions for parsing call those of **babette**. rBEAST was
68developed to test a particular biological hypothesis (Ratmann *et al.* 2016), and
69hence was not designed for general use.

70 Here, we present **babette**: BEAUti 2, BEAST2 and Tracer for R, which
71creates BEAST2 (v.2.4.7) configuration files, runs BEAST2, and analyzes its
72results, all from an R function call. This will save time, tedious mouse clicking
73and reduces the chances of errors in such repetitive actions. The interface of
74**babette** mimics the tools it is based on. This familiarity helps both beginner
75and experienced BEAST2 users to make the step from those tools to **babette**.
76**babette** enables the creation of a single-script pipeline from sequence alignments

77 to posterior analysis in R.

78 2 Description

79 **babette** is written in the R programming language (R Core Team 2013) and
80 enables the full BEAST2 workflow from an R function call, in a similar way
81 to what BEAUti, DensiTree and Tracer do. **babette**'s main function is **run**,
82 which configures BEAST2, runs it and parses its output. **run** needs at least the
83 name of a FASTA file containing a DNA alignment. The default settings for
84 the other arguments of **run** are identical to BEAUti's and BEAST2's default
85 settings. Per alignment, a site model, clock model and tree prior can be chosen.
86 Multiple alignments can be used, each with its own (unlinked) site model, clock
87 model and tree prior.

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

99 Currently, **babette** does not replace all functionality in BEAUti, BEAST2
100 and their many plug-ins. This is reasonable, as these themselves also change
101 in time. **babette** provides the majority of default tree priors and works only
102 on DNA data. **babette** supports the most important command-line arguments

103 of BEAST2, provides the core Tracer analysis options, and has the most basic
104 subset of plotting options of DensiTree. Up until now, the **babette** features
105 implemented are those requested by users. Further extension of **babette** will
106 be based on future user requests.

107 3 Usage

108 **babette** can be installed easily with the **devtools** package (Wickham & Chang
109 2016):

```
110 library(devtools)
111 install_github("richelbilderbeek/babette")
```

112 To start using **babette**, load its functions in the global namespace first:

```
113 library(babette)
```

114 For most convenience, let **babette** install BEAST2 to a default location:

```
115 install_beast2()
```

116 BEAUti, and likewise **babette**, needs at least a FASTA filename to produce a
117 BEAST2 configuration file. In BEAUti, this is achieved by loading a FASTA file,
118 then saving an output file using a common save file dialog. After this, BEAST2
119 needs to be applied to the created configuration file. It creates multiple files
120 storing the posterior. These output files must be parsed by either Tracer or
121 DensiTree. In **babette**, all this is achieved by:

```
122 out <- bbt_run(fasta_filenames = "anthus_aco.fas")
```

123 This code will create a (temporary) BEAST2 configuration file, from the FASTA
124 file with name **anthus_aco.fas** (which is supplied with the package, from
125 (Van Els & Norambuena 2018)), using the same default settings as BEAUti,
126 which are, among others, a Jukes-Cantor site model, a strict clock, and a Yule

127 birth tree prior. `babette` will then execute BEAST2 using that file, and parses
 128 the output. The returned data structure, named `out`, is a list of parameter
 129 estimates (called `estimates`), posterior phylogenies (called `anthus_aco_trees`,
 130 named after the alignment's name) and MCMC operator performance (`operators`).
 131 An example of using a different site model, clock model and tree prior is:

```
132 out <- bbt_run(  
133   fasta_filenames = "anthus_aco.fas",  
134   site_models = create_hky_site_model(),  
135   clock_models = create_rln_clock_model(),  
136   tree_priors = create_bd_tree_prior()  
137 )
```

138 This code uses an HKY site model, a relaxed log-normal clock model and a birth-
 139 death tree prior, each with their default settings in BEAUti. Table 1 shows an
 140 overview of all functions to create site models, clock models and tree priors. Note
 141 that the arguments' names `site_models`, `clock_models` and `tree_priors` are
 142 plural, as each of these can be (a list of) one or more elements. Each of these
 143 arguments must have the same number of elements, so that each alignment has
 144 its own site model, clock model and tree prior. An example of two alignments,
 145 each with its own site model, is:

```
146 out <- bbt_run(  
147   fasta_filenames = c(  
148     "anthus_aco.fas",  
149     "anthus_nd2.fas"  
150   ),  
151   site_models = list(  
152     create_tn93_site_model(),  
153     create_gtr_site_model()  
154   )
```

