Change-point Detection on a Tree to Study Evolutionary Adaptation from Present-day Species

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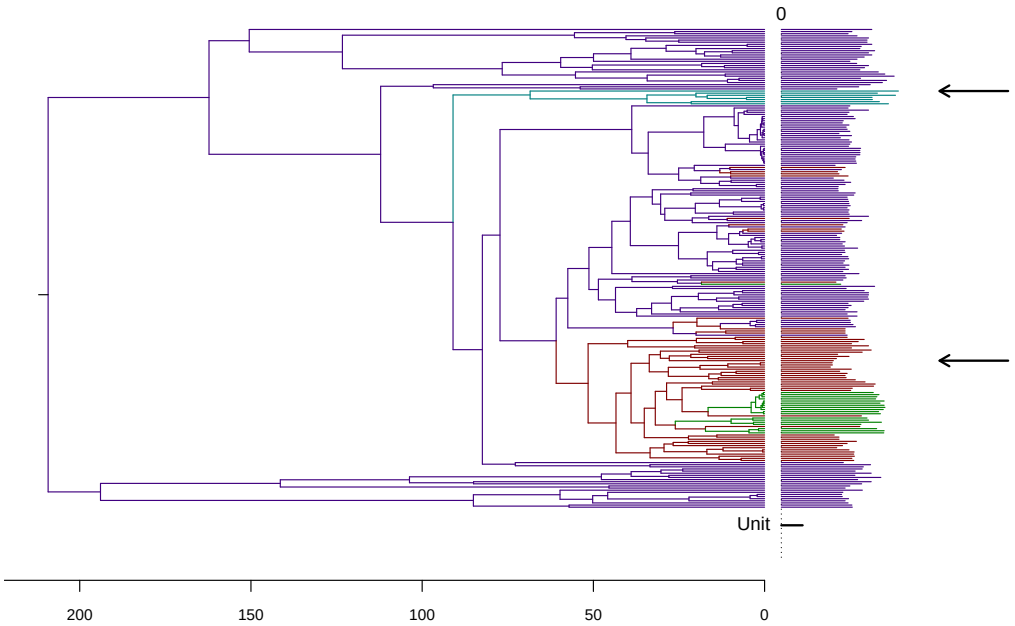
19 April 2016

Introduction



Dermochelys Coriacea

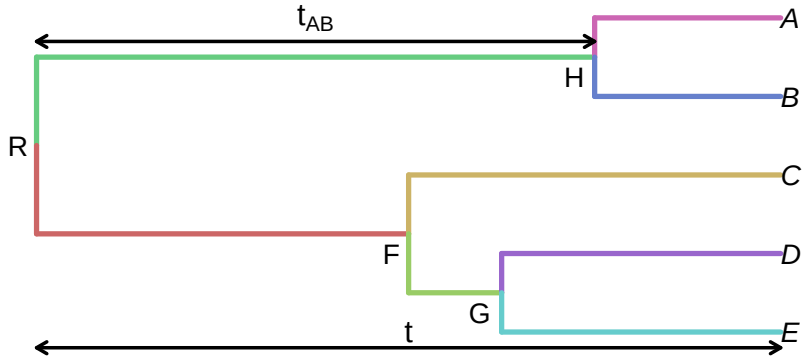
Homopus Areolatus

Turtles phylogenetic tree with habitats.
(Jaffe et al., 2011).

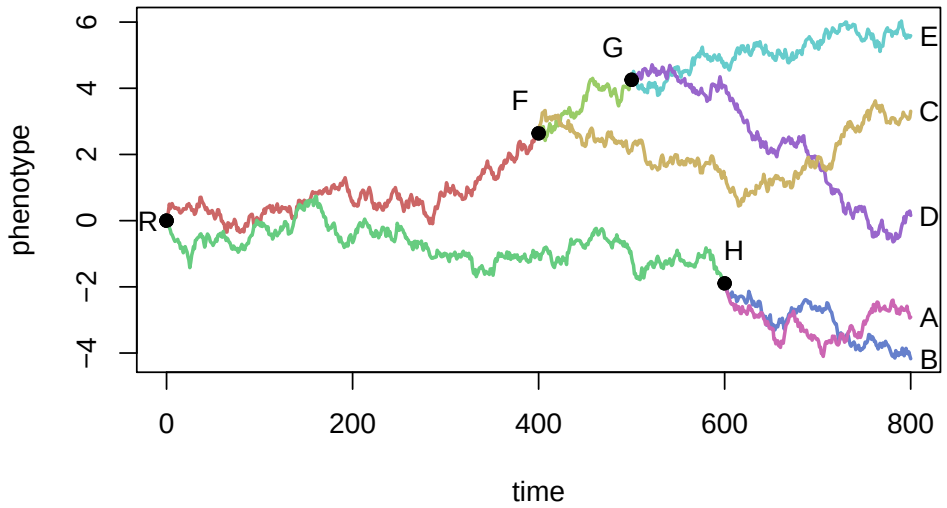
- How can we explain the diversity, while accounting for the phylogenetic correlations ?
- Modelling: a shifted stochastic process on the phylogeny.

Outline

Stochastic Process on a Tree (Felsenstein, 1985)



Only *tip* values are observed

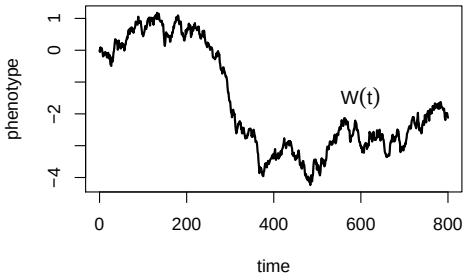
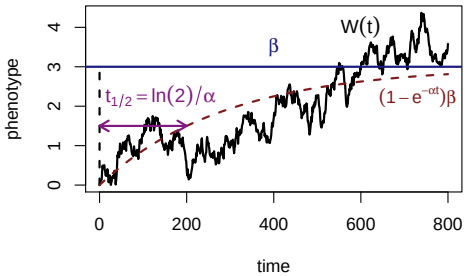


Brownian Motion:

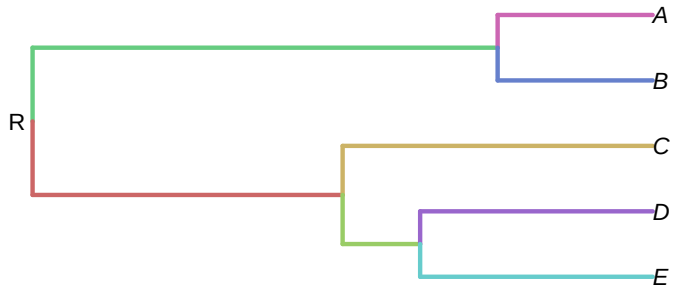
$$\mathbb{V}\mathrm{ar}\left[A \mid R\right] = \sigma^2 t$$

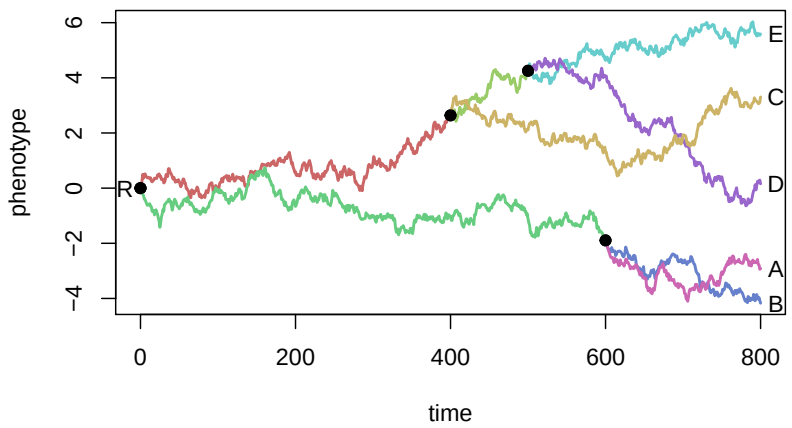
$$\mathbb{C}\mathrm{ov}\left[A; B \mid R\right] = \sigma^2 t_{AB}$$

