PhylogeneticEM: An R Package for Change-point Detection on Phylogenetic Trees

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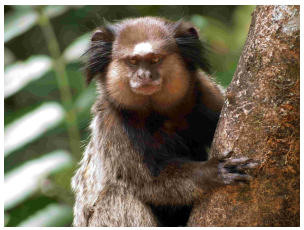
[4] MIA-Paris, INRA - AgroParisTech, Paris, France

8 November 2017



New World Monkeys

(Aristide et al., 2016)



Callithrix penicillata

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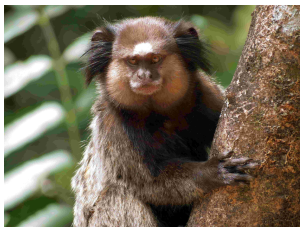

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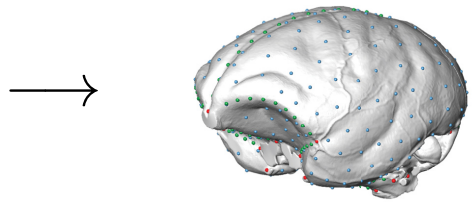

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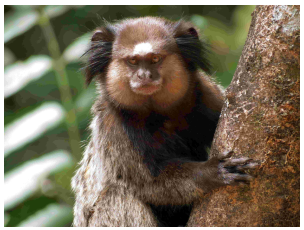

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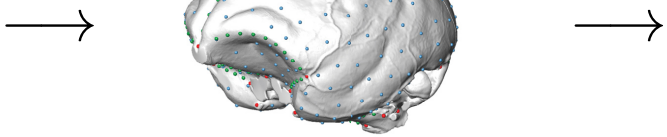

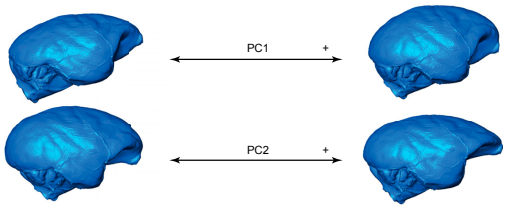

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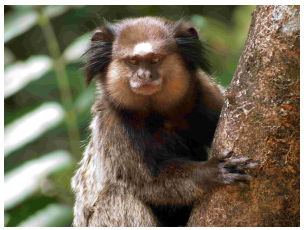

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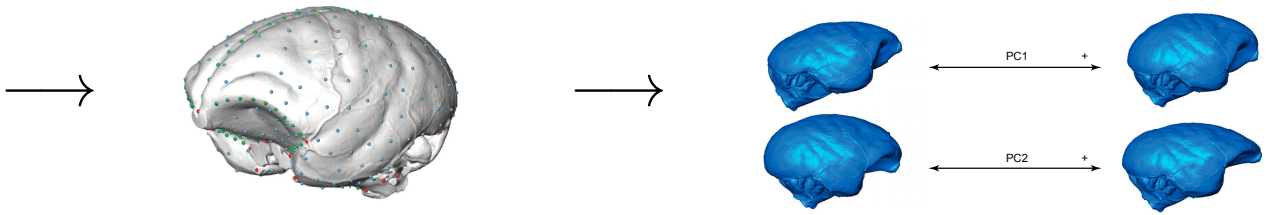

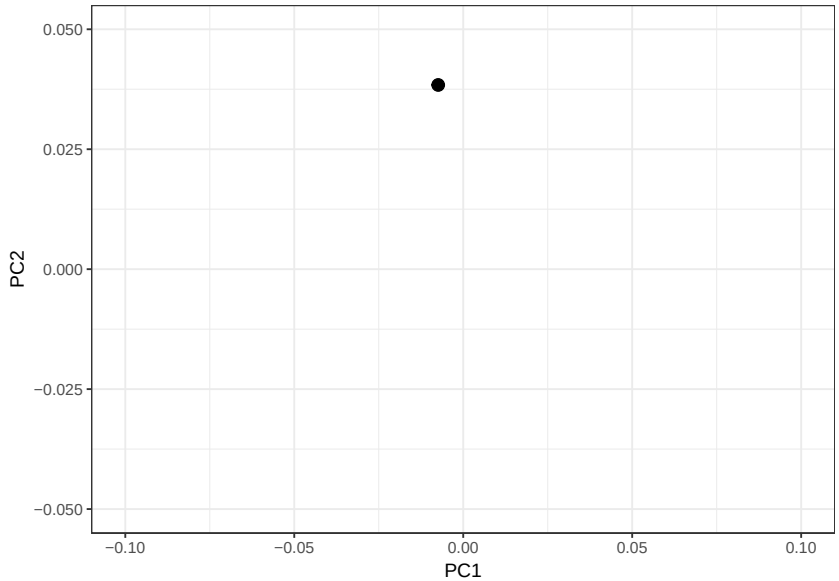

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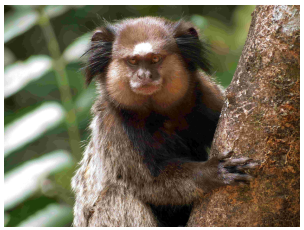

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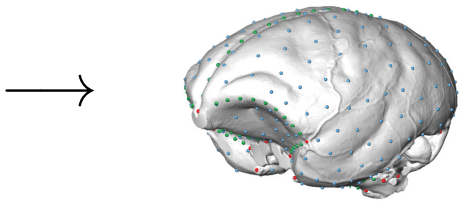
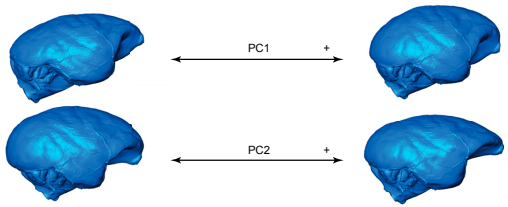
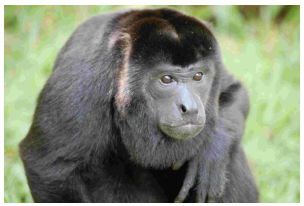
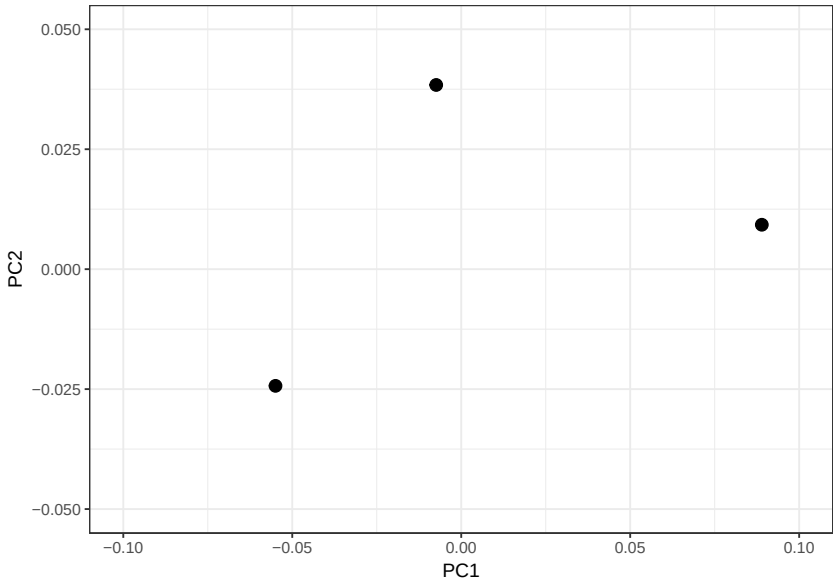
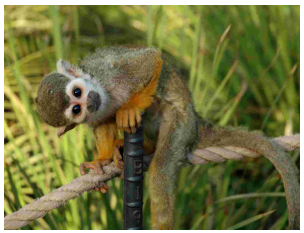






Alouatta palliata





Saimiri sciureus

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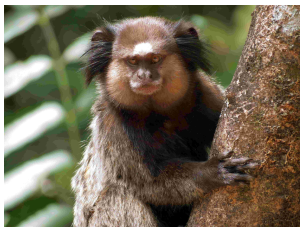

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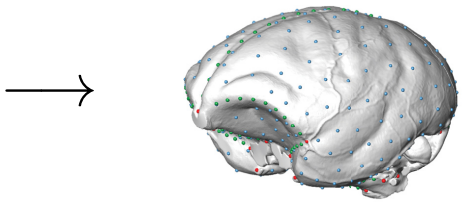

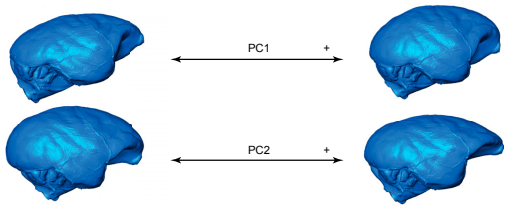

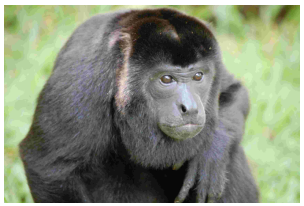

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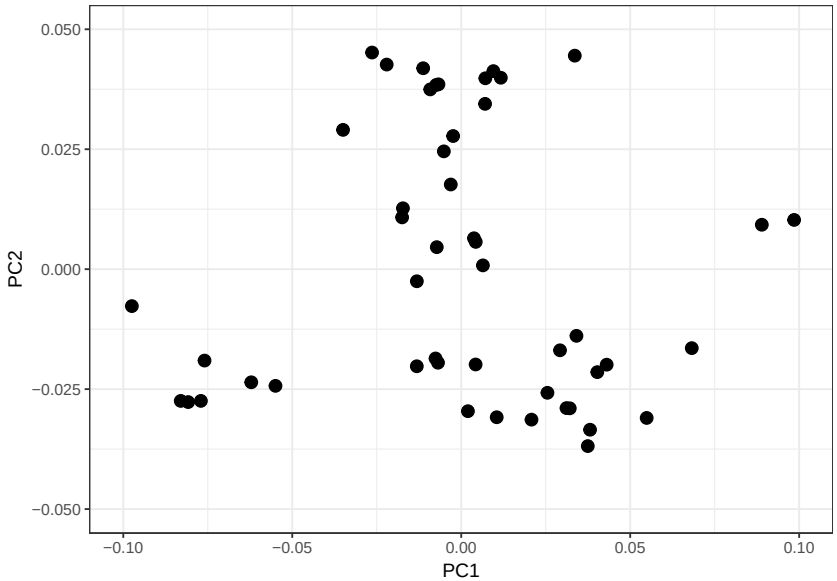

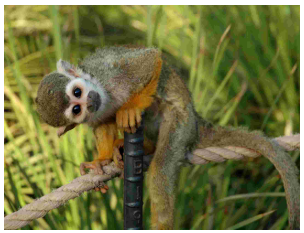

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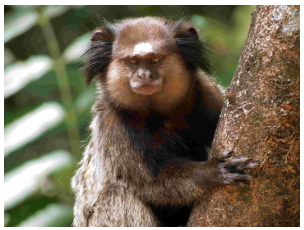