155)

156 **babette** also uses the same default prior distributions as BEAUti for each of
157 the site models, clock models and tree priors. For example, by default, a Yule
158 tree prior assumes that the birth rate follows a uniform distribution, from minus
159 infinity to plus infinity. One may prefer a different distribution instead. Here
160 is an example how to specify an exponential distribution for the birth rate in a
161 Yule tree prior in **babette**:

```
162 out <- bbt_run(  
163   fasta_filenames = "anthus_aco.fas",  
164   tree_priors = create_yule_tree_prior(  
165     birth_rate_distr = create_exp_distr()  
166   )  
167 )
```

168 In this same example, one may specify the initial shape parameters of the expo-
169 nential distribution. In BEAST2's implementation, an exponential distribution
170 has one shape parameter: its mean, which can be set to any value with BEAUti.
171 Within **babette**, to set the mean value of the exponential distribution to a fixed
172 (non-estimated) value, do:

```
173 out <- bbt_run(  
174   fasta_filenames = "anthus_aco.fas",  
175   tree_priors = create_yule_tree_prior(  
176     birth_rate_distr = create_exp_distr(  
177       mean = create_mean_param(  
178         value = 1.0,  
179         estimate = FALSE  
180       )  
181     )  
182   )
```

183)

184 **NOTE: suggest to remove this paragraph until node dating** Our initial
185 motivation to create **babette** was that we wanted to fix the crown age (the
186 time of first divergence) of a phylogeny. BEAUti assumes that a phylogeny has
187 a crown age that needs to be jointly estimated with the phylogeny and other
188 parameters. It does not allow for fixing the crown age. Without **babette**,
189 one needs to manually edit the BEAST2 configuration file, to remove all tree
190 operators that change the height of the root node, which is tedious and prone
191 to errors. Fixing the crown ages is useful when it is unnecessary to accurately
192 model the uncertainty of absolute divergence times. This is how to specify a
193 fixed crown age with **babette**:

```
194 out <- bbt_run(  
195   fasta_filenames = "anthus_aco.fas",  
196   posterior_crown_age = 15  
197 )
```

198 **babette** also supports node dating. Like BEAUti, one can specify Most Recent
199 Common Ancestor ('MRCA') priors. An MRCA prior allows to specify taxa
200 having a common ancestor, including a distribution for the date of that ancestor.
201 An application of such a prior is to specify a (close to) fixed crown age, by
202 including all taxa and assuming a tight normal distribution around the desired
203 crown age. Within **babette**, this is achieved as such:

```
204 out <- bbt_run(  
205   fasta_filenames = "anthus_aco.fas",  
206   mrca_priors = create_mrca_prior(  
207     taxa_names = get_taxa_names("anthus_aco.fas"),  
208     alignment_id = get_alignment_id("anthus_aco.fas"),  
209     mrca_distr = create_normal_distr(  

```



```

210     mean = create_mean_param(value = 15.0, estimate =
211         FALSE),
212     sigma = create_sigma_param(value = 0.01, estimate =
213         FALSE)
214 )
215 )
216 )

```

217 **babette** allows for the same core functionality as Tracer, in which it works on
218 the values of the parameter estimates sampled in the BEAST2 run. This is
219 called the "trace" (hence the name). The start of the trace is usually discarded,
220 as an MCMC algorithm (such as used by BEAST2) first has to converge to
221 its equilibrium. The start of the trace, called the "burn-in", will be removed,
222 because its parameter estimates are not representative. By default, Tracer dis-
223 cards the first 10% of all the parameter estimates. To remove a 20% burn-in
224 from all parameter estimates in **babette**, the following code can be used:

```

225 traces <- remove_burn_ins(
226     traces = out$estimates,
227     burn_in_fraction = 0.2
228 )

