

bgphy, a package for Bayesian analysis of mixed Gaussian phylogenetic models.

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The package at a glance

This package performs Bayesian inference of a class of phylogenetic comparative methods (PCM) which assumes Gaussian processes, specifically Brownian Motion (BM) or Ornstein-Uhlenbeck process (OU), as a model of univariate traits evolution on a phylogenetic tree. Moreover, it performs inferences of mixed Gaussian phylogenetic models (MGPM). In this setting, a phylogenetic tree can be partitioned into multiple different “evolutionary regimes” which consist of different processes along with different parameters.

The package uses [PCMBase](#) (Mitov et al. 2020) as the engine for high-speed likelihood calculations. A user-friendly interface for customizing priors and regime configurations is also provided. The Bayesian inference is done using an importance-sampling based algorithm to compute statistics of the posterior distribution, which utilizes R’s native `parallel` package to accelerate inference time.

Parameters notation

The BM and OU processes can be written by the following stochastic differential equations (SDEs):

- BM: $dx(t) = \sigma dW(t)$,
- OU: $dx(t) = -\alpha(x(t) - \theta)dt + \sigma dW(t)$,

where $x(t)$ is the trait at time t , $W(t)$ is a Wiener process at time t . The parameter α can be interpreted as the strength of random fluctuation, while α is the strength of selection (or convergence rate) into an optimum value θ . Notice that, BM is a specific case of an OU process when $\alpha = 0$. The ancestral state is also considered a parameter, which is denoted by X_0 .

Given measurements on the tips \mathbf{x}_{tips} and a model \mathcal{M} with a fixed regimes configurations and parameters Θ , the goal is to calculate the posterior distribution

$$P(\Theta|\mathbf{x}_{\text{tips}}) \propto P(\mathbf{x}_{\text{tips}}|\Theta)P(\Theta),$$

and compare different configurations, $\mathcal{M}_1(\Theta_1)$ vs $\mathcal{M}_2(\Theta_2)$ vs \dots vs $\mathcal{M}_m(\Theta_m)$.

Installation

```
devtools::install_github("bayubeta/bgphy", build_vignettes = TRUE)
```

Getting started

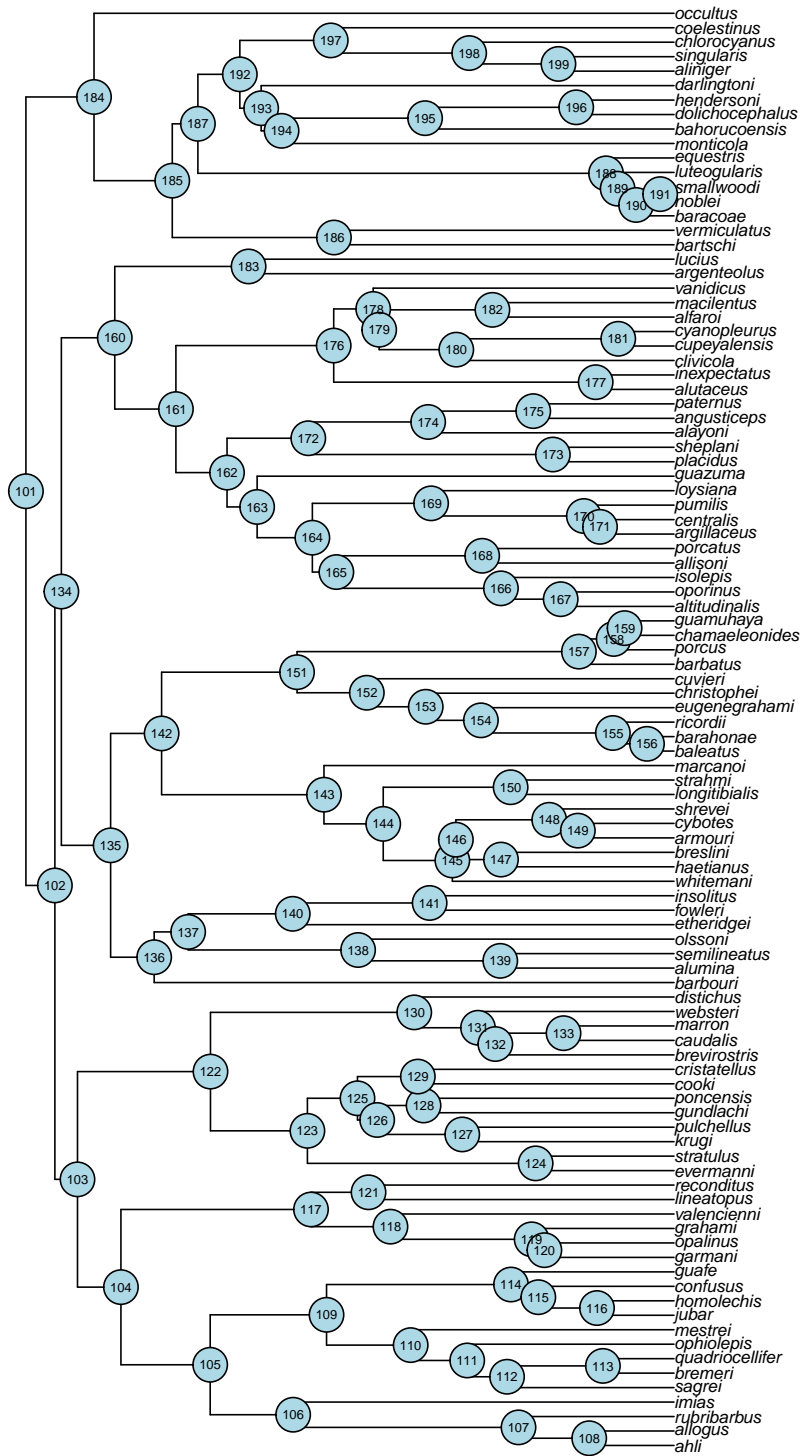
Loading the package:

```
library(bgphy)
library(ape)
```