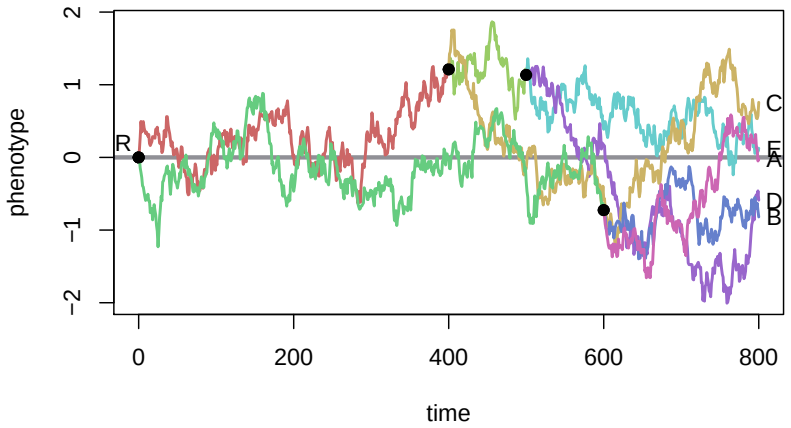
BM vs OU

	Equation	Stationary State	Variance
	$dW(t) = \sigma dB(t)$	None.	$\sigma_{ij} = \sigma^2 t_{ij}$
	$dW(t) = \sigma dB(t)$ $+\alpha[\beta(t) - W(t)]dt$	$\begin{cases} \mu = \beta_0 \\ \gamma^2 = \dfrac{\sigma^2}{2\alpha} \end{cases}$	$\sigma_{ij} = \gamma^2 e^{-\alpha(t_i+t_j)} \times (e^{2\alpha t_{ij}} - 1)$

Shifts







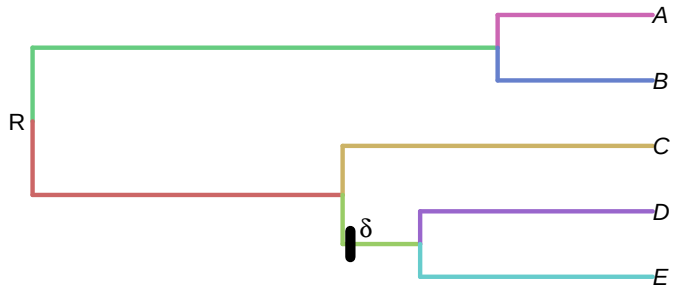
BM Shifts in the **mean**:

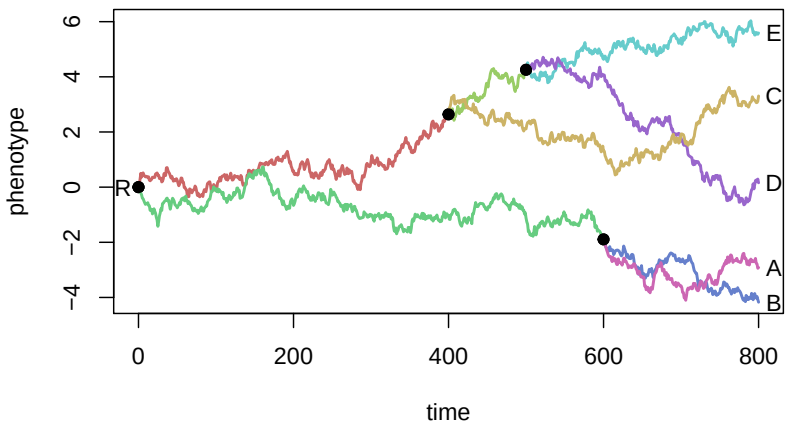
$$m_{\text{child}} = m_{\text{parent}} + \delta$$

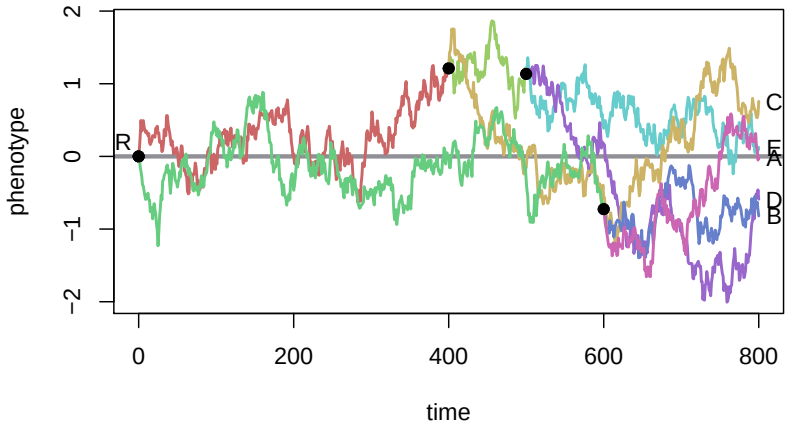
OU Shifts in the **optimal value**:

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

Shifts







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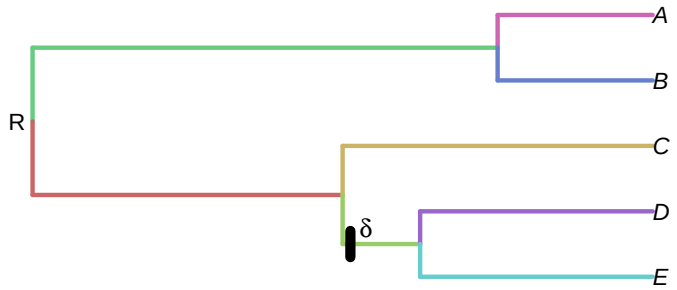