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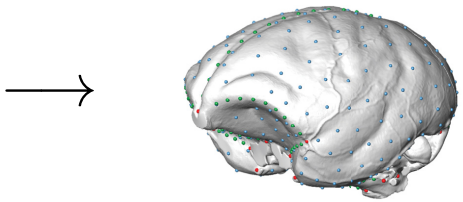

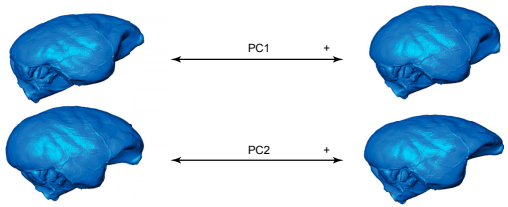

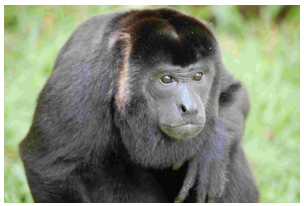

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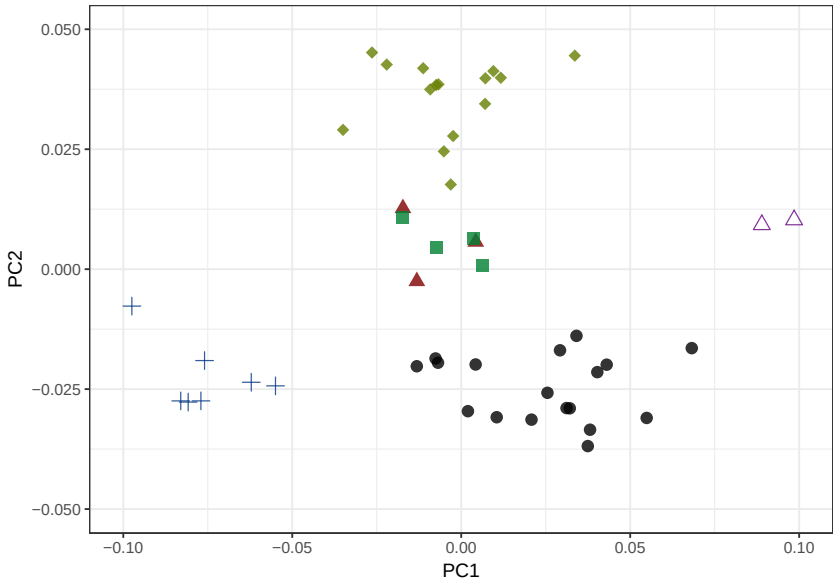

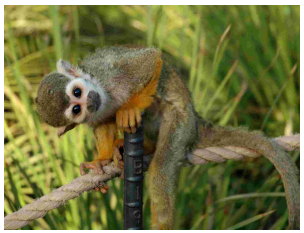

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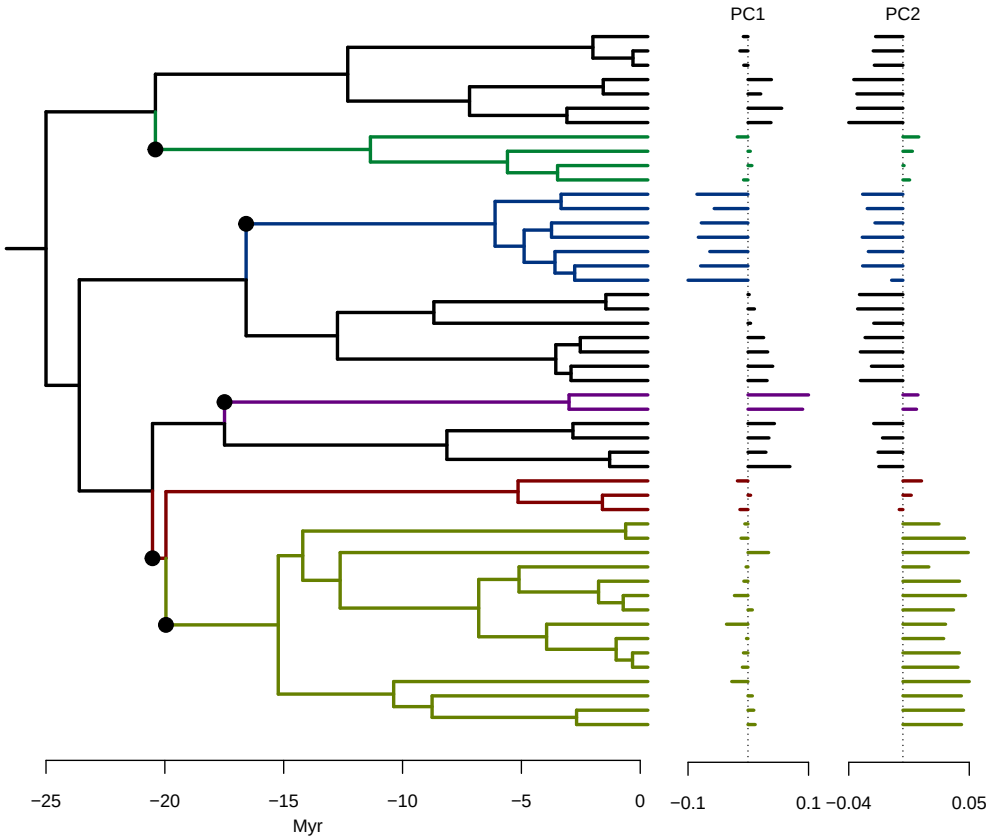

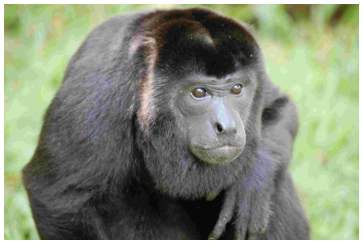

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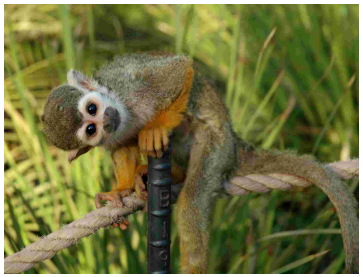

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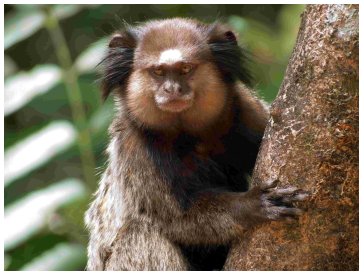
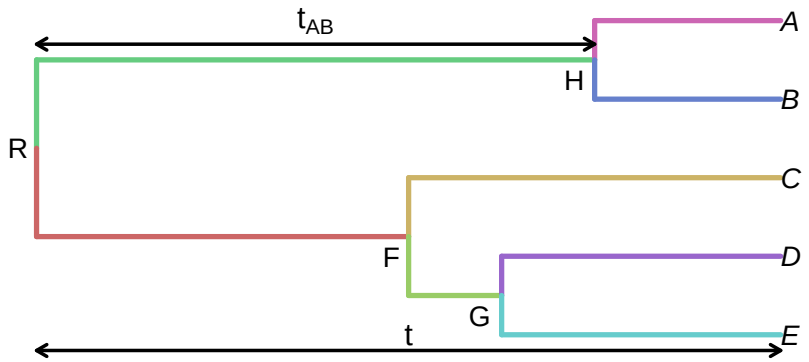
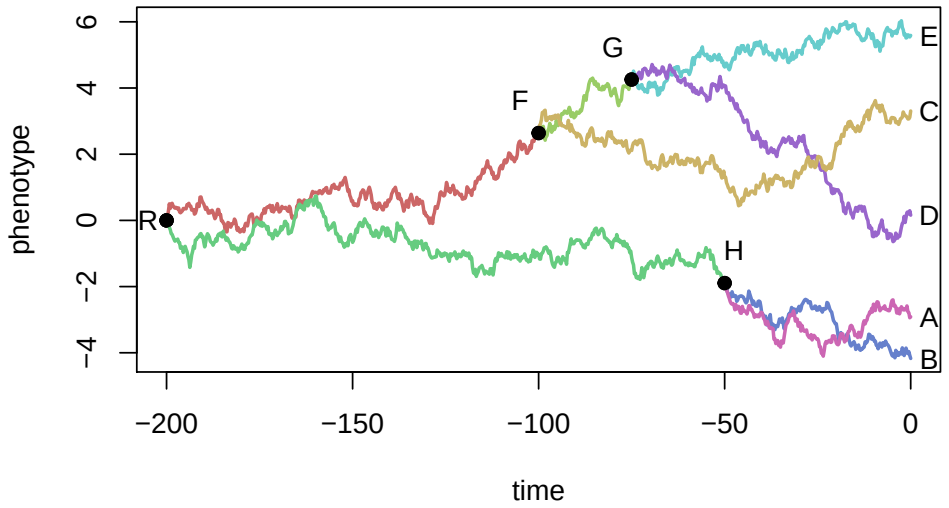


Callithrix penicillata

Outline

Stochastic Process on a Tree (Felsenstein, 1985)





Known tree.

Only **tips** observed.

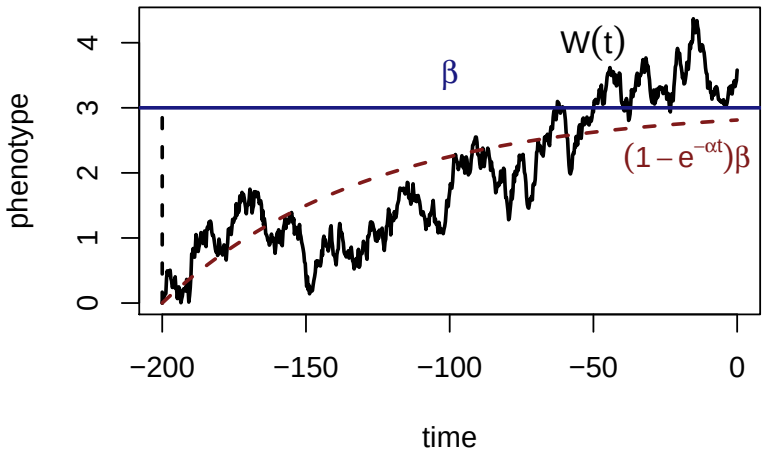
Brownian Motion:

$$\mathbb{V}\mathrm{ar}\left[A \mid R\right] = \sigma^2 t$$

$$\mathbb{C}\mathrm{ov}\left[A; B \mid R\right] = \sigma^2 t_{AB}$$

OU Modeling

(Hansen, 1997)



$$dW(t) = \alpha[\beta(t) - W(t)]dt + \sigma dB(t)$$

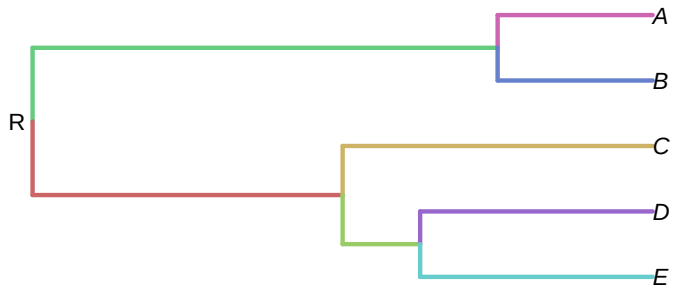
Deterministic part:

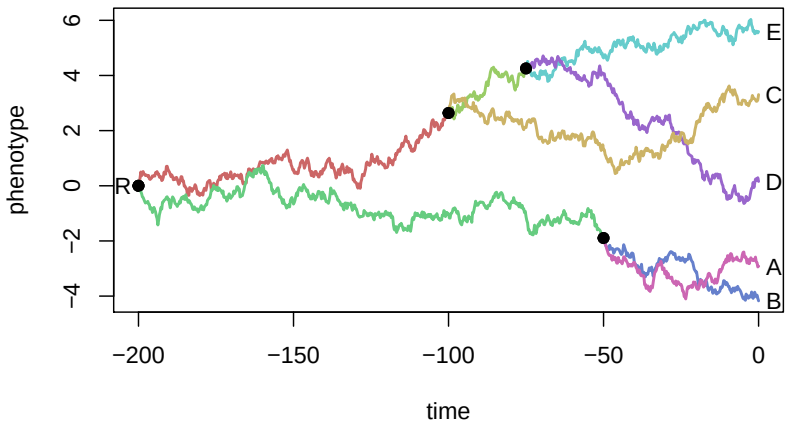
- $\beta(t)$: primary optimum, mechanistically defined.
- α: selection strength.