Constructing a model using `setModel()`

Given a phylogenetic tree of class `phylo`, we can construct a model by using `setModel()` function by specifying the model types ("BM" or "OU") and their position in the tree. For example, we use the phylogenetic tree of Caribbean anoles (Mahler et al. 2013; retrieved from Bastide and Didier 2023) . The tree is available within the package as `lizardTree`. Below is the tree plotted with its node numbers:

```
plot(lizardTree, no.margin = TRUE, cex = 0.7)
nodelabels(cex = 0.5, frame = "circle")
```



Global model

Assume that the traits are evolving under the same process throughout all parts of the tree (BM or OU). To construct such model we can run:

```
# Brownian Motion (BM)
BM <- setModel(tree = lizardTree, regime_names = "R1", modeltypes = "BM")

# Ornstein-Uhlenbeck (OU)
OU <- setModel(tree = lizardTree, regime_names = "R1", modeltypes = "OU")
```

This will return an object of class `bgphy_model` which contains the information of the model in `PCMBase`, the tree, and the default priors for the parameters of the model. The information of the models can be printed:

```
print(BM)
```

Regime	Model
-----	-----
R1	BM(sigma)

```
Priors:
X0 ~ normal(mean = 0, sd = 10)
sigma ~ halft(nu = 1, sigma = 3)
```

```
print(OU)
```

Regime	Model
-----	-----
R1	OU(alpha, theta, sigma)

```
Priors:
X0 ~ normal(mean = 0, sd = 10)
alpha ~ halfnormal(sigma = 6.931472)
theta ~ normal(mean = 0, sd = 10)
sigma ~ halft(nu = 1, sigma = 3)
```

Mixed model

Suppose we are interested in splitting the tree into two regimes:

- Ancestral: starts from the ancestral node (101).
- New: starts from node 135.

Furthermore, the ancestral regime is assumed to follow a BM process while the New regime follows an OU process. The model is constructed as:

```
BMOU <- setModel(tree = lizardTree, regime_names = c("Ancestral", "New"),
                 modeltypes = c("BM", "OU"),
                 startNodes = list(Ancestral = "101", New = "135"))
print(BMOU)
```