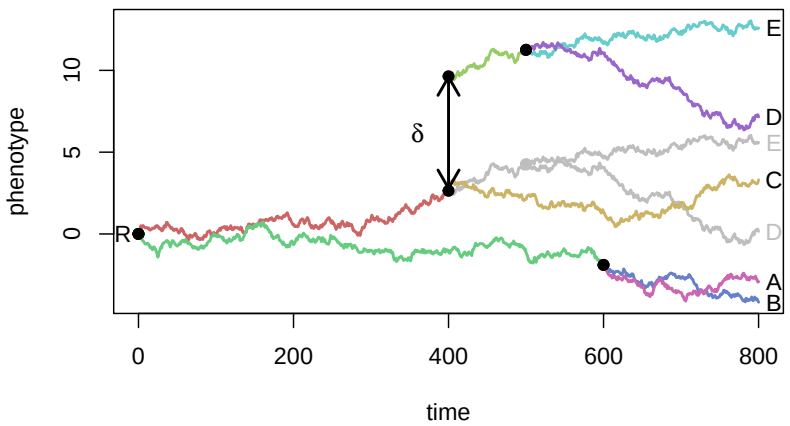

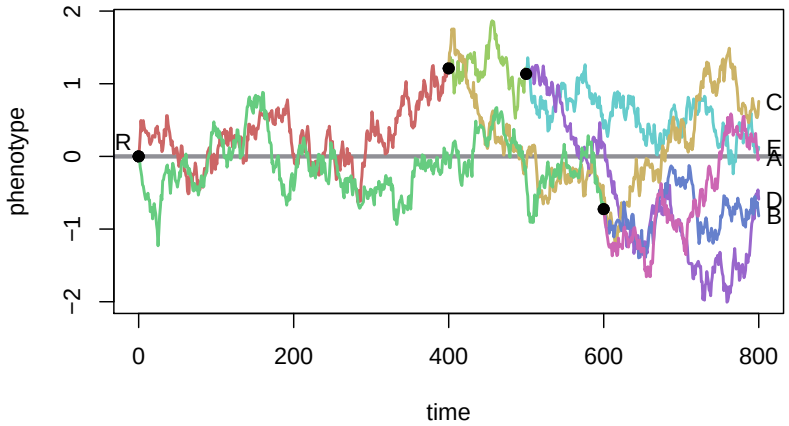

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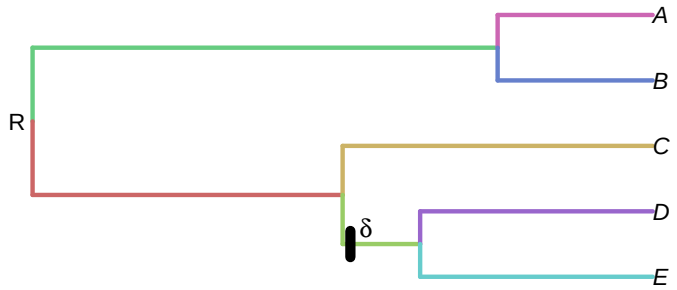

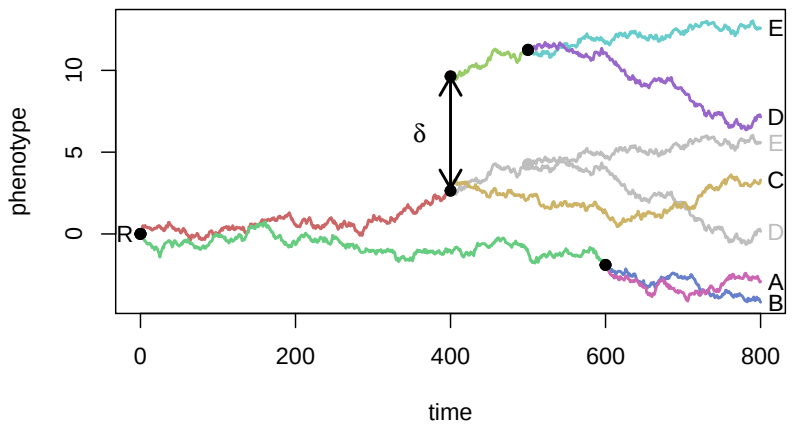

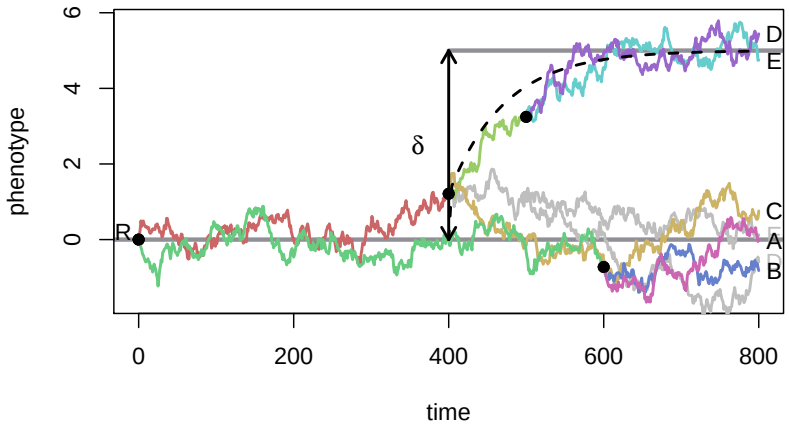

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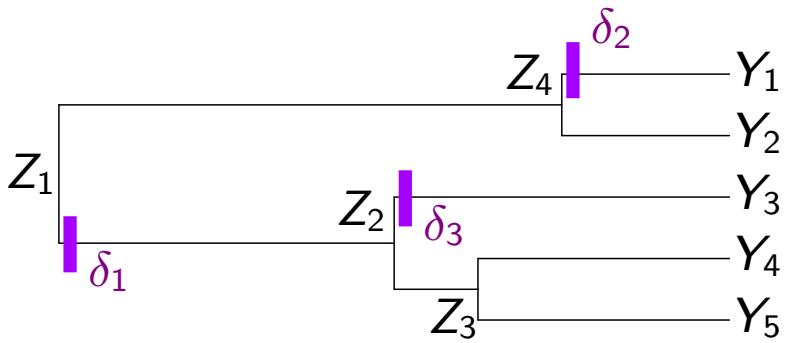
Linear Regression Model

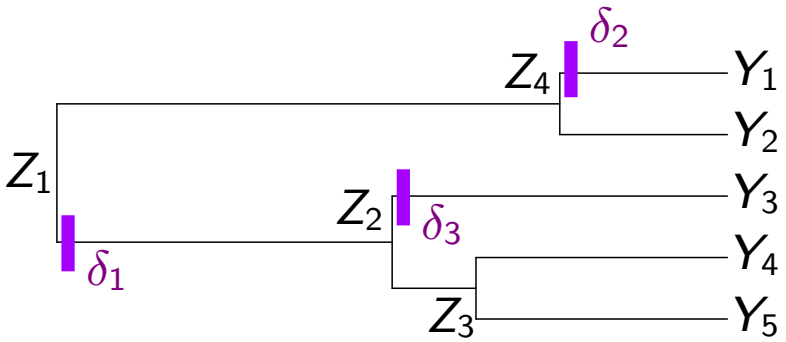


$$\Delta = \begin{pmatrix} \mu \\ \delta_1 \\ 0 \\ 0 \\ \delta_2 \\ 0 \\ \delta_3 \\ 0 \\ 0 \end{pmatrix} \qquad T\Delta = \begin{pmatrix} \mu + \delta_2 \\ \mu \\ \mu + \delta_1 + \delta_3 \\ \mu + \delta_1 \\ \mu + \delta_1 \end{pmatrix}$$

$$T = \begin{array}{c} \\ Y_1 \\ Y_2 \\ Y_3 \\ Y_4 \\ Y_5 \end{array} \begin{array}{c} \begin{array}{ccccccccc} Z_1 & Z_2 & Z_3 & Z_4 & Y_1 & Y_2 & Y_3 & Y_4 & Y_5 \end{array} \\ \begin{pmatrix} 1 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 & 0 & 0 & 1 & 0 \\ 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \end{array}$$

$$BM: \quad Y = T\Delta^{BM} + E^{BM}$$

Linear Regression Model



$$\Delta = \begin{pmatrix} \lambda \\ \delta_1 \\ 0 \\ 0 \\ \delta_2 \\ 0 \\ \delta_3 \\ 0 \\ 0 \end{pmatrix} \qquad TW(\alpha)\Delta = \begin{pmatrix} \lambda + w_5\delta_2 \\ \lambda \\ \lambda + w_2\delta_1 + w_7\delta_3 \\ \lambda + w_2\delta_1 \\ \lambda + w_2\delta_1 \end{pmatrix}$$

$$W(\alpha) = \text{Diag}(1 - e^{-\alpha(h - t_{\text{pa}(i)})}, 1 \leq i \leq m+n)$$

