

# 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 phylogenetic tree of a given set of species. BEAST2 (Bouckaert *et al.* 2014) is one of the most widely used ones. It creates a posterior of jointly 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 manageable 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 BEAST2 model configuration and a Microsoft Excel file to specify alignment files.

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

59 However, for exploring the output of many BEAST2 runs, one would like a  
 60script to collect all parameters’ ESSes, parameter traces and posterior phyloge-  
 61nies. There is no single package that offers a complete solution, but examples  
 62of R packages that offer a partial solution are rBEAST (Ratmann 2015) and  
 63RBeast (Faria & Suchard 2015). RBeast provides some plotting options and  
 64parsing of BEAST2 output files, but the plotting functions are too specific for  
 65general use, where the functions for parsing call those of **babette**. rBEAST was  
 66developed to test a particular biological hypothesis (Ratmann *et al.* 2016), and  
 67hence was not designed for general use.

68 Here, we present **babette**: BEAUti 2, BEAST2 and Tracer for R, which  
 69creates BEAST2 (v.2.4.7) configuration files, runs BEAST2, and analyzes its  
 70results, all from an R function call. This will save time, tedious mouse clicking  
 71and reduces the chances of errors in such repetitive actions. The interface of  
 72**babette** mimics the tools it is based on. This familiarity helps both beginner  
 73and experienced BEAST2 users to make the step from those tools to **babette**.  
 74**babette** enables the creation of a single-script pipeline from sequence alignments  
 75to posterior analysis in R.

## 76 2 Description

77 **babette** is written in the R programming language (R Core Team 2013) and en-  
78 ables the full BEAST2 workflow from an R function call, in a similar way to what  
79 BEAUti, DensiTree and Tracer do. **babette**'s main function is `run_beast2`,  
80 which configures BEAST2, runs it and parses its output. `run_beast2` needs  
81 at least the name of a FASTA file containing a DNA alignment. The default  
82 settings for the other arguments of `run_beast2` are identical to BEAUti's and  
83 BEAST2's default settings. Per alignment, a site model, clock model and tree  
84 prior can be chosen. Multiple alignments can be used, each with its own (un-  
85 linked) site model, clock model and tree prior.

86 **babette** currently has 100 exported functions to set up a BEAST2 config-  
87 uration file. **babette** can currently handle a majority of BEAUti use cases.  
88 Because of BEAUti's high number of plugins, **babette** uses a software architec-  
89 ture that is designed to be extended. Furthermore, **babette** has 12 exported  
90 functions to run and help run BEAST2. One function is used to run BEAST2,  
91 others allow the user to check if a BEAST2 configuration file is indeed valid.  
92 Finally, **babette** has 21 exported function to parse the BEAST2 output files  
93 and analyze the created posterior. **babette** gives the same ESSes and summary  
94 statistics as Tracer. The data is formatted such that it can easily be visualized  
95 using `ggplot2` (for a trace, similar to Tracer) or `phangorn` (Schliep 2011) (for  
96 the phylogenies in a posterior, similar to DensiTree).

97 Currently, **babette** does not replace all functionality in BEAUti, as it does  
98 not provide 3 out of 7 tree priors, nor does it support RNA alignments or  
99 use of morphological data. The many plug-ins of BEAUti are not yet sup-  
100 ported by **babette**. **babette** does not support all command-line arguments of  
101 BEAST2, does not provide the more specialized Tracer analysis options, nor is it  
102 as feature-rich in plotting options as DensiTree. Up until now, the **babette** fea-

103 tures implemented are those requested by users. Further extension of **babette**  
104 will be based on future user requests.

### 105 **3 Usage**

106 In R, the functions of a package need to be loaded in the global namespace first:

```
107 library(babette)
```

108 BEAUti, and likewise **babette**, needs at least a FASTA filename to produce a  
109 BEAST2 configuration file. In BEAUti, this is achieved by loading a FASTA file,  
110 then saving an output file using a common save file dialog. After this, BEAST2  
111 needs to be applied to the created configuration file. It creates multiple files  
112 storing the posterior. These output files must be parsed by either Tracer of  
113 DensiTree. In **babette**, all this is achieved by:

```
114 out <- run_beast2("anthus_aco.fas")
```

115 This code will create a (temporary) BEAST2 configuration file, from the FASTA  
116 file with name **anthus\_aco.fas** (which is supplied with the package, from  
117 (Van Els & Norambuena 2018)), using the same default settings as BEAUti,  
118 which are, among others, a Jukes-Cantor site model, a strict clock, and a Yule  
119 birth tree prior. **babette** will then execute BEAST2 using that file, and parses  
120 the output. The returned data structure, named **out**, is a list of parameter  
121 estimates (called **estimates**), posterior phylogenies (called **anthus\_aco\_trees**,  
122 named after the alignment's name) and MCMC operator performance (**operators**).  
123 An example of using a different site model, clock model and tree prior is:

```
124 out <- run_beast2(  
125   "anthus_aco.fas",  
126   site_models = create_hky_site_model(),  
127   clock_models = create_rln_clock_model(),
```

```

128     tree_priors = create_bd_tree_prior()
129 )