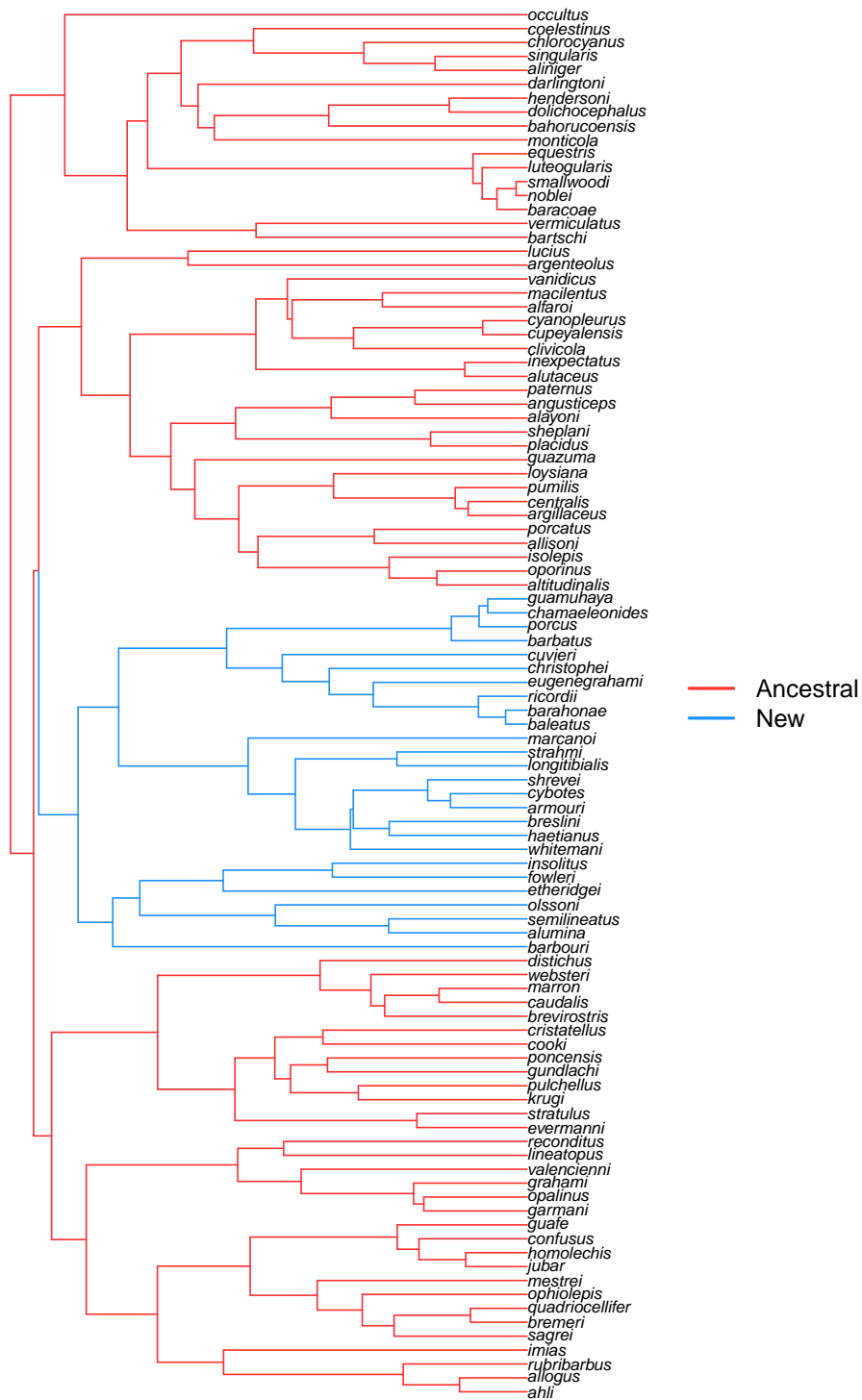
Regime	Model
-----	-----
Ancestral	BM(sigma_1)
New	OU(alpha_2, theta_2, sigma_2)

Priors:

```
X0 ~ normal(mean = 0, sd = 10)
sigma_1 ~ halft(nu = 1, sigma = 3)
alpha_2 ~ halfnormal(sigma = 6.931472)
theta_2 ~ normal(mean = 0, sd = 10)
sigma_2 ~ halft(nu = 1, sigma = 3)
```

Using the function `plot_regimes()`, the regimes can be visualized on top of the tree:

```
plot_regimes(BMOU$tree, no.margin = TRUE, x.lim = c(0,1.6), cex = 0.7)
```



A more complicated configuration

Let's say that there are three regimes:

- R1: starts from the ancestral node (101), but includes the taxa *ahli*, *lucius*, and *darlingtoni*. Follows a BM process.
- R2: starts from node 104 and 160, follows an OU process.
- R3: starts from node 184, follows an OU process.