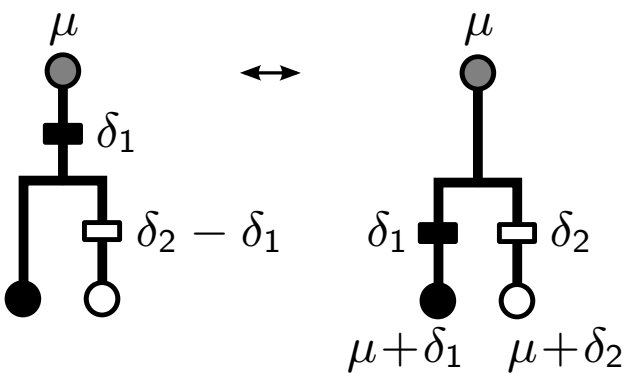
$$\lambda = \mu e^{-\alpha h} + \beta_0(1 - e^{-\alpha h})$$

$$BM: \quad Y = T\Delta^{BM} + E^{BM}$$

$$OU: \quad Y = TW(\alpha)\Delta^{OU} + E^{OU}$$

Equivalencies

- Number of shifts K fixed, several equivalent solutions.



- Problem of over-parametrization: parsimonious configurations.

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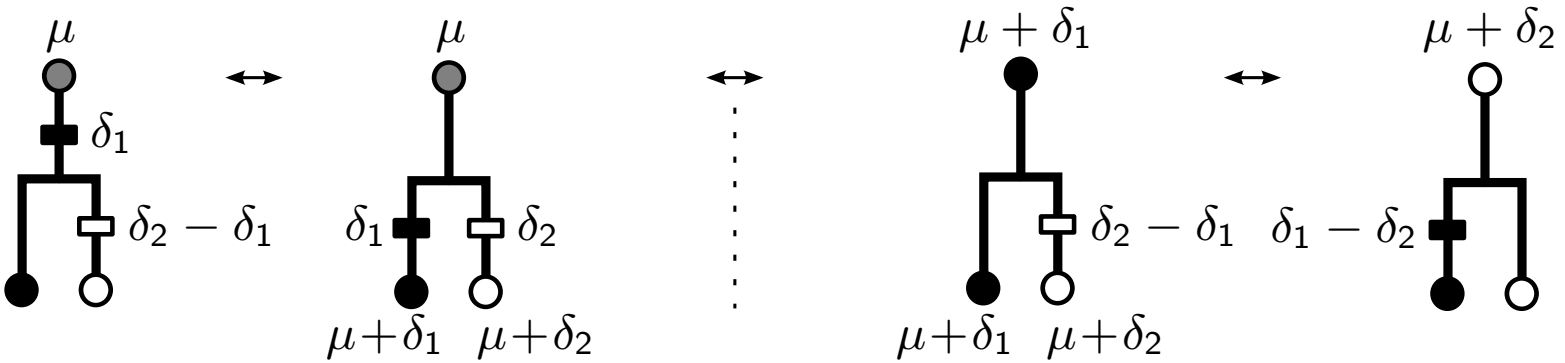

- Problem of over-parametrization: parsimonious configurations.

Parsimonious Solution : Definition

Definition (Parsimonious Allocation)

A coloring of the tips being given, a *parsimonious* allocation of the shifts is such that it has a minimum number of shifts.

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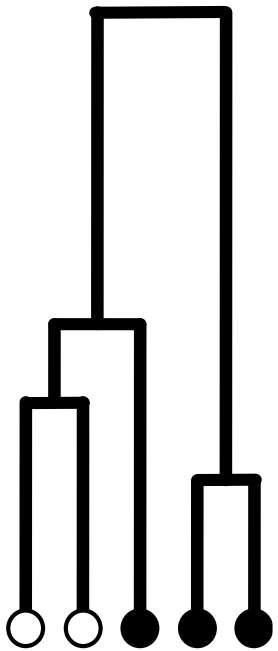

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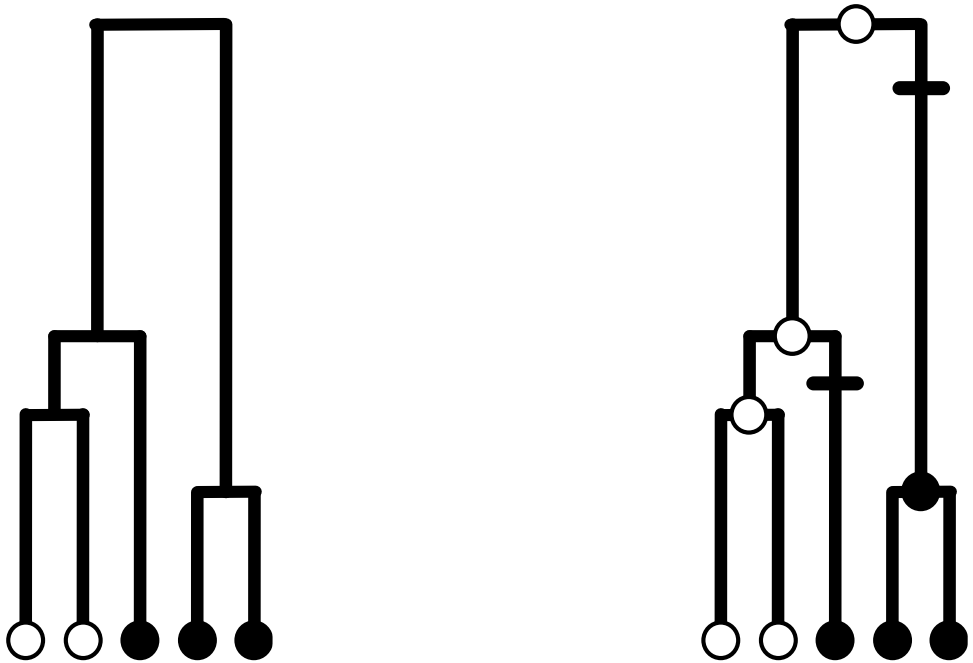