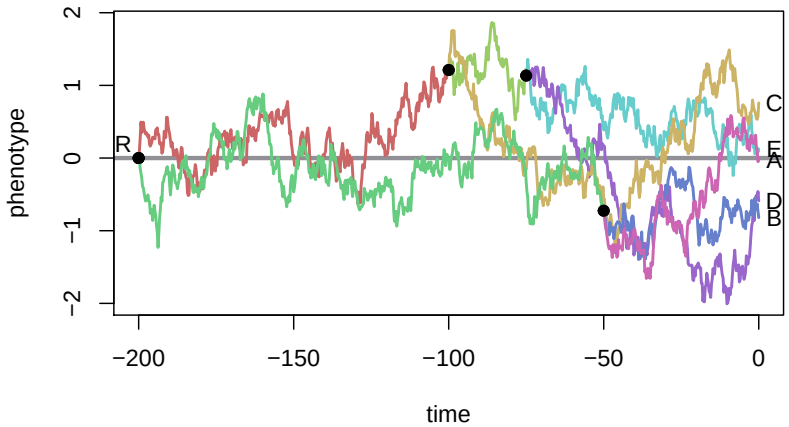
Stochastic part:

- $W(t)$: actual optimum (trait value).
- $\sigma dB(t)$ Brownian fluctuations.

Shifts







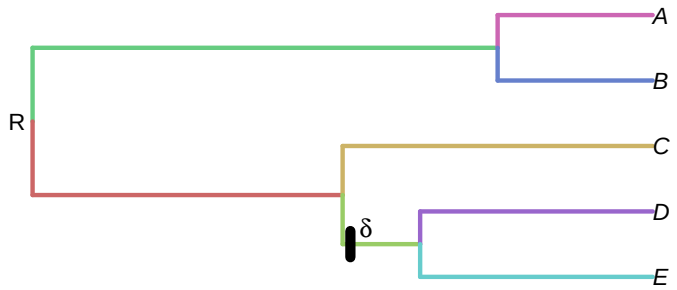
BM Shifts in the **mean**:

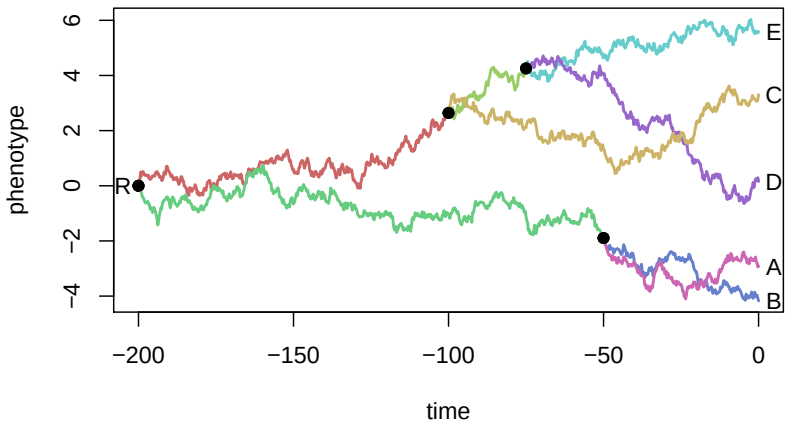
$$m_{\text{child}} = m_{\text{parent}} + \delta$$

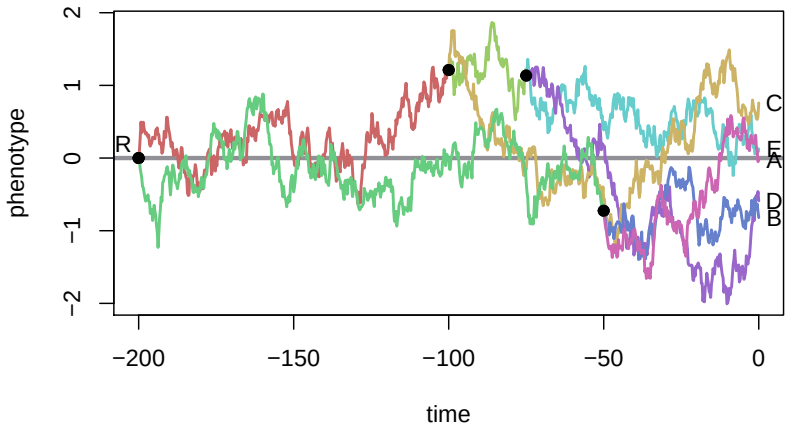
OU Shifts in the **optimal value**:

$$\beta_{\text{child}} = \beta_{\text{parent}} + \delta$$

Shifts







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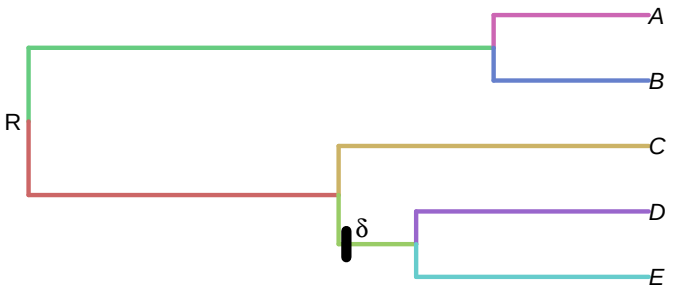

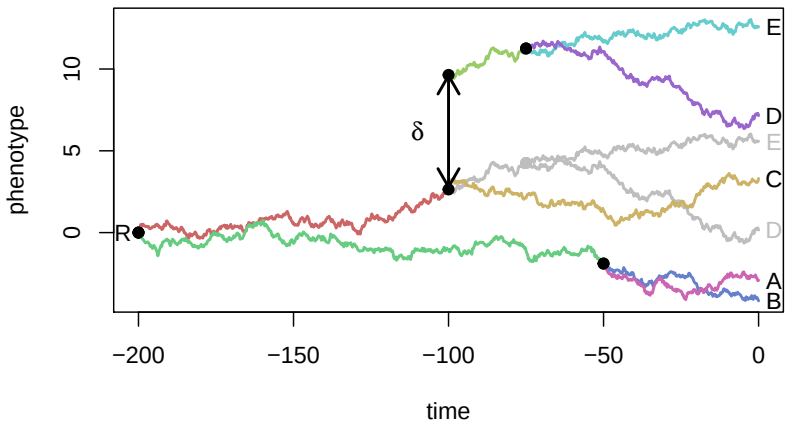

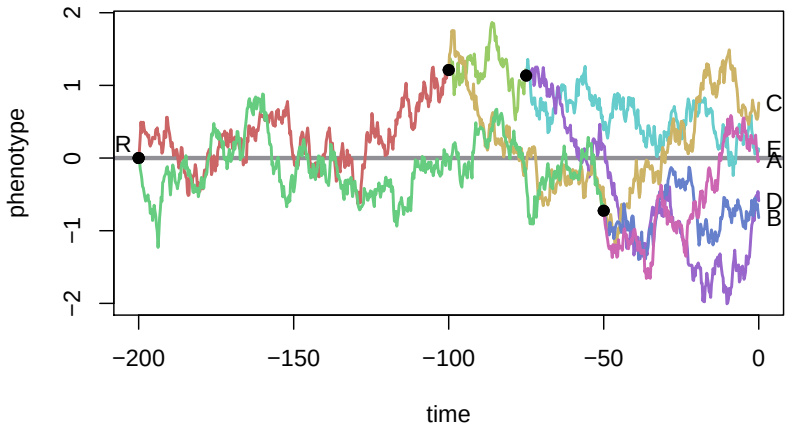

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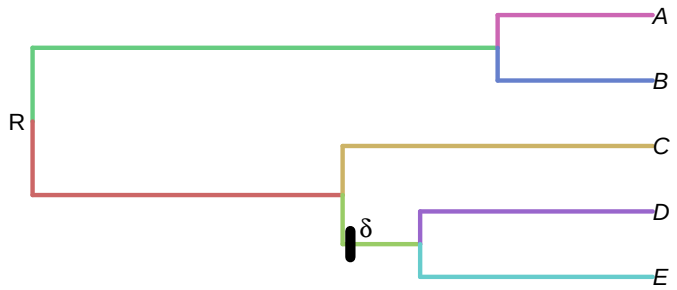