The model can be constructed as follows:

```
model3 <- setModel(tree = lizardTree, regime_names = c("R1", "R2", "R3"),
                  modeltypes = c("BM", "OU", "OU"),
                  startNodes = list(R1 = c("101", "ahli", "lucius", "darlingtoni"),
                                   R2 = c("104", "160"),
                                   R3 = c("184")))

print(model3)
```

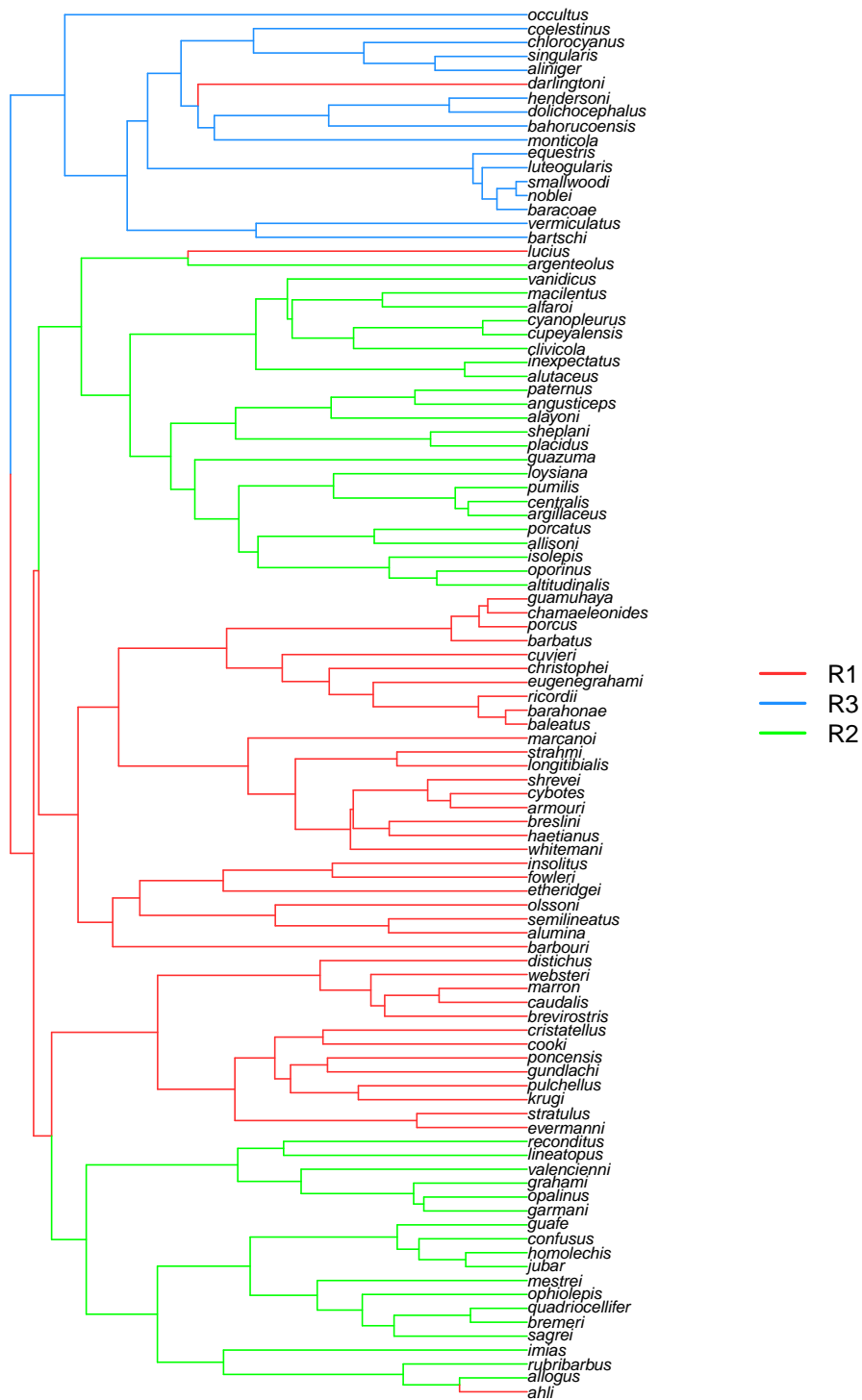
Regime	Model
-----	-----
R1	BM(sigma_1)
R2	OU(alpha_2, theta_2, sigma_2)
R3	OU(alpha_3, theta_3, sigma_3)