```

229 Tracer shows the ESSes of each posterior's variables. These ESSes are important
230 to determine the strength of the inference. As a rule of thumb, an ESS of 200 is
231 acceptable for any parameter estimate. To calculate the effective sample sizes
232 (of all estimated variables) in **babette**:

```

233 esses <- calc_esses(
234     traces = traces,
235     sample_interval = 1000
236 )

```

237 Tracer displays multiple summary statistics for each estimated variable: the
238 mean and its standard error, standard deviation, variance, median, mode, geo-
239 metric mean, 95% highest posterior density interval, auto-correlation time and
240 effective sample size. It displays these statistics per variable. In **babette**, these
241 summary statistics are collected for all estimated parameters at once:

```
242 sum_stats <- calc_summary_stats(  
243   traces = traces,  
244   sample_interval = 1000  
245 )
```

246 **babette** allows for the same functionality as DensiTree. DensiTree displays the
247 phylogenies in a posterior at the same time scale, drawn one over one another,
248 allowing to see the uncertainty in topology and branch lengths. Within the
249 object **out**, the posterior phylogenies are stored as **anthus_aco_trees**, and can
250 be plotted as such:

```
251 plot_densitree(phylos = out$anthus_aco_trees)
```

252 Instead of running the full pipeline, **babette** also allows to only create a BEAST2
253 configuration file. To create a BEAST2 configuration file, with all settings to
254 default, use:

```
255 create_beast2_input_file(  
256   input_filenames = babette::get_babette_path("anthus_aco.  
257     fas"),  
258   output_filename = "beast2.xml"  
259 )
```

260 This file can then be loaded and edited by BEAUti, or run by BEAST2. **babette**
261 also allows to only run BEAST2 from a BEAST2 configuration file:

```
262 run_beast2(  
263   input_filename = "beast2.xml",
```

```

264     output_log_filename = "run.log",
265     output_trees_filenames = "posterior.trees",
266     output_state_filename = "final.xml.state"
267 )

```

268 In this example, we specify the names of the desired BEAST2 output files. These
 269 output files can then be inspected with other tools, or to be used to continue a
 270 BEAST2 run. Also `bbt_run` supports to specify these filenames, and these files
 271 are put in a temporary folder by default.

272 4 **babette** resources

273 **babette** is free, libre and open source software available at [http://github.](http://github.com/richelbilderbeek/babette)
 274 [com/richelbilderbeek/babette](http://github.com/richelbilderbeek/babette) and is licensed under the GNU General Pub-
 275 lic License v3.0. **babette** uses the Travis CI (<https://travis-ci.org>) con-
 276 tinuous integration service, which is known to significantly increase the number
 277 of bugs exposed (Vasilescu *et al.* 2015) and increases the speed at which new
 278 features are added (Vasilescu *et al.* 2015). **babette** has a 100% code cover-
 279 age, which correlates with code quality (Horgan *et al.* 1994; Del Frate *et al.*
 280 1995). **babette** follows Hadley Wickham’s style guide (Wickham 2015), which
 281 improves software quality (Fang 2001). **babette** depends on multiple packages,
 282 which are **ape** (Paradis *et al.* 2004), **beautier** (Bilderbeek 2018b), **beastier**
 283 (Bilderbeek 2018a), **devtools** (Wickham & Chang 2016), **geiger** (Harmon *et al.*
 284 2008), **ggplot2** (Wickham 2009), **knitr** (Xie 2017), **phangorn** (Schliep 2011),
 285 **rmarkdown** (Allaire *et al.* 2017), **seqinr** (Charif & Lobry 2007), **stringr** (Wick-
 286 ham 2017), **testit** (Xie 2014) and **tracerer** (Bilderbeek 2018c). We tested
 287 **babette** to give a clean error message for incorrect input, by calling **babette**
 288 one million times with random or random sensible inputs, using the Peregrine
 289 high performance computer cluster. The scripts to do so are supplied with

290 **babette**.

291 **babette**'s development takes place on GitHub, <https://github.com/richelbilderbeek/>
292 **babette**, which accommodates collaboration (Perez-Riverol *et al.* 2016) and im-
293 proves transparency (Gorgolewski & Poldrack 2016). **babette**'s GitHub facili-
294 tates feature requests and has guidelines how to do so.