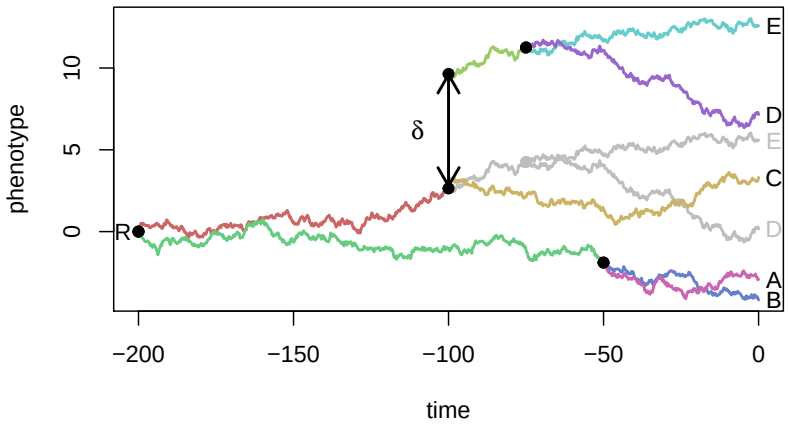

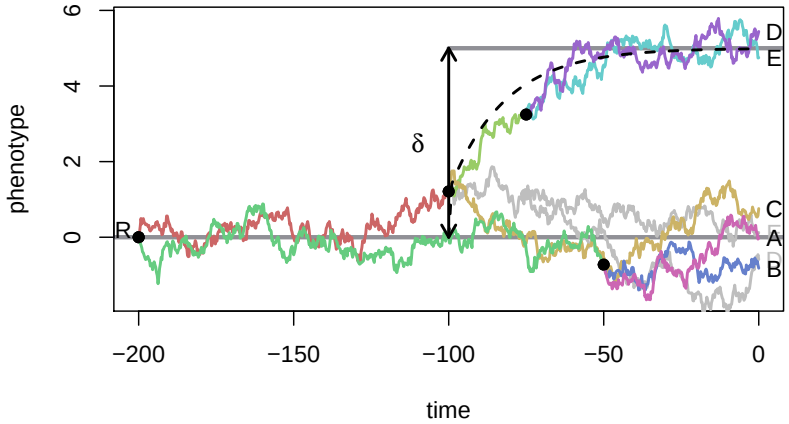

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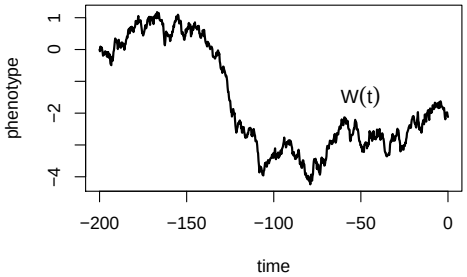
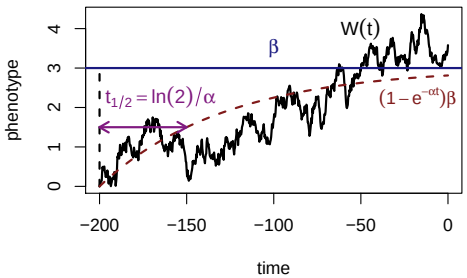
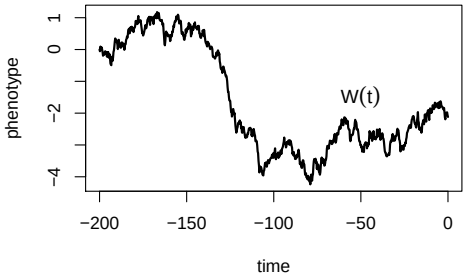
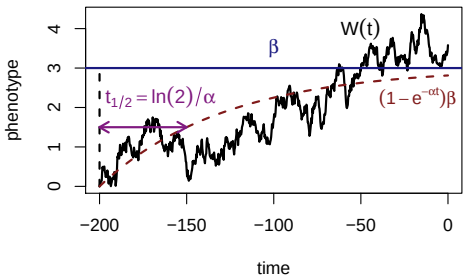
Univariate BM vs OU

	Equation	$\mathbb{C}\mathrm{ov}[Y_i; Y_j]$	Inference
	$dW(t) = \sigma dB(t)$	$t_{ij} \times \sigma^2$	:-)
	$dW(t) = \sigma dB(t)$ $+\alpha[\beta(t) - W(t)]dt$	$\frac{1}{2\alpha} e^{-2\alpha h}(e^{2\alpha t_{ij}} - 1) \times \sigma^2$	:-(

Univariate BM vs OU

	Equation	$\mathbb{C}\mathrm{ov}[Y_i; Y_j]$	Inference
	$dW(t) = \sigma dB(t)$	$t_{ij} \times \sigma^2$	:-)
	$dW(t) = \sigma dB(t)$ $+\alpha[\beta(t) - W(t)]dt$	$\underbrace{\frac{1}{2\alpha} e^{-2\alpha h}(e^{2\alpha t_{ij}} - 1)}_{t'_{ij}(\alpha)} \times \sigma^2$	:-)

Multivariate BM vs OU

$\mapsto$ All the traits shift at the same time

Equation	$\mathbb{C}\text{ov}\left[\mathbf{Y}_i; \mathbf{Y}_j\right]$	Inference
$d\mathbf{W}(t) = \mathbf{\Sigma} d\mathbf{B}_t$	$t_{ij} \times \mathbf{\Sigma}\mathbf{\Sigma}^T$	:-)
$d\mathbf{W}(t) = -\mathbf{A}(\mathbf{W}(t) - \beta(t))dt + \mathbf{\Sigma} d\mathbf{B}_t$	$\int \dots$	:'-(

Multivariate BM vs **scOU**

$\mapsto$ All the traits shift at the same time

$\mapsto$ All the traits shift have the same α.

Equation	$\mathbb{C}\text{ov}\left[\mathbf{Y}_i; \mathbf{Y}_j\right]$	Inference
$d\mathbf{W}(t) = \mathbf{\Sigma} d\mathbf{B}_t$	$t_{ij} \times \mathbf{\Sigma}\mathbf{\Sigma}^T$	:-)
$d\mathbf{W}(t) = -\alpha(\mathbf{W}(t) - \beta(t))dt + \mathbf{\Sigma} d\mathbf{B}_t$	$t'_{ij}(\alpha) \times \mathbf{\Sigma}\mathbf{\Sigma}^T$	:-)

Outline

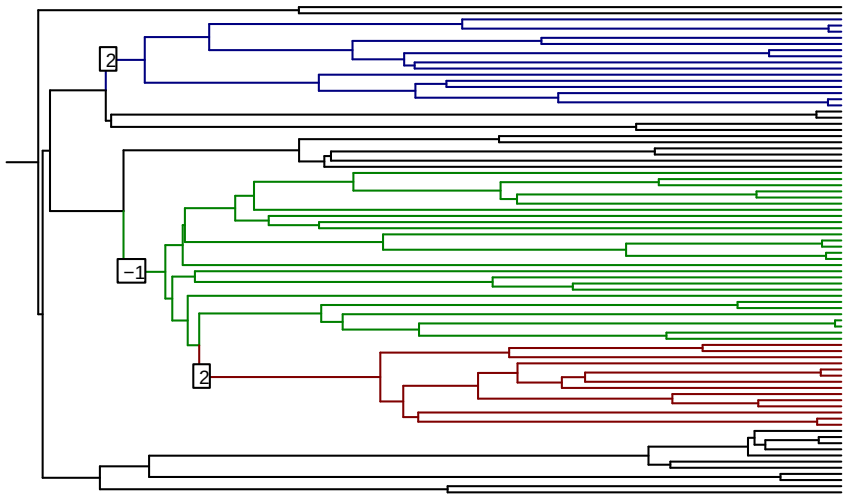
Simulation: Tree

```
library(PhylogeneticEM)
```

```
set.seed(17920902)
ntaxa = 80
tree <- TreeSim::sim.bd.taxa.age(n=ntaxa, numbsim=1, lambda=0.1, mu=0, age=1, mrca=TRUE)[[1]]
```

```
params <- params_process("OU",                                          ## Process
                         p = 2,                                         ## Dimension
                         variance = diag(0.5, 2, 2) + 0.5,              ## Rate matrix
                         selection.strength = 3,                        ## Selection Strength
                         edges = c(29, 25, 127),                        ## Position of the shifts
                         values = cbind(c(2,  1), c(-1,  2), c(2, -1))) ## Values of the shifts
```

```
plot(params, phylo = tree, traits = 1, value_in_box = TRUE, shifts_bg = "white")
```



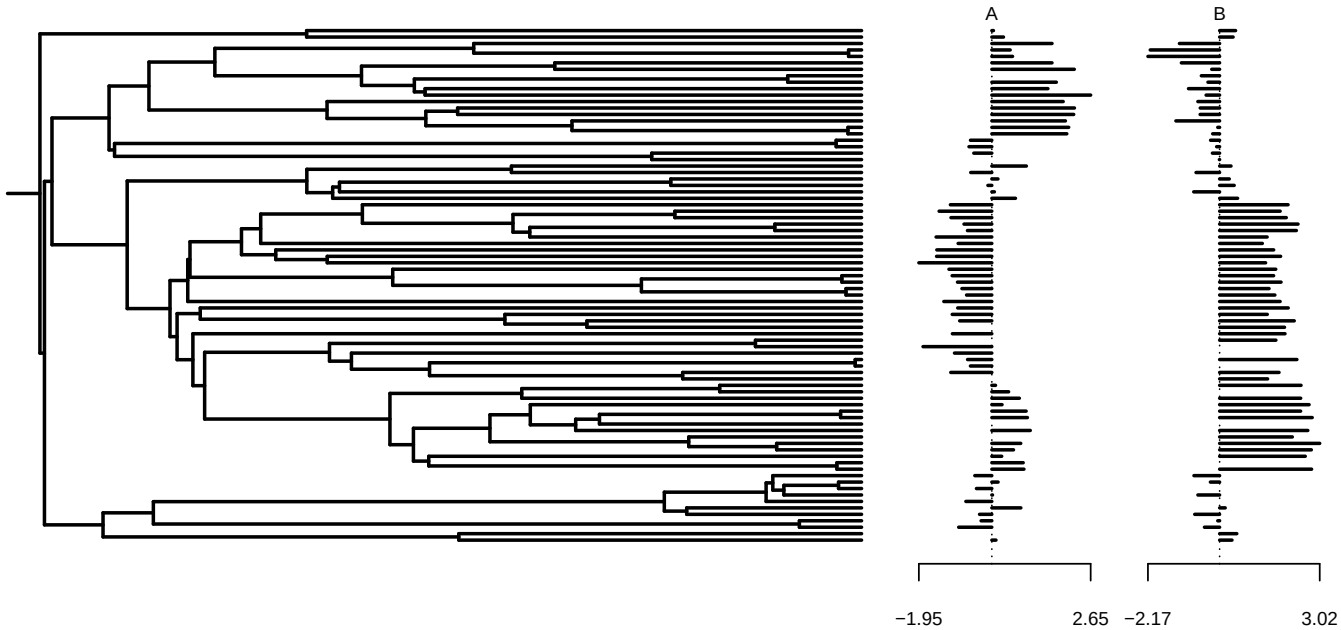
Simulation: Data

```
sim <- simul_process(params, tree)
```

```
data <- extract(sim,              ## A simul_process object
                what = "states", ## We want the actual values
                where = "tips")  ## Only at the tips of the tree
rownames(data) <- c("A", "B")
```

```
nMiss <- floor(ntaxa * 2 * 0.1)                                  ## 10% of missing data
data[sample(c(rep(F, 2*ntaxa - nMiss), rep(T, nMiss)))] <- NA    ## forget some values
```

```
plot(params_BM(p=2), phylo = tree, data = data, edge.width=2)
```