Priors:

```
X0 ~ normal(mean = 0, sd = 10)
sigma_1 ~ halft(nu = 1, sigma = 3)
alpha_2 ~ halfnormal(sigma = 6.931472)
theta_2 ~ normal(mean = 0, sd = 10)
sigma_2 ~ halft(nu = 1, sigma = 3)
alpha_3 ~ halfnormal(sigma = 6.931472)
theta_3 ~ normal(mean = 0, sd = 10)
sigma_3 ~ halft(nu = 1, sigma = 3)
```

And the regimes configuration can be shown by:

```
plot_regimes(model3$tree, no.margin = TRUE, x.lim = c(0,1.6), cex = 0.7)
```



Specifying the priors

By default, the priors for each parameters are given as follows:

- $X_0 \sim \text{Normal}(\mu = 0, \sigma^2 = 100)$,
- $\alpha \sim \text{Half-Normal}(\sigma = \log(2)/(2 \cdot 0.05 \cdot \ell_T))$,
- $\theta \sim \text{Normal}(\mu = 0, \sigma^2 = 100)$,
- $\sigma \sim \text{Half-t}(\nu = 1, \sigma = 3\ell_T)$,

in which ℓ_T is the height of the tree.

We can customize the priors by changing the elements of the `model$priors` by `priorpdf` objects provided by `bgphy`:

`?bgphy::priorpdf`

For example, we want to modify priors of the regime “New” in the BMOU model:

```
BMOU$priors$alpha_2 <- prior_halfnormal(sigma = 2)
BMOU$priors$theta_2 <- prior_normal(mean = 2, sd = 5)
BMOU$priors$sigma_2 <- prior_halfnormal(nu = 1, sigma = 2)
print(BMOU$priors)
```

```
X0 ~ normal(mean = 0, sd = 10)
sigma_1 ~ halft(nu = 1, sigma = 3)
alpha_2 ~ halfnormal(sigma = 2)
theta_2 ~ normal(mean = 2, sd = 5)
sigma_2 ~ halft(nu = 1, sigma = 2)
```

Running the posterior inference using `bgphy()`

The main function of the package is the `bgphy()` function, which takes arguments:

- `model`: an object of class `bgphy_model`, constructed by using `setModel()`.
- `X`: a data matrix of dimension $1 \times N$, where N is the number of tips of the tree. The column names of `X` must match the tip labels, that can be accessed by `model$tree$tip.label`.
- `nsample`: number of particles for the importance sampling method (the default is 10000).

- **parallel**: a Boolean variable determining the use of paralleled computing for the algorithm. By default is set to **TRUE**.

For this example, let us use simulated dataset **XOU** that is available in the package. This dataset contains 100 realizations of simulation under a certain OU process on the same tree that we currently use (Caribbean anoles). Since the data matrix needs to have column names that match the names on the tips of the tree, and since **XOU** consists of 100 realizations of the simulation, we can pick only one row for our example, and turn it into a format that the **bgphy()** accepts:

```
X <- matrix(XOU[1,], nrow = 1, dimnames = list(NULL, colnames(XOU)))
```

Let us run a Bayesian inference of the model specified by **BMOU** and using the data **X**, and using 10000 particles. The processing time of the algorithm is also recorded.

```
set.seed(1234, kind = "L'Ecuyer-CMRG")
start <- Sys.time()
post_BMOU <- bgphy(model = BMOU, X = X)
end <- Sys.time()
```

The **bgphy()** function outputs an object of class **bgphy_posterior**, and the posterior information can be seen by:

```
print(post_BMOU)
```

	mean	std_error	std	2.5%	50%	97.5%
X0	1.6497361	0.0017670605	0.14828686	1.3695102	1.649160	1.9371391
sigma_1	0.6561341	0.0004564267	0.03856066	0.5878940	0.654138	0.7393092
alpha_2	2.1116874	0.0092210576	0.75019883	0.8576021	2.061707	3.7467182
theta_2	1.3602997	0.0019099498	0.17924395	0.9305668	1.366556	1.7346952
sigma_2	1.2422369	0.0022161494	0.18558202	0.9294802	1.227065	1.6435897

```
Posterior predictive loss: 66.62103
ESS: 4692.53792
```

Where **mean** denotes the posterior mean, as seen from each parameter, with **std_error** determines the standard error of the **mean**. The column **std** shows the standard deviation of the posterior distribution, while the last three columns describe the 2.5-th, 50-th (median), and 97.5-th percentile of the marginal posterior distribution. The posterior predictive loss score is also shown, where a lower value indicates a better fit to the data, along with the effective sample size.