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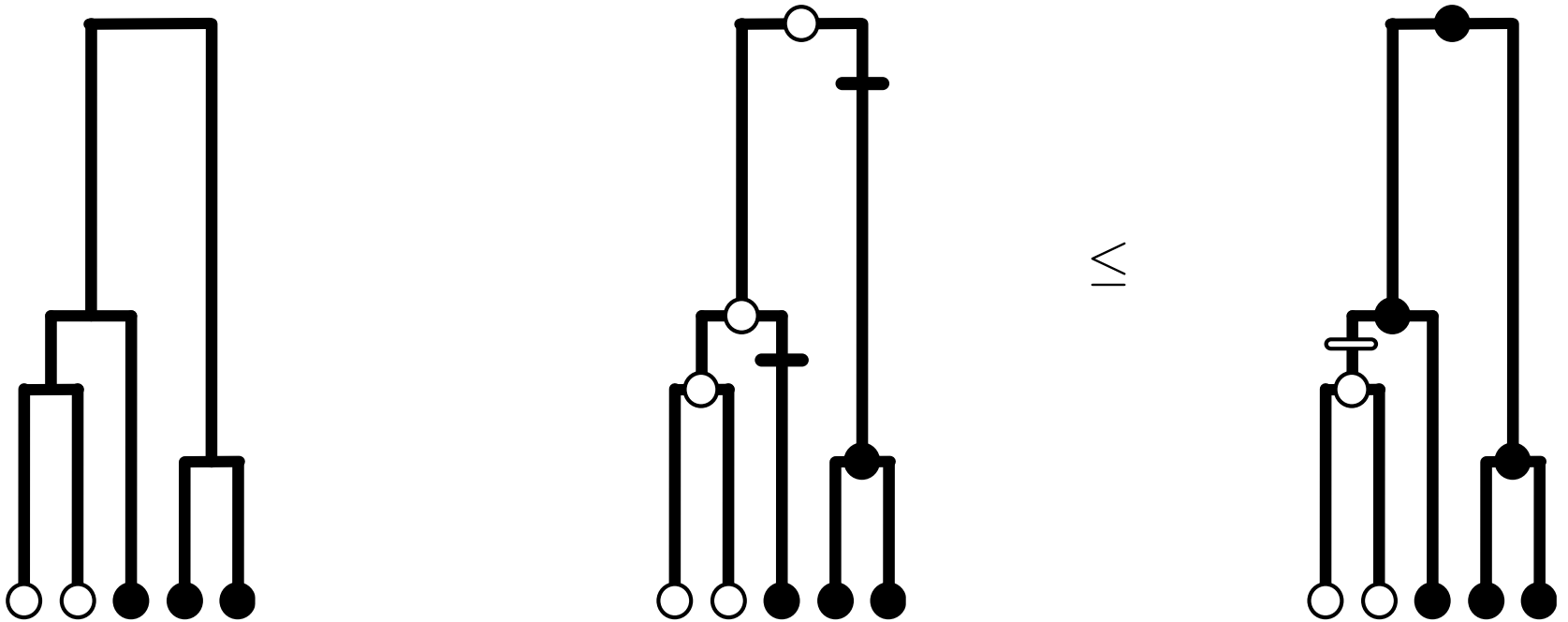

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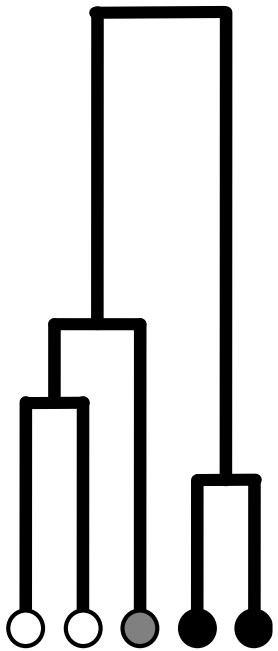

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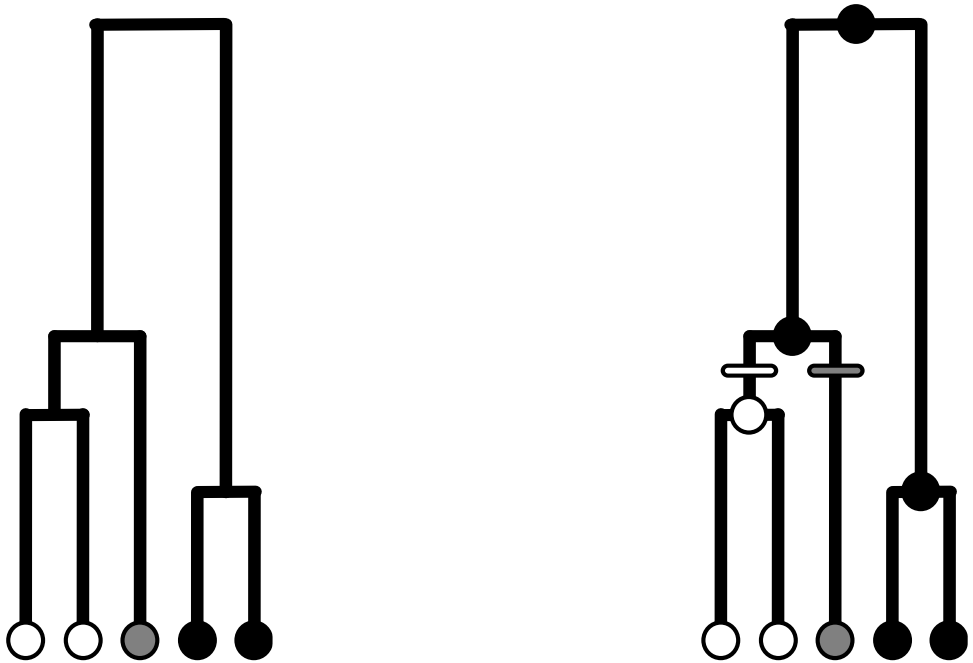

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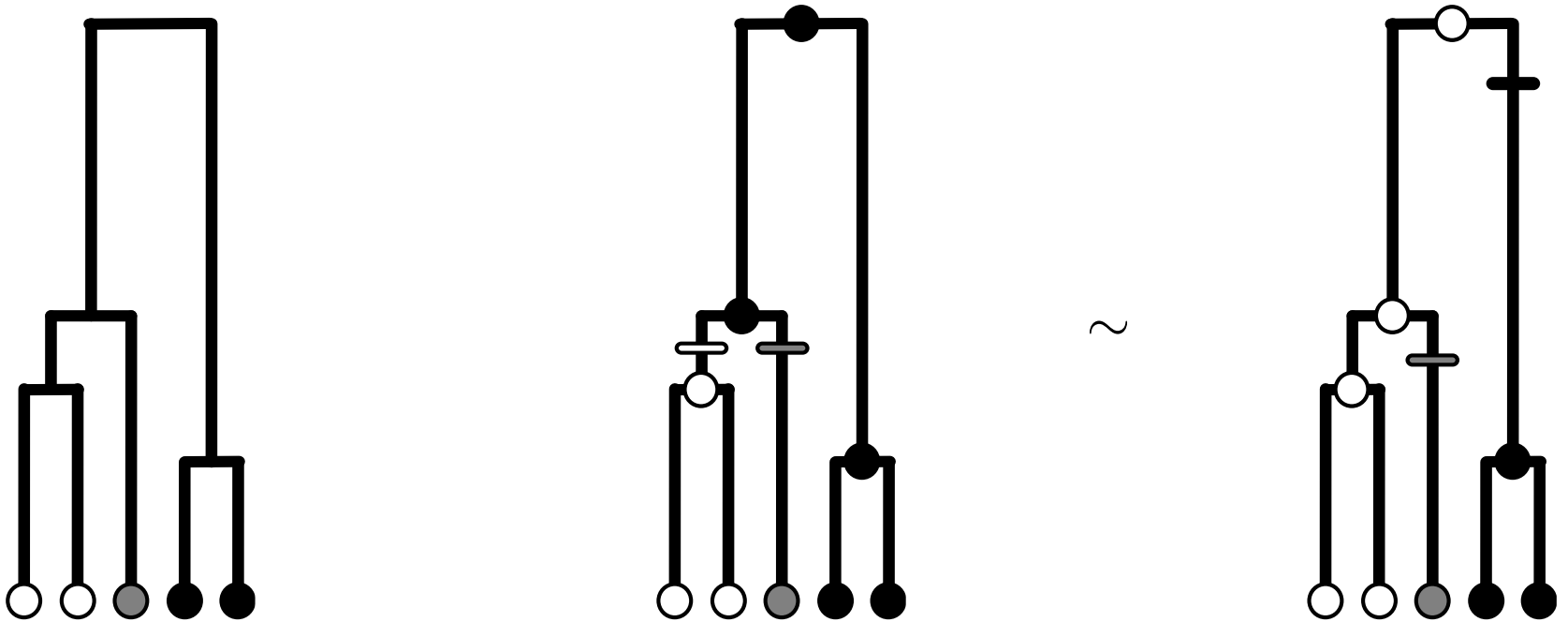