Inference

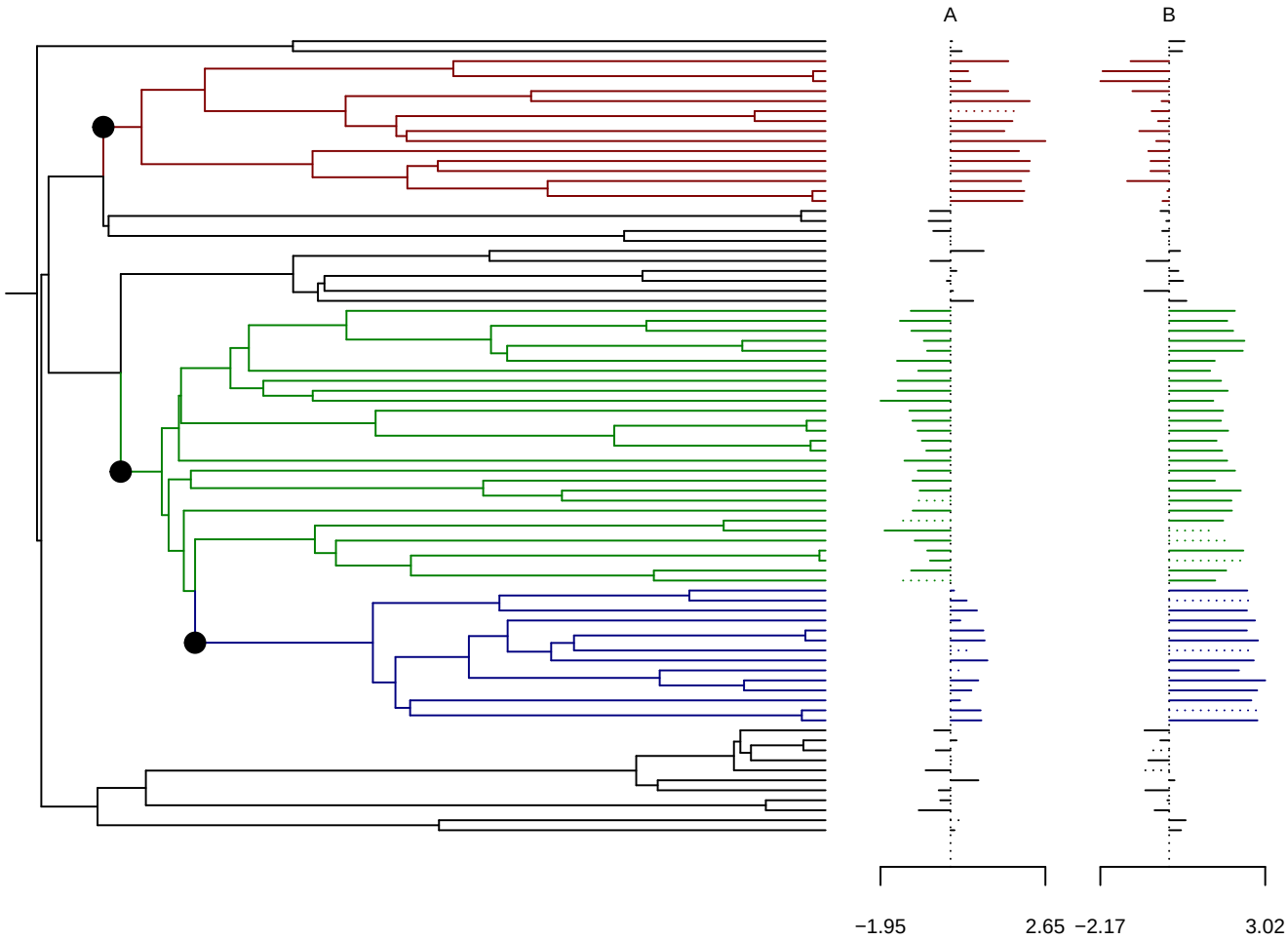
```
## Grid on alpha
alpha_grid <- c(2, 2.5, 3, 3.5)

## Run algorithm
system.time(
res <- PhyloEM(phylo = tree,
               Y_data = data,
               process = "scOU",                ## scalar OU model
               alpha = alpha_grid,              ## On a grid of alpha
               K_max = 10,                      ## Maximal number of shifts
               parallel_alpha = TRUE,           ## This can be set to TRUE for
               Ncores = 2)                      ## parallel computations
)


##    user  system elapsed
##   0.536   0.004  57.126
```

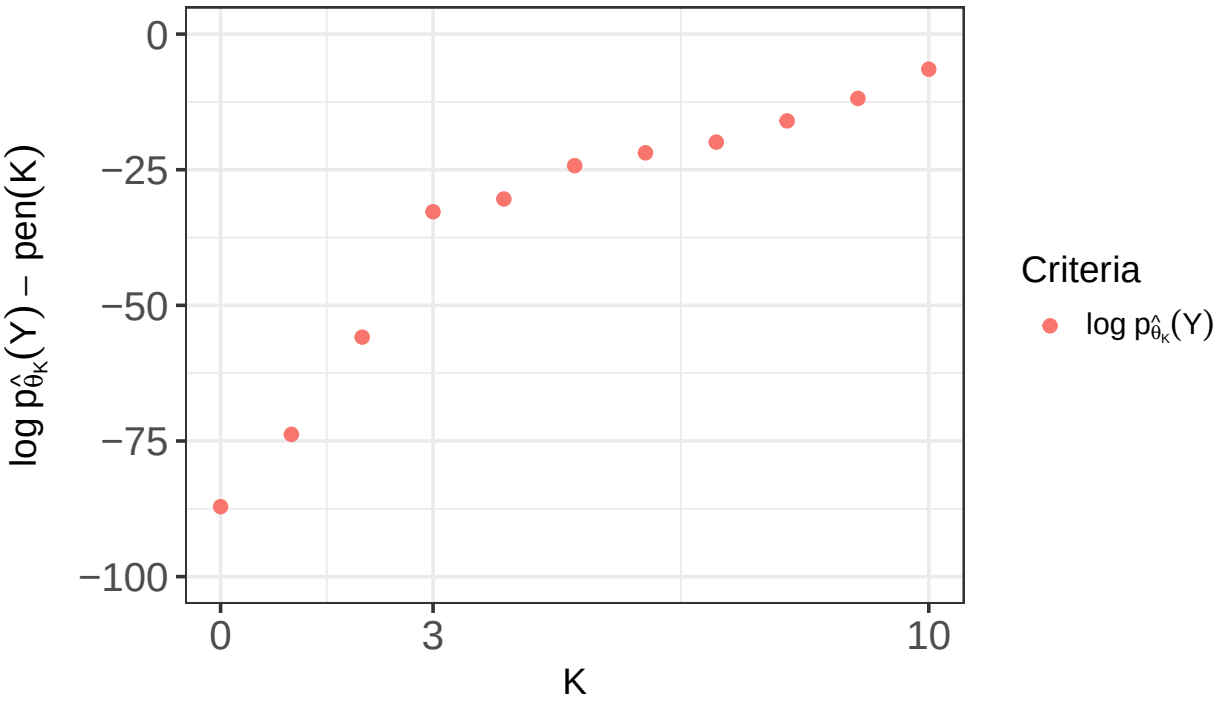
Analysis

```
plot(res)
```



Model Selection: Penalized Likelihood

Idea $\hat{K} = \underset{0 \leq K \leq K_{\max}}{\operatorname{argmax}} \left\{ \log\ p_{\hat{\theta}_K}(Y) - \text{pen}(K) \right\}$ (Univariate)



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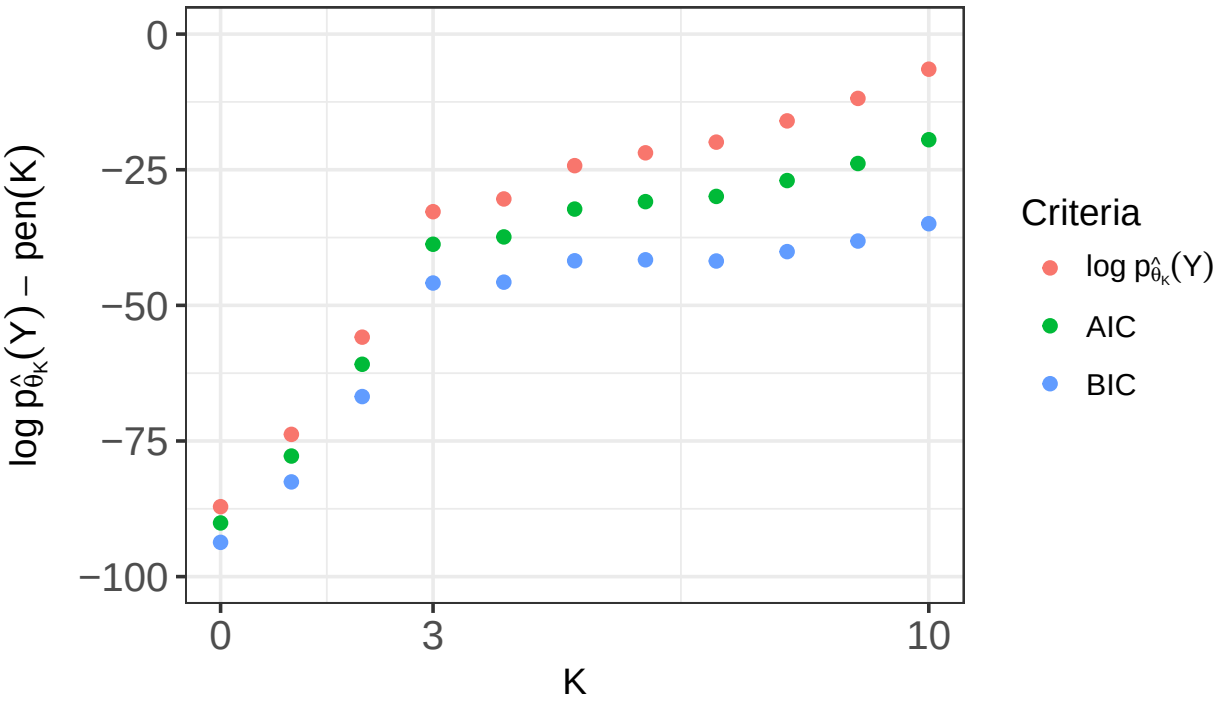

Penalties:

AIC $K + 3$

BIC $\frac{1}{2}(K + 3)\log(n)$

Model Selection: Penalized Likelihood

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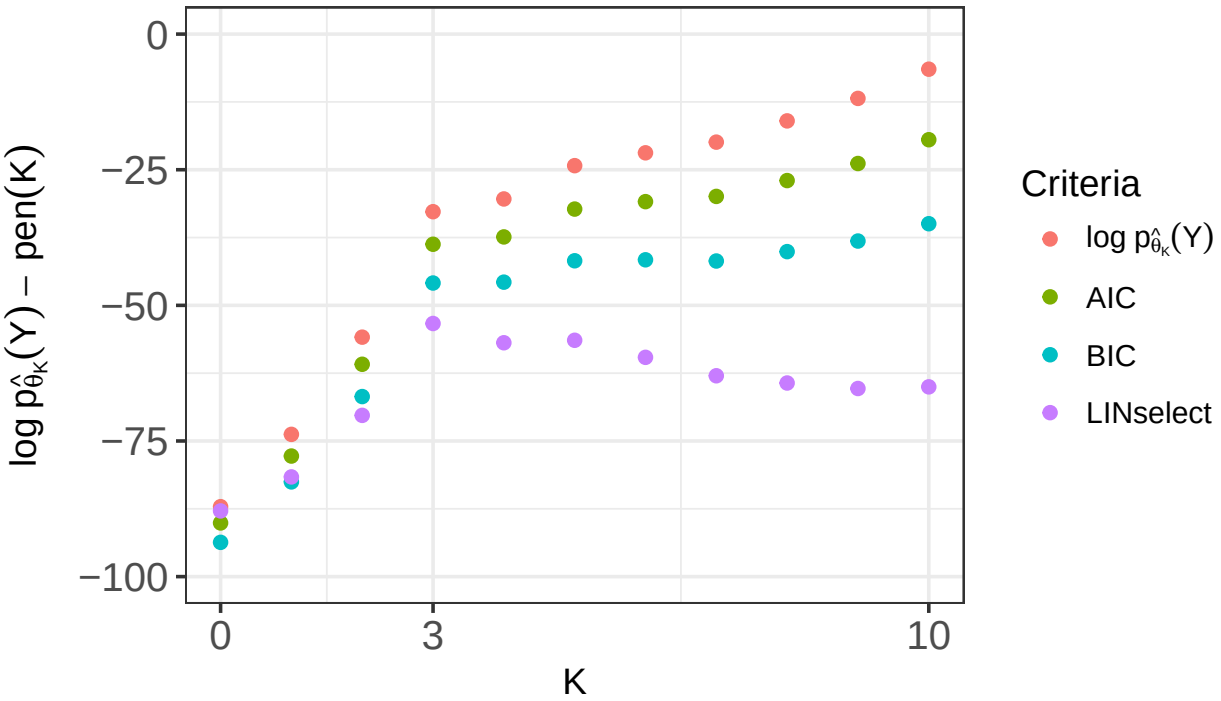