295 **babette**'s documentation is extensive. All functions are documented in the
296 package's internal documentation. For quick use, each exported function shows
297 a minimal example. For easy exploration, each exported function's documen-
298 tation links to related functions. Additionally, **babette** has a vignette that
299 demonstrates extensively how to use it. There is documentation on the GitHub
300 to get started, with a dozen examples of BEAUti screenshots with equivalent
301 **babette** code. Finally, **babette** has tutorial videos that can be downloaded or
302 viewed on YouTube, <https://goo.gl/weKaaU>.

303 5 Citation of babette

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

```
307 > citation("babette")
```

308 6 Acknowledgements

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317 to the Peregrine high performance computing cluster.

318 7 Authors’ contributions

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

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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

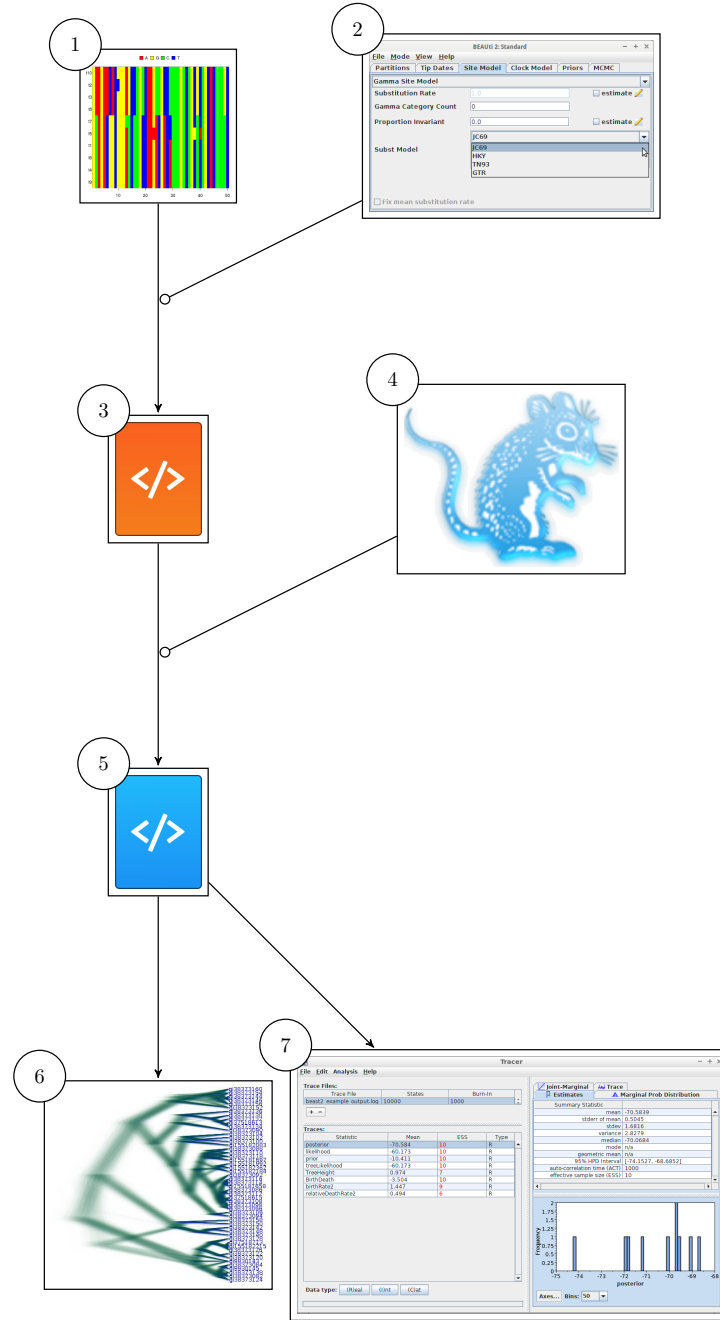


Figure 1: Workflow using GUI tools. From an alignment (1) and BEAUti (2), a BEAST2 configuration file (3) is created. BEAST2 (4) uses that file to infer a posterior, storing it in multiple files (5). These results are visualized using DensiTree (6) and Tracer (7). babette allows for the same workflow, all from an R function call.