```

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

```

138 out <- run_beast2(
139   c("anthus_aco.fas", "anthus_nd2.fas"),
140   site_models = list(
141     create_tn93_site_model(),
142     create_gtr_site_model()
143   )
144 )

```

**babette** also uses the same default prior distributions as BEAUti for each of the site models, clock models and tree priors. For example, by default, a Yule tree prior assumes that the birth rate follows a uniform distribution, from minus infinity to plus infinity. This assumption implies that negative and positive birth rates are just as likely, where a negative birth rate is biologically impossible (note that in practice, this usually works out just fine). One may prefer an exponential distribution instead, as this would assume only positive birth rates, and makes high birth rates unlikely. To do this in **babette**:

```

153 out <- run_beast2(
154   "anthus_aco.fas",

```

```

155     tree_priors = create_yule_tree_prior(
156         birth_rate_distr = create_exp_distr()
157     )
158 )

```

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

```

164 out <- run_beast2(
165     "anthus_aco.fas",
166     tree_priors = create_yule_tree_prior(
167         birth_rate_distr = create_exp_distr(
168             mean = create_mean_param(
169                 value = 1.0,
170                 estimate = FALSE
171             )
172         )
173     )
174 )

```

175 Our initial motivation to create **babette** was that we wanted to fix the crown  
176 age of a phylogeny. BEAUti assumes that a phylogeny has a crown age that  
177 needs to be jointly estimated with the phylogeny and other parameters. It does  
178 not allow for fixing the crown age. Without **babette**, one needs to manually edit  
179 the BEAST2 configuration file (Bouckaert & Vaughan 2017), which is tedious  
180 and prone to errors. Fixing the crown ages is especially useful for theoretical  
181 experiments, as this allows for one less source of variation. This is how to specify  
182 a fixed crown age with **babette**:

```

183 out <- run_beast2(
184   "anthus_aco.fas",
185   posterior_crown_age = 15
186 )

```

187 **babette** allows for the same functionality as Tracer. Tracer works on the values  
188 of the parameter estimates sampled in the BEAST2 run. This is called the  
189 "trace" (hence the name). The start of the trace is usually discarded, as an  
190 MCMC algorithm (such as used by BEAST2) first has to converge to its equi-  
191 librium. The start of the trace, called the "burn-in", will be removed, because  
192 its parameter estimates are not representative. By default, Tracer discards the  
193 first 10% of all the parameter estimates. To remove a 20% burn-in from all  
194 parameter estimates in **babette**, the following code can be used:

```

195 traces <- remove_burn_ins(
196   out$estimates,
197   burn_in_fraction = 0.2
198 )

```

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

```

203 esses <- calc_esses(
204   traces,
205   sample_interval = 1000
206 )

```

207 Tracer displays multiple summary statistics for each estimated variable: the  
208 mean and its standard error, standard deviation, variance, median, mode, geo-  
209 metric mean, 95% highest posterior density interval, auto-correlation time and



210 effective sample size. It displays these statistics per variable. In **babette**, these  
211 summary statistics are collected for all estimated parameters at once:

```
212 sum_stats <- calc_summary_stats(  
213   traces ,  
214   sample_interval = 1000  
215 )
```

216 **babette** allows for the same functionality as **DensiTree**. **DensiTree** displays the  
217 phylogenies in a posterior at the same time scale, drawn one over one another,  
218 allowing to see the uncertainty in topology and branch lengths. Within the  
219 object **out**, the posterior phylogenies are stored as **anthus\_aco\_trees**, and can  
220 be plotted as such:

```
221 plot_densitree(out$anthus_aco_trees)
```

## 222 4 **babette** resources

223 **babette** is free, libre and open source software available from the official R pack-  
224 age archive at <http://cran.r-project.org/src/contrib/PACKAGES.html#babette>  
225 and is licensed under the GNU General Public License v3.0. **babette** uses the  
226 Travis CI (<https://travis-ci.org>) continuous integration service, which is  
227 known to significantly increase the number of bugs exposed (Vasilescu *et al.*  
228 2015) and increases the speed at which new features are added (Vasilescu *et al.*  
229 2015). **babette** has a 100% code coverage, which correlates with code quality  
230 (Horgan *et al.* 1994; Del Frate *et al.* 1995). **babette** follows Hadley Wickham's  
231 style guide (Wickham 2015), which improves software quality (Fang 2001).  
232 **babette** depends on multiple packages, which are **ape** (Paradis *et al.* 2004),  
233 **beautier** (Bilderbeek 2018b), **beastier** (Bilderbeek 2018a), **devtools** (Wick-  
234 ham & Chang 2016), **geiger** (Harmon *et al.* 2008), **ggplot2** (Wickham 2009),

235 `knitr` (Xie 2017), `phangorn` (Schliep 2011), `rmarkdown` (Allaire *et al.* 2017),  
236 `seqinr` (Charif & Lobry 2007), `stringr` (Wickham 2017), `testit` (Xie 2014)  
237 and `tracerer` (Bilderbeek 2018c). `babette` is tested to give a clean error mes-  
238 sage for incorrect input, by calling `babette` one million times with random or  
239 random sensible inputs, using the Peregrine high performance computer cluster.  
240 The scripts to do so, are supplied with `babette`.