Equivalent Parsimonious Allocations

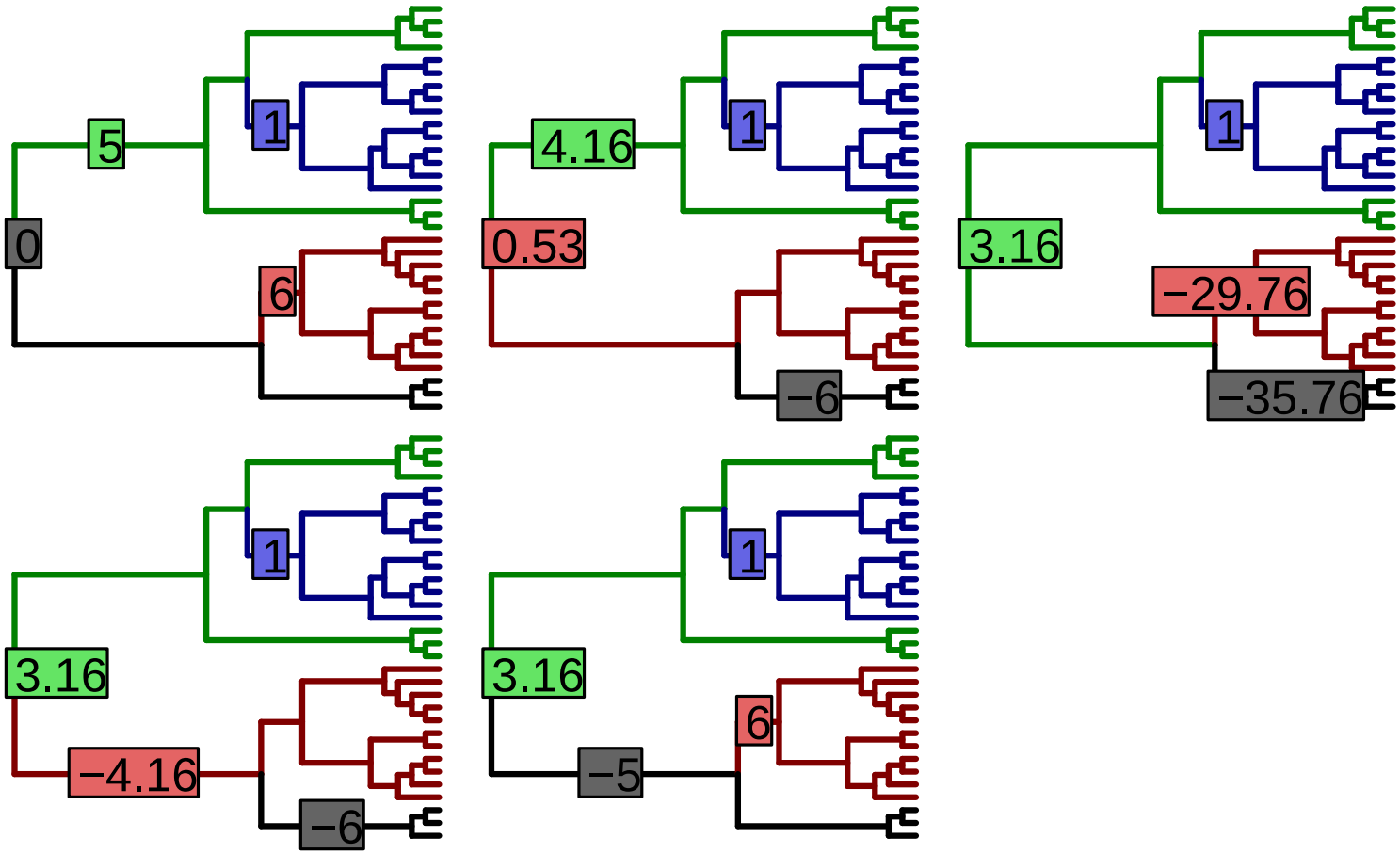
Definition (Equivalency)

Two allocations are said to be *equivalent* (noted $\sim$) if they are both parsimonious and give the same colors at the tips.

Find one solution Several existing Dynamic Programming algorithms (Fitch, Sankoff, see Felsenstein, 2004).

Enumerate all solutions New recursive algorithm, adapted from previous ones (and implemented in R).

Equivalent Parsimonious Solutions for an OU Model.



Equivalent allocations and values of the shifts - OU.

Collection of Models

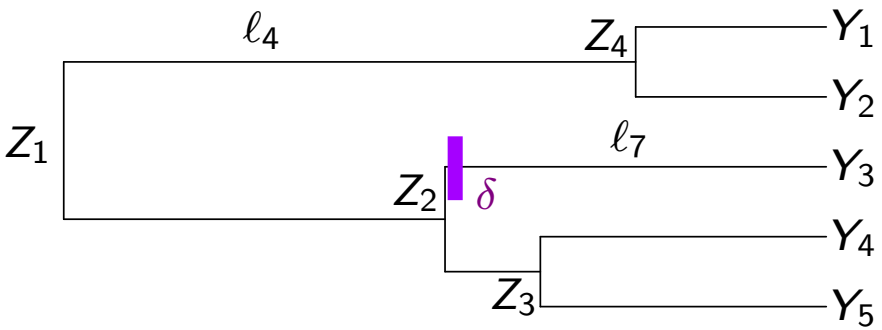
New Problem Number of Equivalence Classes: $\left|\mathcal{S}_K^{PI}\right|$?

- $\left|\mathcal{S}_K^{PI}\right| \leq \binom{m+n-1}{K} = \binom{\#\text{ of edges}}{\#\text{ of shifts}}$
- A recursive algorithm to compute $\left|\mathcal{S}_K^{PI}\right|$ (implemented in R).

$\mapsto$ Generally dependent on the topology of the tree.

- Binary tree: $\left|\mathcal{S}_K^{PI}\right| = \binom{2n-2-K}{K} = \binom{\#\text{ of edges}-\#\text{ of shifts}}{\#\text{ of shifts}}$

EM Algorithm: number of shifts K fixed



$$Y_3 \mid Z_2 \sim \mathcal{N}\Big(Z_2 + \delta,\ \ell_7\sigma^2\Big)$$

$$Z_4 \mid Z_1 \sim \mathcal{N}\Big(Z_1,\ \ell_4\sigma^2\Big)$$

$$\log p_\theta(Y) = \mathbb{E}_\theta[\log p_\theta(Z, Y) \mid Y] - \mathbb{E}_\theta[\log p_\theta(Z) \mid Y]$$