Furthermore, it contains a matrix \mathbf{Q} and a vector \mathbf{W} which are samples from the proposal distribution (multivariate Normal) and the (normalized) importance weights.

The processing time takes around

```
end - start
```

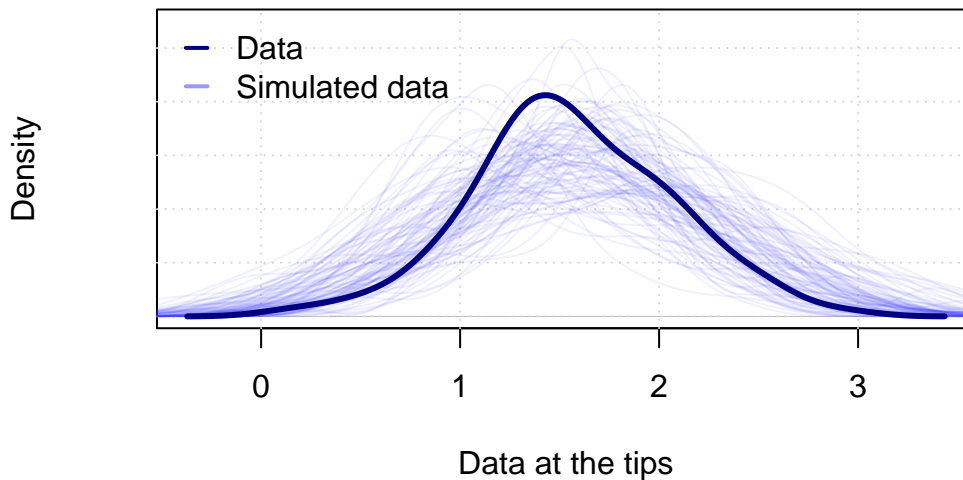
Time difference of 2.326678 mins

on a personal computer with 6-cores AMD Ryzen 5 PRO 4650U with Radeon Graphics 2.10 GHz processor, and 16 GB of RAM.

Posterior predictive distribution check using `post_pred_check()`

We can also see how the posterior distribution of our model fits the original data by simulating data from the posterior predictive distribution using `post_pred_check()`:

```
post_pred_check(post_BMOU)
```



As we can see, the simulated data do not look very similar to the original data, since we assumed a mixed BM to OU model while the original data was simulated from a global OU model.

Let us now do the same procedure, but with an OU model defined in `OU`:

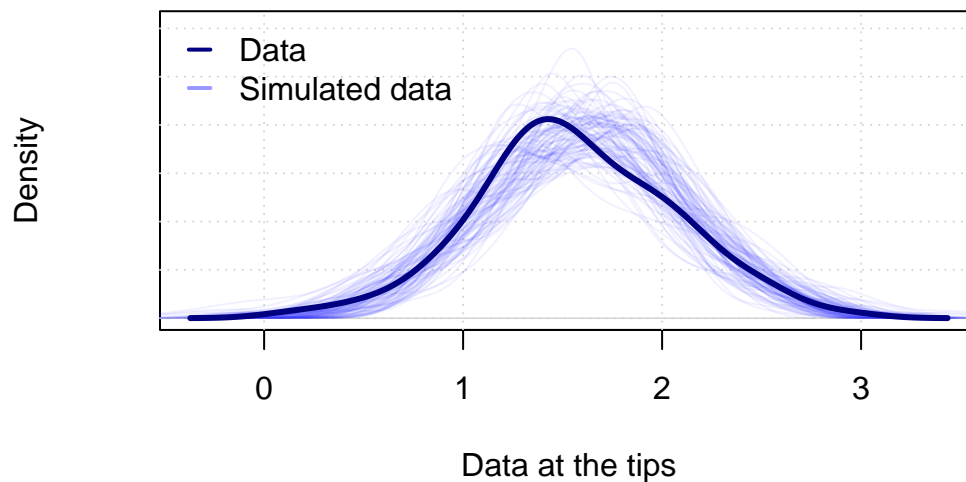
```
set.seed(1234, kind = "L'Ecuyer-CMRG")
post_OU <- bgphy(model = OU, X = X)
print(post_OU)
```

	mean	std_error	std	2.5%	50%	97.5%
X0	-0.143531	0.0579929496	5.3412588	-11.0693785	-0.01421786	10.133323
alpha	2.625908	0.0048023139	0.4757488	1.8203813	2.60379288	3.724987
theta	1.738204	0.0047071941	0.4362034	0.9166749	1.70047103	2.662816
sigma	1.100510	0.0009972653	0.1009060	0.9101860	1.09575100	1.318059