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

245 `babette`'s documentation is extensive. All functions are documented in the  
246 package's internal documentation. For quick use, each exported function shows  
247 a minimal example. For easy exploration, each exported function's documen-  
248 tation links to related functions. Additionally, `babette` has a vignette that  
249 demonstrates extensively how to use it. There is documentation on the GitHub  
250 to get started, with a dozen examples of BEAUti screenshots with equivalent  
251 `babette` code. Finally, `babette` has some tutorial video's that can be down-  
252 loaded or viewed on YouTube, <https://goo.gl/weKaaU>.

## 253 5 Citation of `babette`

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

```
257 > citation("babette")
```

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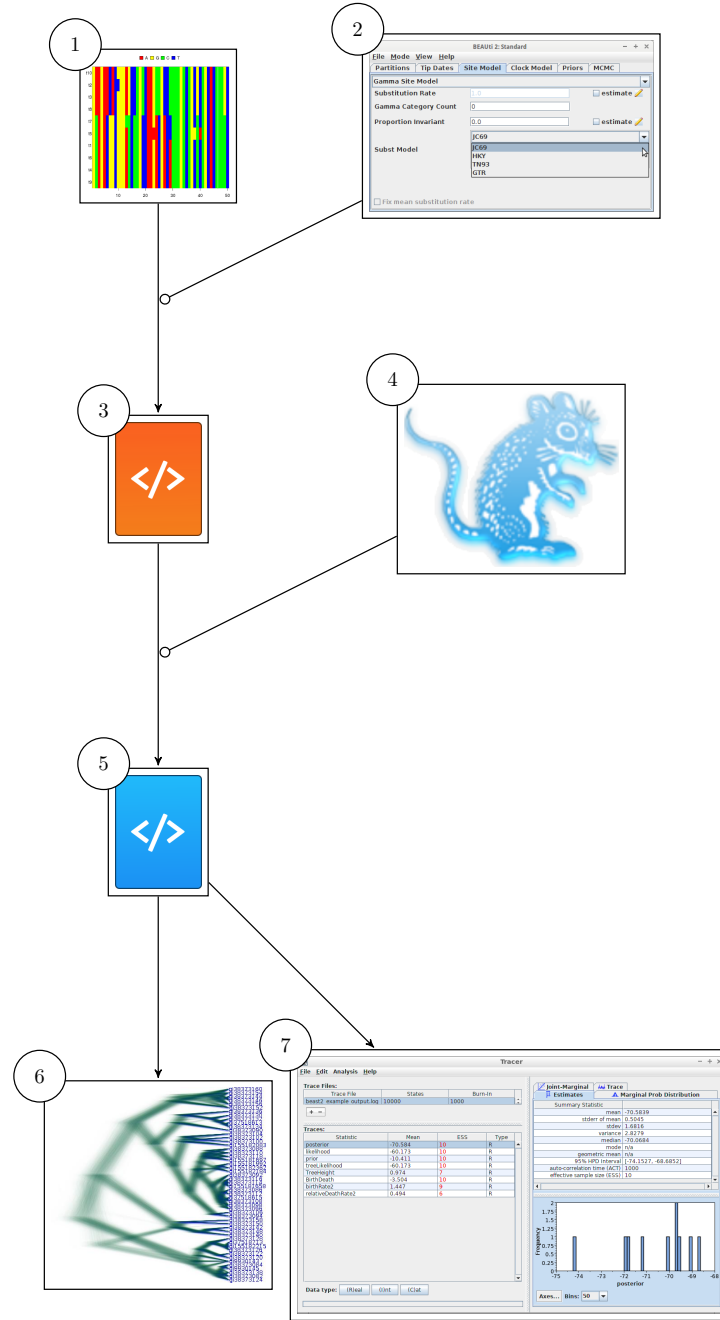


Figure 1: Workflow using GUI tools. From an alignment (1) and BEAUti (2), a BEAST2 configuration file (3) is created. BEAST2 (4) uses that file to infer a posterior, storing it in multiple files (5). These results are visualized using DensiTree (6) and Tracer (7). babette allows for the same workflow,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

Name	Description
run_beast2	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