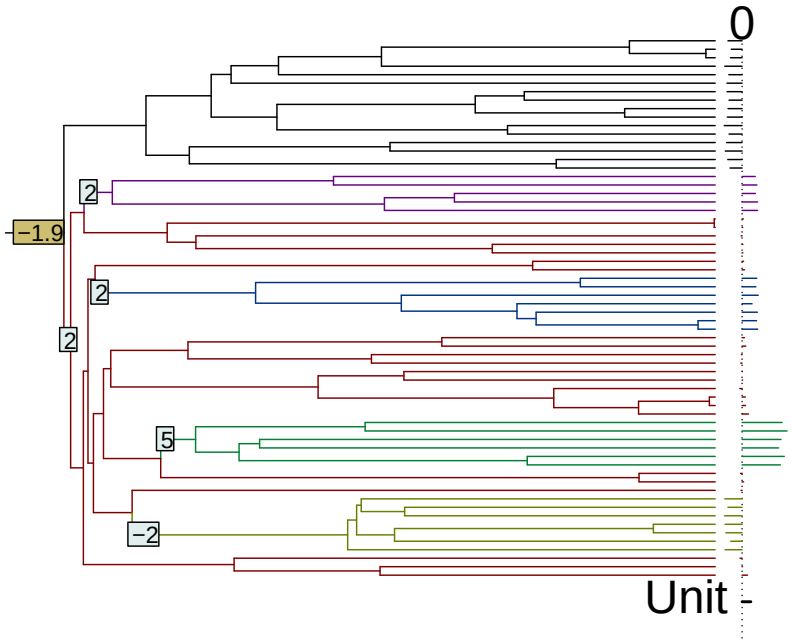
$$p_\theta(Z, Y) = p_\theta(Z_1) \prod_{1<j\leq m} p_\theta(Z_j|Z_{\text{parent}(j)}) \prod_{1\leq i\leq n} p_\theta(Y_i|Z_{\text{parent}(i)})$$

EM Algorithm Maximize $\mathbb{E}_\theta[\log p_\theta(Z, Y) \mid Y]$

E step Given θ^h, compute $p_{\theta^h}(Z \mid Y)$

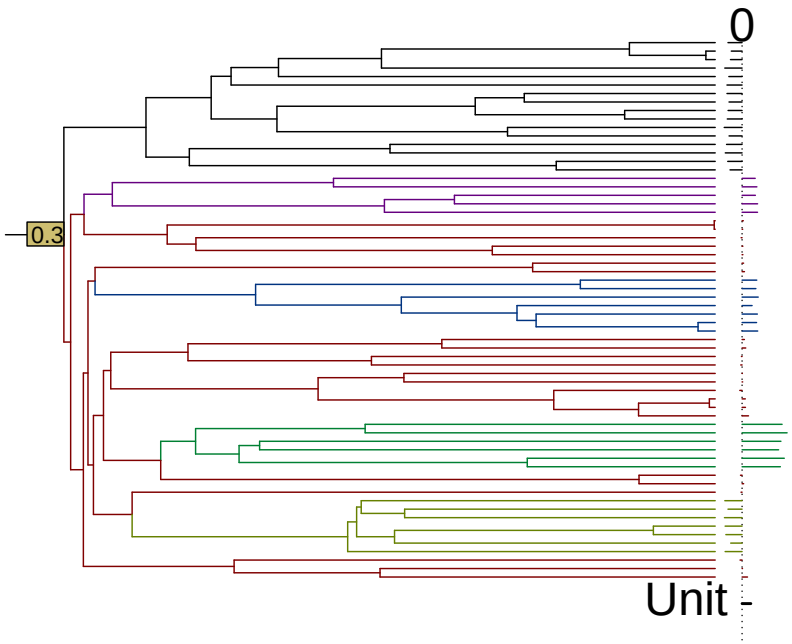
M step $\theta^{h+1} = \text{argmax}_\theta\, \mathbb{E}_{\theta^h}[\log p_\theta(Z, Y) \mid Y]$

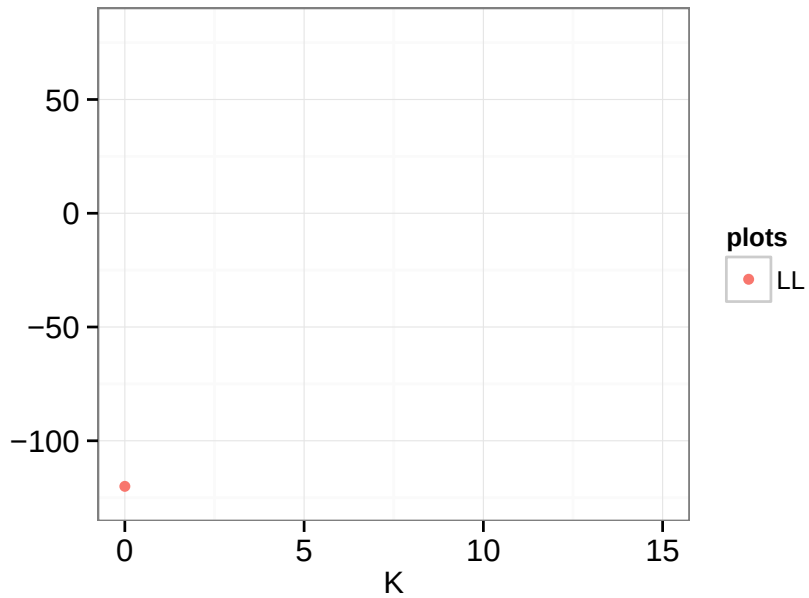
Model Selection on K



Simulated OU (α =3, γ^2 =0.1)

Model Selection on K

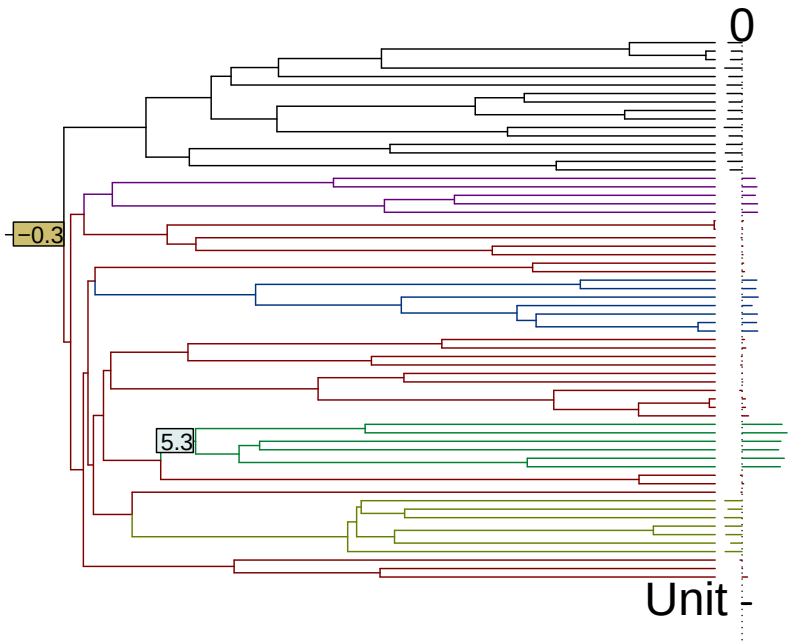


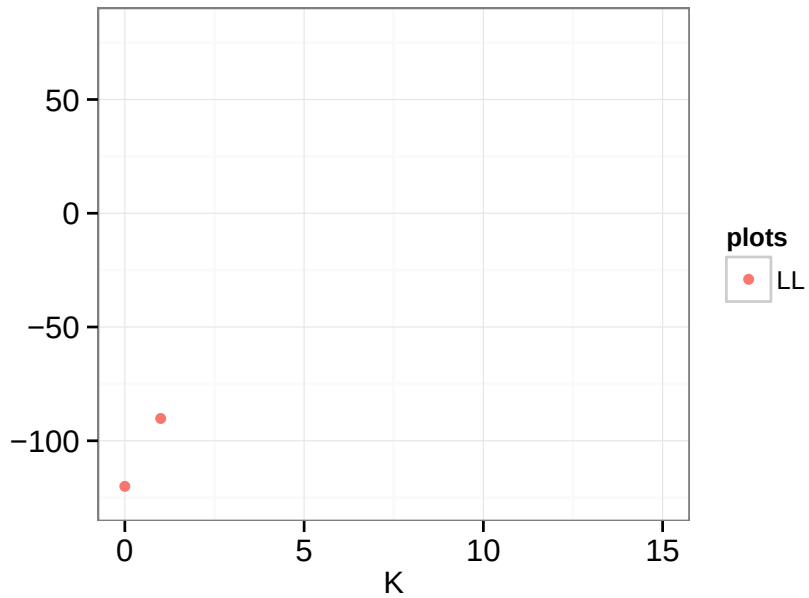


$$\hat{Y}_K = \underset{\eta \in \mathcal{S}_K^{PI}}{\text{argmax}} -\frac{n}{2} \log \left(\frac{\left\| Y - \hat{Y}_\eta \right\|_V^2}{n} \right)$$

$$LL = -\frac{n}{2} \log \left(\frac{\left\| Y - \hat{Y}_K \right\|_V^2}{n} \right)$$