Posterior predictive loss: 48.34376
ESS: 6566.27953

As we can see, the posterior predictive loss is lower (better) than the previous mixed-model. The simulated data curves from the posterior predictive distribution also resemble the original data curve better, as shown on the following plot:

```
post_pred_check(post_OU)
```



Simulating posterior samples using `post_simulate()`

To simulate samples from the posterior distribution, we can use sampling-importance resampling by sampling samples (with replacement) from proposal distribution with importance weights as the probabilities. This can be done by using `post_simulate()` function on the `bgphy_posterior` object:

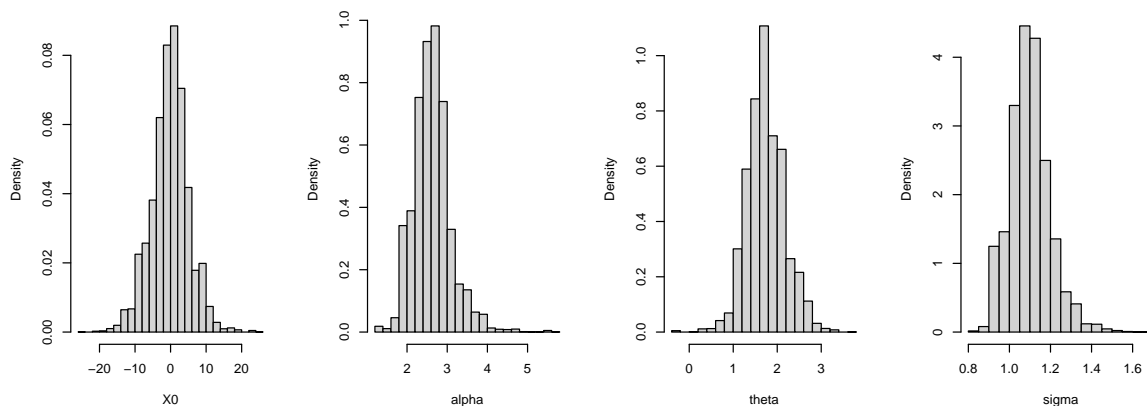
```
set.seed(1234, kind = "L'Ecuyer-CMRG")
post_OU_samples <- post_simulate(post_OU)
head(post_OU_samples)
```

	X0	alpha	theta	sigma
[1,]	-1.39702587	4.774145	1.625119	1.425720
[2,]	0.02594832	2.433787	1.783246	1.120322
[3,]	0.09169699	2.617716	1.637923	1.183824
[4,]	-2.35770360	2.683058	1.846299	1.055465
[5,]	-3.36877944	2.584163	2.016505	1.042770
[6,]	-8.97698136	2.741947	2.277882	1.152775

The marginals of the posterior distribution can then be visualized:

```
parnames <- names(post_OU$mean)
par(mfrow = c(1,4))

for (i in 1:4){
  hist(post_OU_samples[,i], freq = FALSE, breaks = 25, xlab = parnames[i], main = "")
}
```



References

- Bastide, Paul, and Gilles Didier. 2023. “The Cauchy Process on Phylogenies: A Tractable Model for Pulsed Evolution.” *Systematic Biology*, August, syad053. <https://doi.org/10.1093/sysbio/syad053>.
- Mahler, D Luke, Travis Ingram, Liam J Revell, and Jonathan B Losos. 2013. “Exceptional Convergence on the Macroevolutionary Landscape in Island Lizard Radiations.” *Science* 341 (6143): 292–95.
- Mitov, Venelin, Krzysztof Bartoszek, Georgios Asimomitis, and Tanja Stadler. 2020. “Fast Likelihood Calculation for Multivariate Gaussian Phylogenetic Models with Shifts.” *Theoretical Population Biology* 131: 66–78.