

# 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 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

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. rBEAST was developed to test a particular biological hypothesis  
68(Ratmann *et al.* 2016), and hence was not designed for general use.

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

## 77 2 Description

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

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

98 Currently, **babette** does not contain all functionality in BEAUti, BEAST2  
99 and their many plug-ins, because these tools themselves also change in time.  
100 **babette** currently works only on DNA data, because this is the most common  
101 use case. Nevertheless, **babette** provides the majority of default tree priors and  
102 supports the most important command-line arguments of BEAST2, provides the  
103 core Tracer analysis options, and has the most basic subset of plotting options of

104 DensiTree. Up till now, the **babette** features implemented are those requested  
105 by users. Further extension of **babette** will be based on future user requests.

## 106 **3 Usage**

107 **babette** can be installed easily from CRAN:

```
108 install.packages("babette")
```

109 For the most up-to-date version, one can download and install the package from  
110 **babette**'s GitHub repository:

```
111 devtools::install_github("richelbilderbeek/babette")
```

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

```
113 library(babette)
```

114 Because **babette** calls BEAST2, BEAST2 must be installed. This can be done  
115 from R, using:

```
116 install_beast2()
```

117 This will install BEAST2 to the default user data folder, but a different path  
118 can be specified as well. BEAUti, and likewise **babette**, needs at least a FASTA  
119 filename to produce a BEAST2 configuration file. In BEAUti, this is achieved  
120 by loading a FASTA file, then saving an output file using a common save file  
121 dialog. After this, BEAST2 needs to be applied to the created configuration  
122 file. It creates multiple files storing the posterior. These output files must be  
123 parsed by either Tracer or DensiTree. In **babette**, all this is achieved by:

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

125 This code will create a (temporary) BEAST2 configuration file, from the FASTA  
126 file with name **anthus\_aco.fas** (which is supplied with the package, from  
127 (Van Els & Norambuena 2018)), using the same default settings as BEAUti,

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

```
134 out <- bbt_run(  
135   fasta_filenames = "anthus_aco.fas",  
136   site_models = create_hky_site_model(),  
137   clock_models = create_rln_clock_model(),  
138   tree_priors = create_bd_tree_prior()  
139 )
```

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

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

```
156     )
```

```
157 )
```

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

```
164 out <- bbt_run(  
165   fasta_filenames = "anthus_aco.fas",  
166   tree_priors = create_yule_tree_prior(  
167     birth_rate_distr = create_exp_distr()  
168   )  
169 )
```

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

```
175 out <- bbt_run(  
176   fasta_filenames = "anthus_aco.fas",  
177   tree_priors = create_yule_tree_prior(  
178     birth_rate_distr = create_exp_distr(  
179       mean = create_mean_param(  
180         value = 1.0,  
181         estimate = FALSE  
182       )  
183     )  
184   )  
185 )
```

184     )

185     )

186 **babette** also supports node dating. Like BEAUti, one can specify Most Recent  
187 Common Ancestor ('MRCA') priors. An MRCA prior allows to specify taxa  
188 having a common ancestor, including a distribution for the date of that ancestor.  
189 With **babette**, this is achieved as follows:

```
190 out <- bbt_run(  
191   fasta_filenames = "anthus_aco.fas",  
192   mrca_priors = create_mrca_prior(  
193     taxa_names = sample(get_taxa_names("anthus_aco.fas"),  
194       size = 2),  
195     alignment_id = get_alignment_id("anthus_aco.fas"),  
196     is_monophyletic = TRUE,  
197     mrca_distr = create_normal_distr(  
198       mean = create_mean_param(value = 15.0, estimate =  
199         FALSE),  
200       sigma = create_sigma_param(value = 0.025, estimate =  
201         FALSE)  
202     )  
203   )  
204 )
```

205 Instead of dating the ancestor of two random taxa, any subset of taxa can  
206 be selected, and multiple sets are allowed. **babette** allows for the same core  
207 functionality as Tracer to show the values of the parameter estimates sampled  
208 in the BEAST2 run. This is called the "trace" (hence the name). The start  
209 of the trace, called the "burn-in", is usually discarded, as an MCMC algorithm  
210 (such as used by BEAST2) first has to converge to its equilibrium and hence  
211 the parameter estimates are not representative. By default, Tracer discards the



212 first 10% of all the parameter estimates. To remove a 20% burn-in from all  
213 parameter estimates in **babette**, the following code can be used:

```
214 traces <- remove_burn_ins(  
215   traces = out$estimates,  
216   burn_in_fraction = 0.2  
217 )
```