Penalties:

AIC $K + 3$

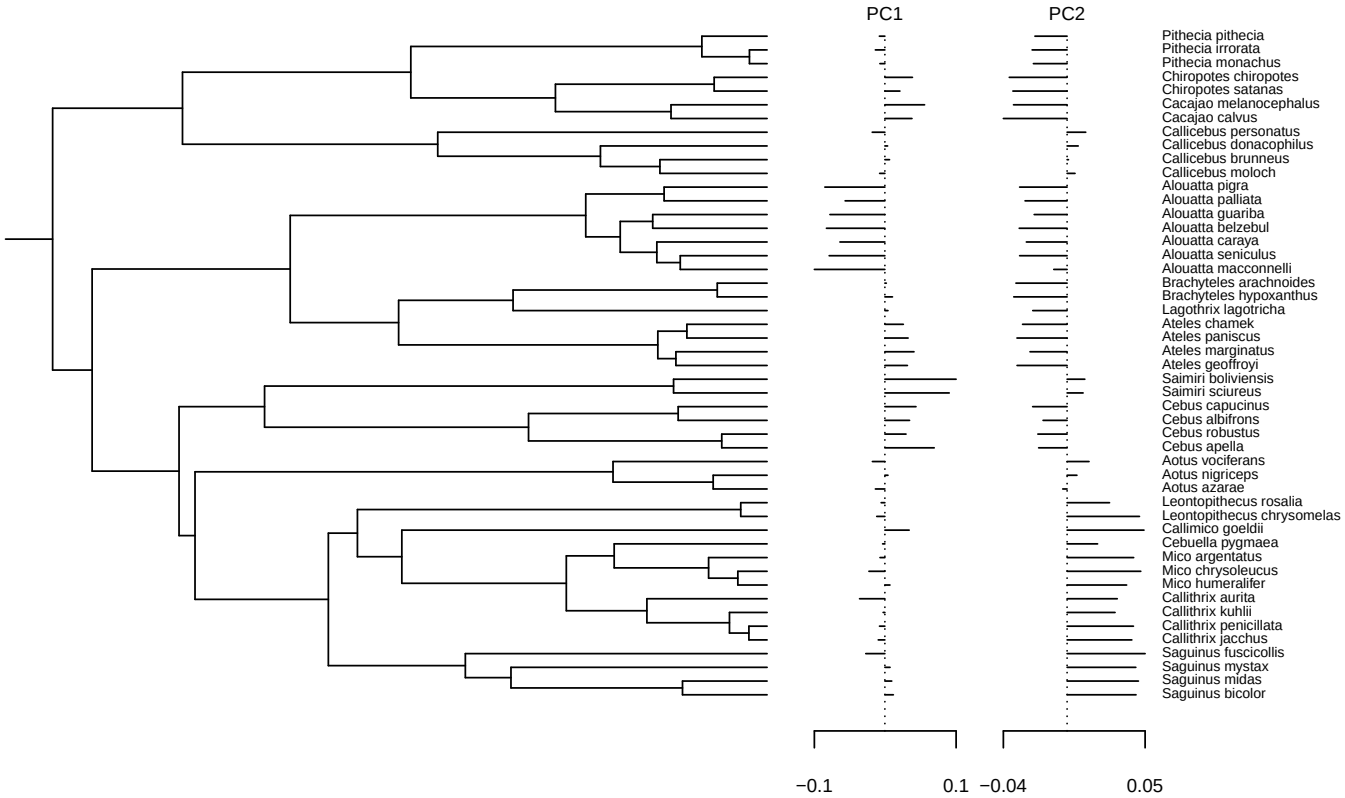
BIC $\frac{1}{2}(K+3)\log(n)$

LINselect $\mathrm{pen}(n, K, |\mathcal{S}_K^{PI}|)$

Monkey Dataset

(Aristide et al., 2016)

```
data(monkeys)

plot(params_BM(p=2), data = monkeys$dat, phylo = monkeys$phy, show.tip.label = TRUE)
```



Analysis

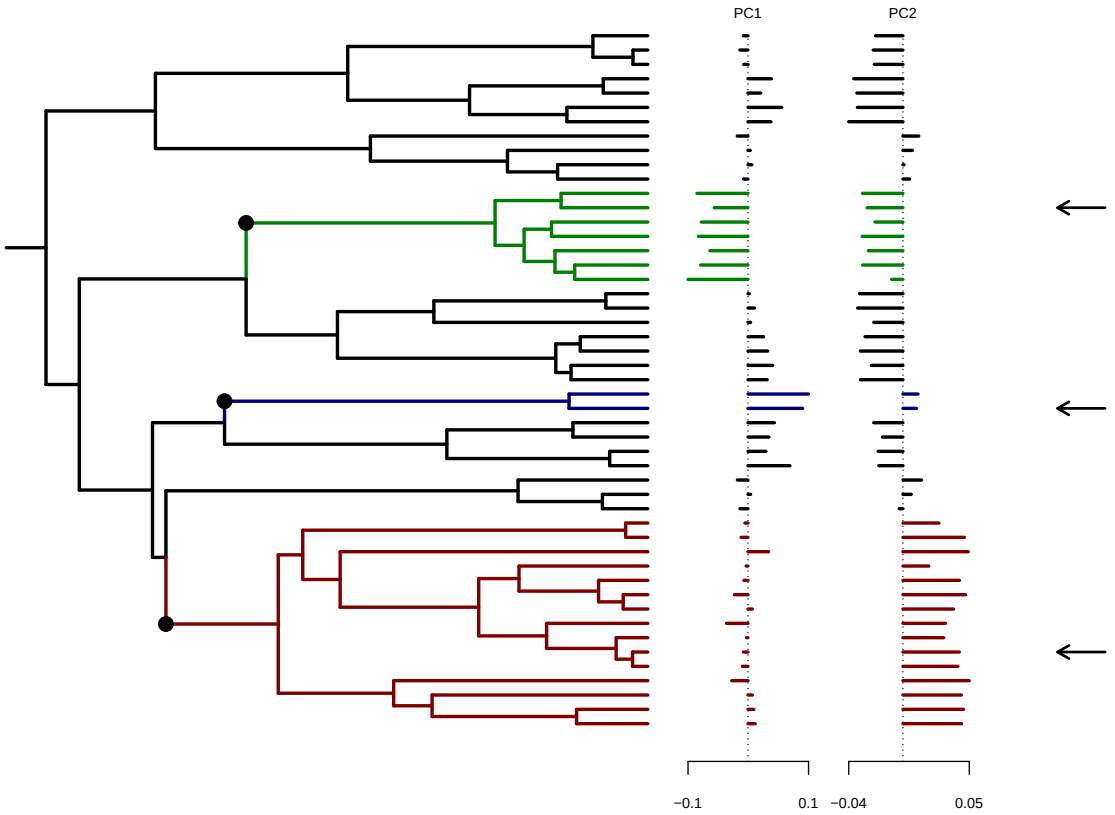
We use function `PhyloEM`:

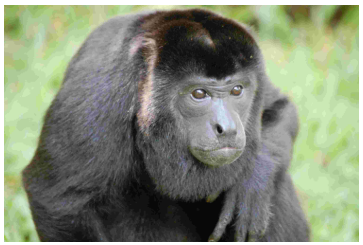
```
system.time(
res <- PhyloEM(Y_data = monkeys$dat,          ## data
               phylo = monkeys$phy,           ## phylogeny
               process = "scOU",              ## scalar OU
               K_max = 10,                    ## maximal number of shifts
               nbr_alpha = 4,                 ## number of alpha values
               parallel_alpha = TRUE,         ## parallelize on alpha values
               Ncores = 2)
)


##    user  system elapsed
##   0.440   0.004  14.957
```

Then plot the solution selected by the default method:

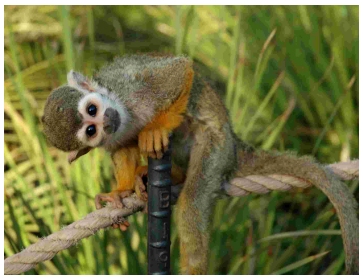
```
plot(res, edge.width = 2)
```

Result

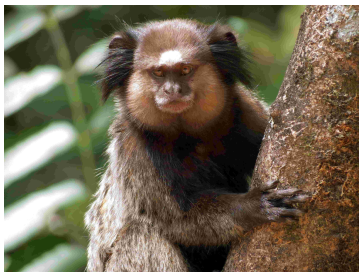




Alouatta palliata



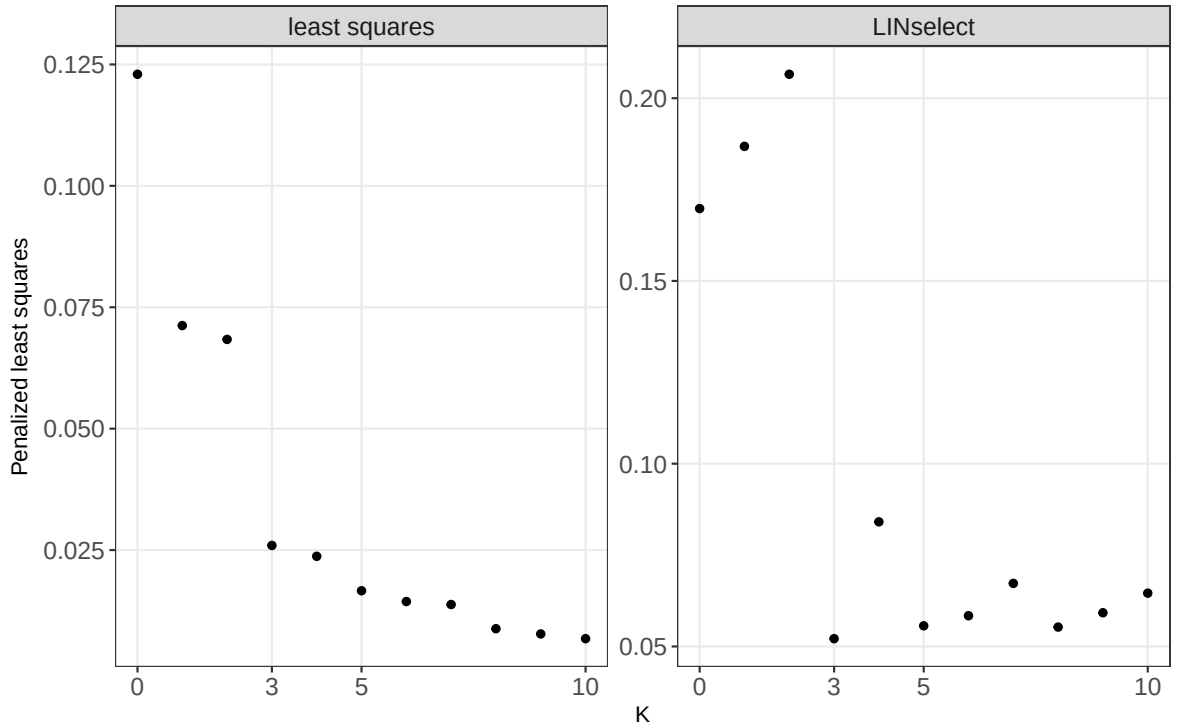
Saimiri sciureus



Callithrix penicillata

Model Selection

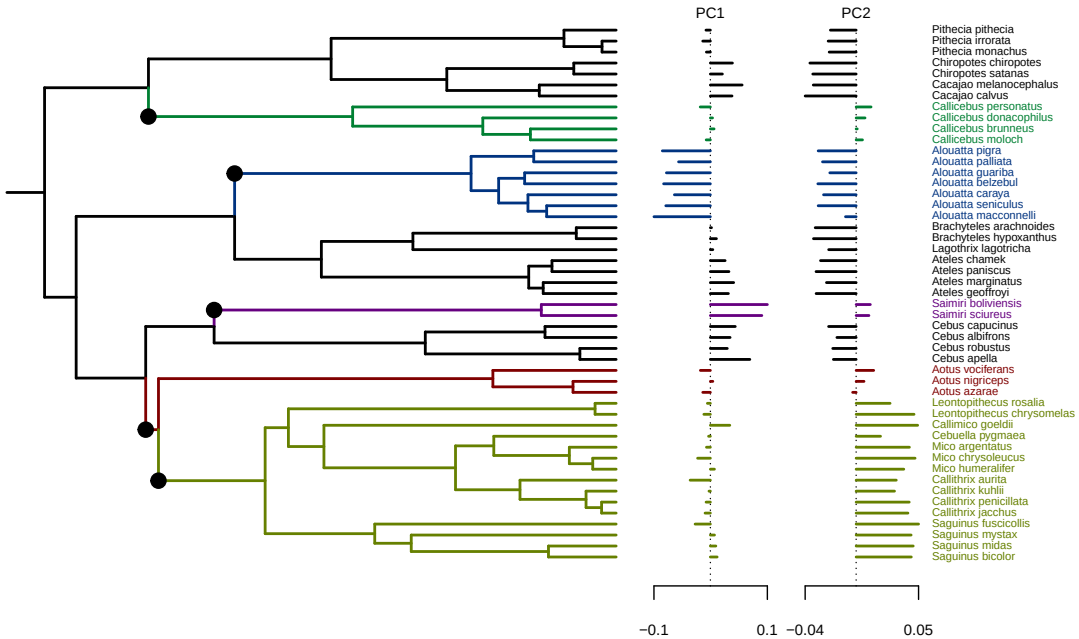
Solution with $K = 5$ seems to be a good solution too.



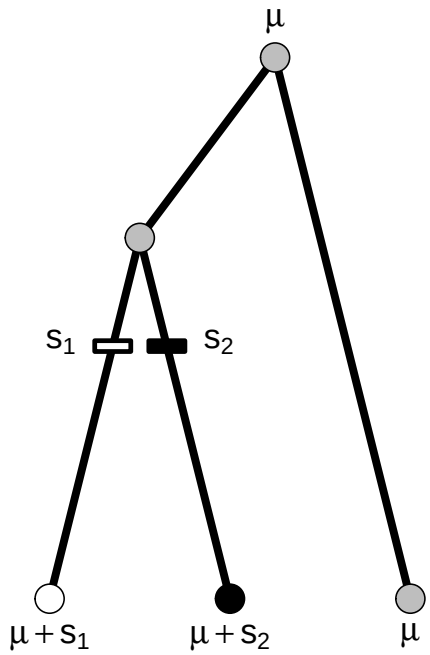
Solution for $K = 5$

```
plot(res, params = params_process(res, K = 5), edge.width = 2, show.tip.label = TRUE)
```

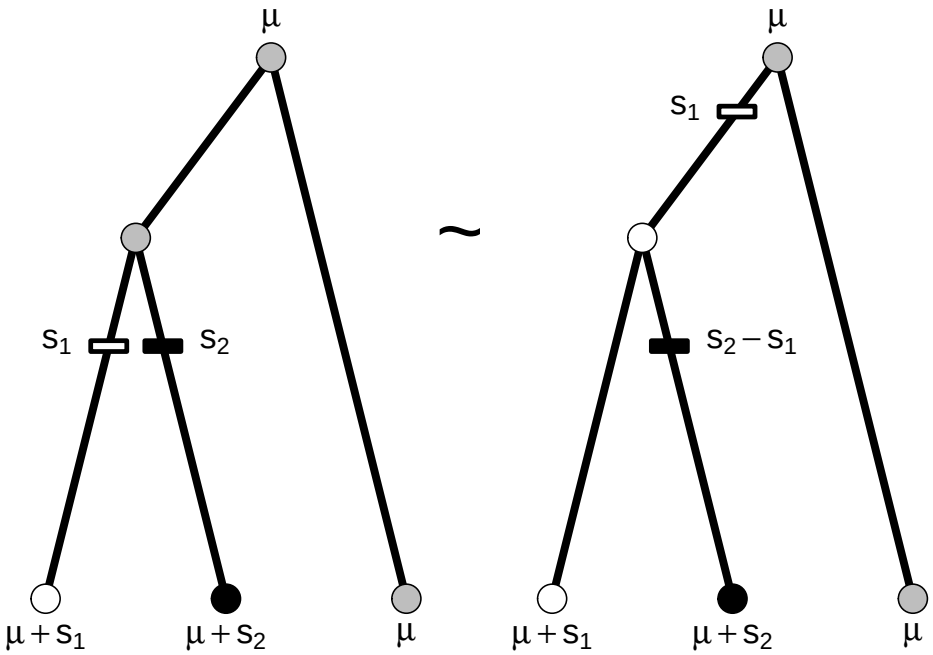
```
## Warning in params_process.PhyloEM(res, K = 5): There are several equivalent solutions for
this shift position.
```