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

```
222 esses <- calc_esses(  
223   traces = traces,  
224   sample_interval = 1000  
225 )
```

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

```
231 sum_stats <- calc_summary_stats(  
232   traces = traces,  
233   sample_interval = 1000  
234 )
```

235 **babette** allows for the same functionality as **DensiTree**. **DensiTree** displays the  
236 phylogenies in a posterior at the same time scale, drawn one over one another,  
237 allowing to see the uncertainty in topology and branch lengths. The posterior  
238 phylogenies are stored as **anthus\_aco\_trees** in the object **out**, and can be

239 plotted as follows:

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

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

```
244 create_beast2_input_file(  
245     input_filenames = babette::get_babette_path("anthus_aco.  
246         fas"),  
247     output_filename = "beast2.xml"  
248 )
```

249 This file can then be loaded and edited by BEAUti, run by BEAST2, or run by  
250 **babette**:

```
251 run_beast2(  
252     input_filename = "beast2.xml",  
253     output_log_filename = "run.log",  
254     output_trees_filenames = "posterior.trees",  
255     output_state_filename = "final.xml.state"  
256 )
```

257 In this example, we specify the names of the desired BEAST2 output files.  
258 These output files can then be inspected with other tools, or used to continue a  
259 BEAST2 run. **bbt\_run** supports specifying the folder and name of these files,  
260 which defaults to a temporary folder to keep the working directory clean of  
261 intermediate and temporary files.

## 262 4 **babette** resources

263 **babette** is free, libre and open source software available at [http://github.](http://github.com/richelbilderbeek/babette)  
264 [com/richelbilderbeek/babette](http://github.com/richelbilderbeek/babette) and is licensed under the GNU General Pub-

265 lic License v3.0. **babette** uses the Travis CI (<https://travis-ci.org>) con-  
 266 tinuous integration service, which is known to significantly increase the number  
 267 of bugs exposed (Vasilescu *et al.* 2015) and increases the speed at which new  
 268 features are added (Vasilescu *et al.* 2015). **babette** has a 100% code cover-  
 269 age, which correlates with code quality (Horgan *et al.* 1994; Del Frate *et al.*  
 270 1995). **babette** follows Hadley Wickham’s style guide (Wickham 2015), which  
 271 improves software quality (Fang 2001). **babette** depends on multiple packages,  
 272 which are **ape** (Paradis *et al.* 2004), **beautier** (Bilderbeek 2018b), **beastier**  
 273 (Bilderbeek 2018a), **devtools** (Wickham & Chang 2016), **geiger** (Harmon *et al.*  
 274 2008), **ggplot2** (Wickham 2009), **knitr** (Xie 2017), **phangorn** (Schliep 2011),  
 275 **rmarkdown** (Allaire *et al.* 2017), **seqinr** (Charif & Lobry 2007), **stringr** (Wick-  
 276 ham 2017), **testit** (Xie 2014) and **tracerer** (Bilderbeek 2018c). We tested  
 277 **babette** to give a clean error message for incorrect input, by calling **babette**  
 278 one million times with random or random sensible inputs, using the Peregrine  
 279 high performance computer cluster. The test scripts are supplied with **babette**.  
 280 **babette**’s development takes place on GitHub, <https://github.com/richelbilderbeek/>  
 281 **babette**, which accommodates collaboration (Perez-Riverol *et al.* 2016) and im-  
 282 proves transparency (Gorgolewski & Poldrack 2016). **babette**’s GitHub facili-  
 283 tates feature requests and has guidelines how to do so.  
 284 **babette**’s documentation is extensive. All functions are documented in the  
 285 package’s internal documentation. For quick use, each exported function shows  
 286 a minimal example. For easy exploration, each exported function’s documen-  
 287 tation links to related functions. Additionally, **babette** has a vignette that  
 288 demonstrates extensively how to use it. There is documentation on the GitHub  
 289 to get started, with a dozen examples of BEAUti screenshots with equivalent  
 290 **babette** code. Finally, **babette** has tutorial videos that can be downloaded or  
 291 viewed on YouTube, <https://goo.gl/weKaaU>.

## 292 5 Citation of babette

293 Scientists using **babette** in a published paper can cite this article, and/or cite  
294 the **babette** package directly. To obtain this citation from within an R script,  
295 use:  
296 `> citation("babette")`

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## 307 7 Authors’ contributions

308 RJCB and RSE conceived the idea for the package. RJCB created and tested  
309 the package, and wrote the first draft of the manuscript. RSE contributed  
310 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