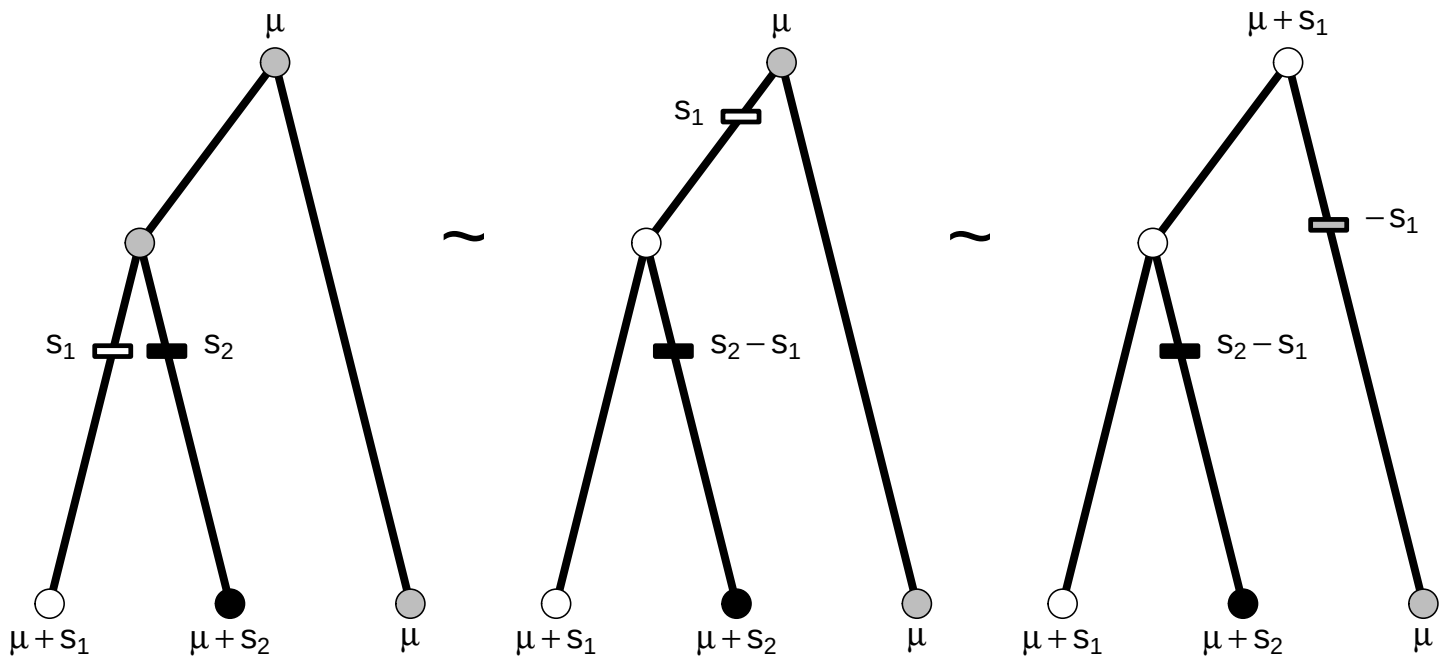
Equivalencies



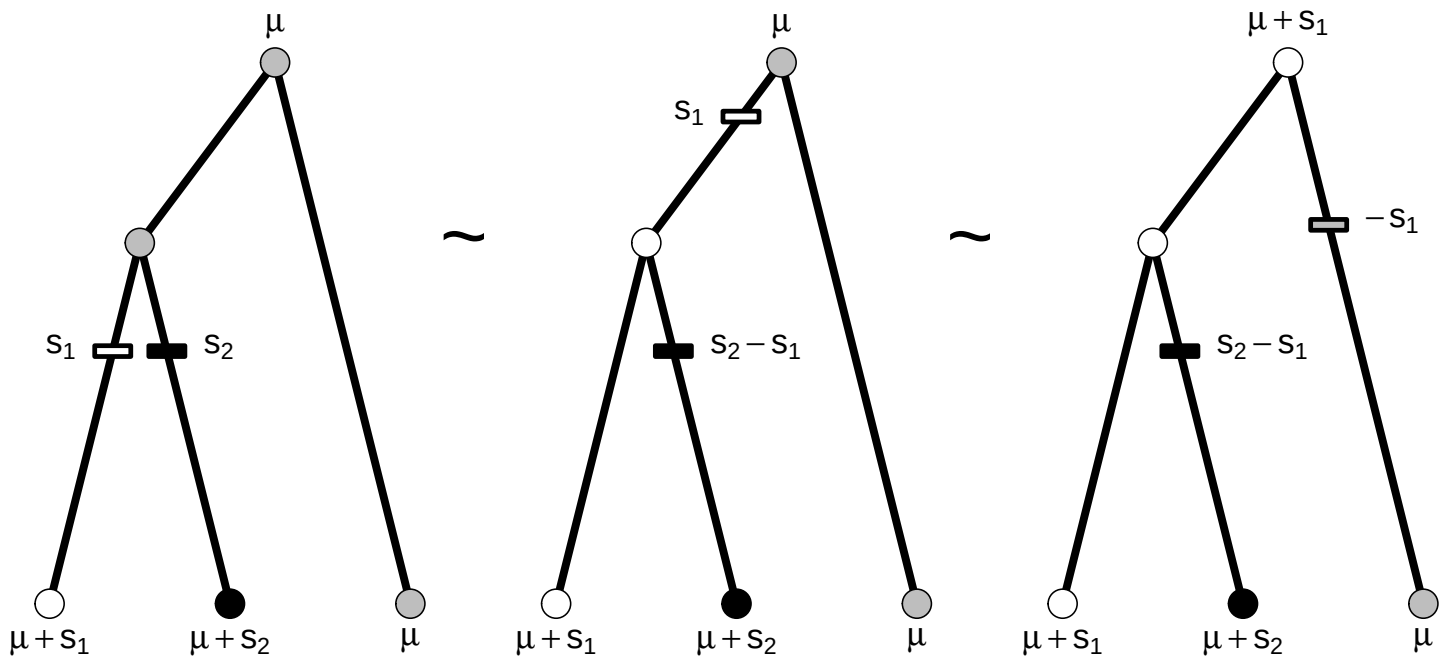
Equivalencies



Equivalencies

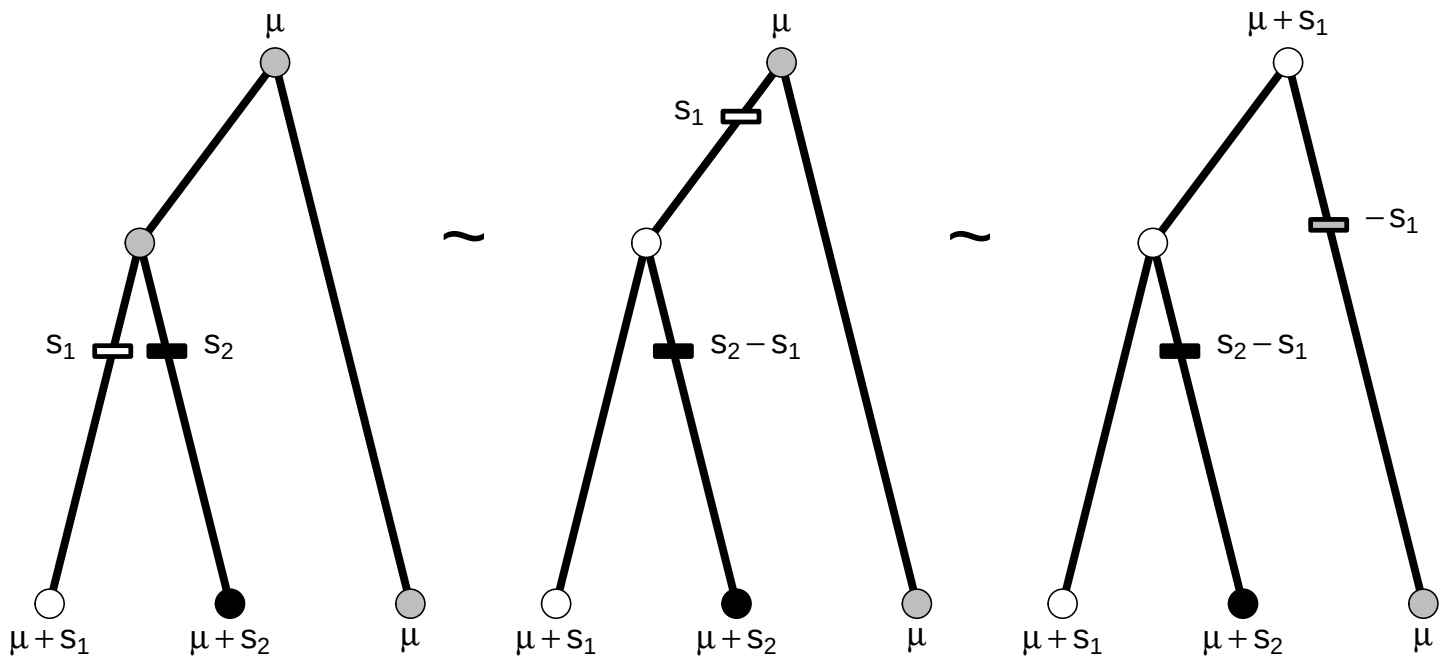


Equivalencies



Equivalent allocations *cannot* be distinguished from the data.

Equivalencies



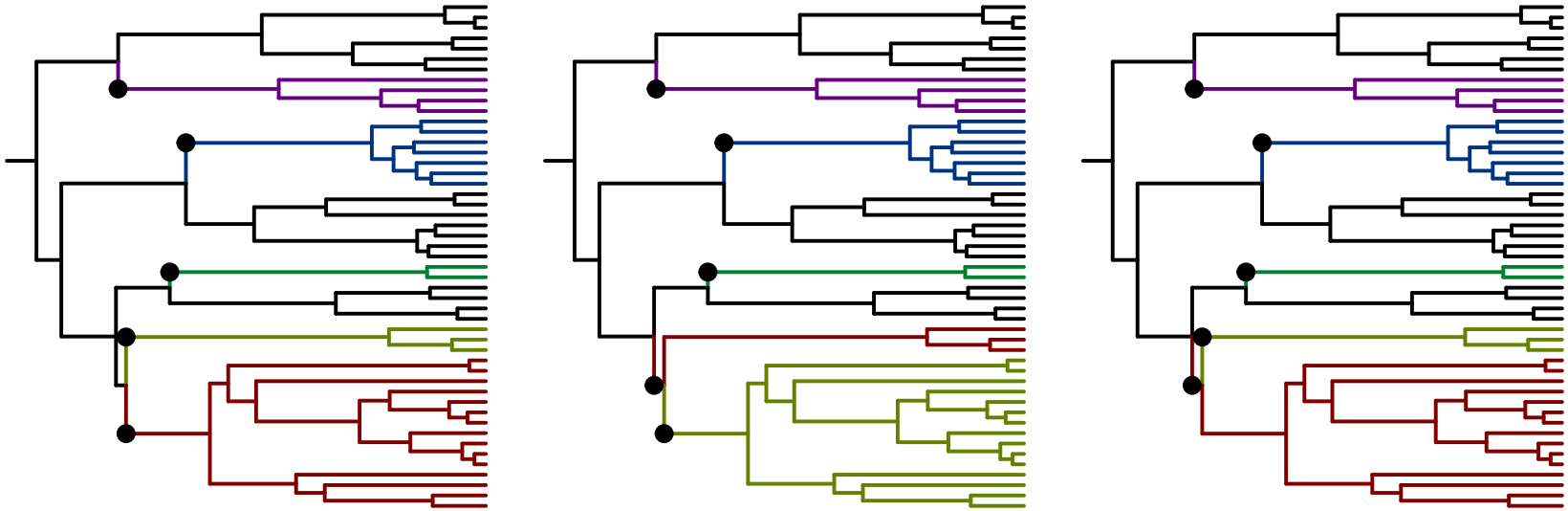
Equivalent allocations *cannot* be distinguished from the data.

`PhylogeneticEM` Enumerate all solutions
(Adaptation of Fitch, Sankoff, see Felsenstein, 2004).

Solution for $K = 5$

```
params_5 <- params_process(res, K = 5)
eq_shifts <- equivalent_shifts(monkeys$phy, params_5)
```

```
plot(eq_shifts, show_shifts_values = FALSE, shifts_cex = 0.5)
```

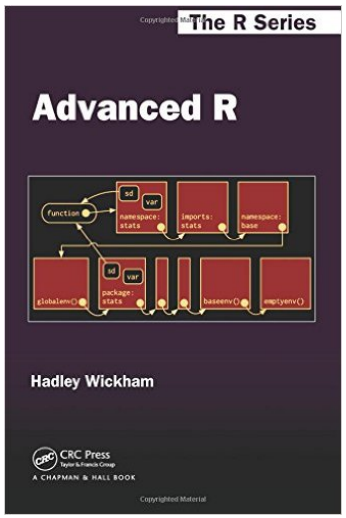


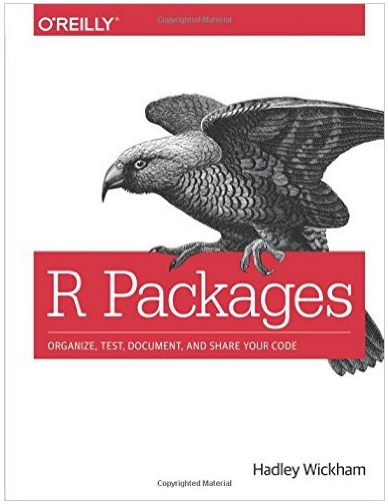
Outline

References

I used mainly these two books by Hadley Wickham:

- Advanced R: `http://adv-r.had.co.nz/`
- R Packages: `http://r-pkgs.had.co.nz/`





- Intensive use of `devtools` and `Rstudio`.

Implementation

Transparency

GitHub	`https://github.com/pbastide/PhylogeneticEM`
CRAN	Version `1.1.0`
Doc	Automatically build with `pkgdown`.

Efficiency

Profiling	Find bottleneck with `lineprof`
Optimizing	Speed up with `C++` and `RcppArmadillo`
	Avoid memory leaks with `valgrind`.
	Use the `Armadillo` library.

Robustness

Tests	Unitary tests with `testthat`.
CI	Continuous Integration with `Travis CI`.
Coverage	With `covr` and `codecov`.

Conclusion and Perspectives

A general inference framework for trait evolution models.

Conclusions

- A complete maximum likelihood procedure
- Taking identifiability problems into account
- With model selection

R Package

- Available on the CRAN and on GitHub
- Can scale up to big datasets ($\sim$ 1200 species)

Perspectives

- Deal with uncertainty (data, tree, shifts).
- Phylogenetic networks: See `julia` package `PhyloNetworks`.
- Combine with factor analysis.

Bibliography

Bastide P, Mariadassou M, Robin S. 2017. Detection of adaptive shifts on phylogenies by using shifted stochastic processes on a tree. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, 79(4), 1067–1093.

Bastide P, Ané C, Robin S, Mariadassou M. 2017. Inference of Adaptive Shifts for Multivariate Correlated Traits. *Systematic Biology, under minor revisions*.

Aristide L, dos Reis SF, Machado AC, Lima I, Lopes RT, Perez SI. 2016. Brain shape convergence in the adaptive radiation of New World monkeys. *Proceedings of the National Academy of Sciences*. 113:2158–2163.

Felsenstein J. 1985. Phylogenies and the Comparative Method. *The American Naturalist*. 125:1–15.

Felsenstein J. 2004. Inferring Phylogenies.

Hansen TF. 1997. Stabilizing Selection and the Comparative Analysis of Adaptation. *Evolution*. 51:1341.

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Thank you for listening

pbastide.github.io