Model Selection on K





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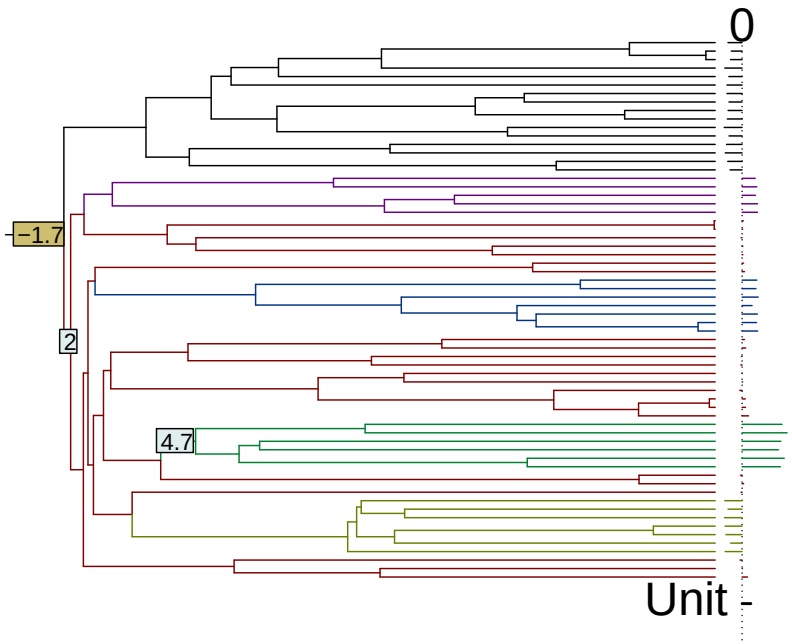

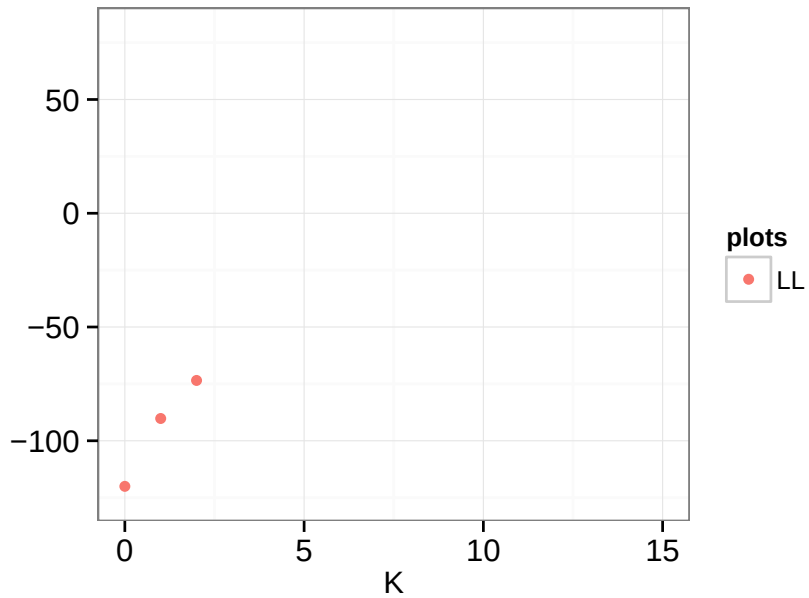

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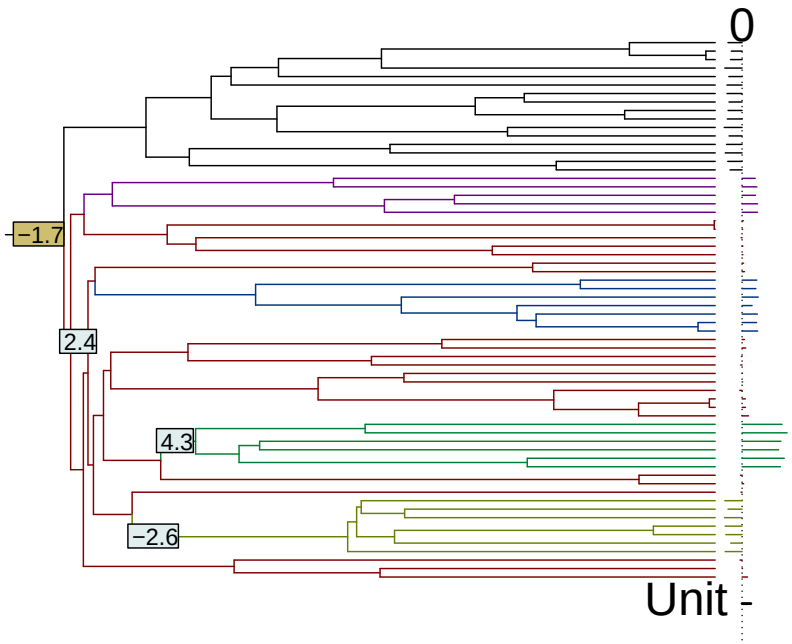

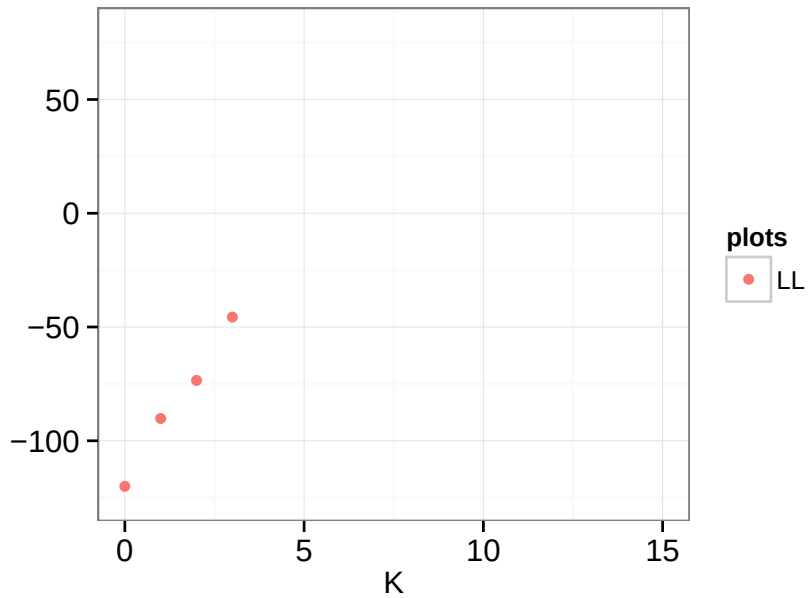

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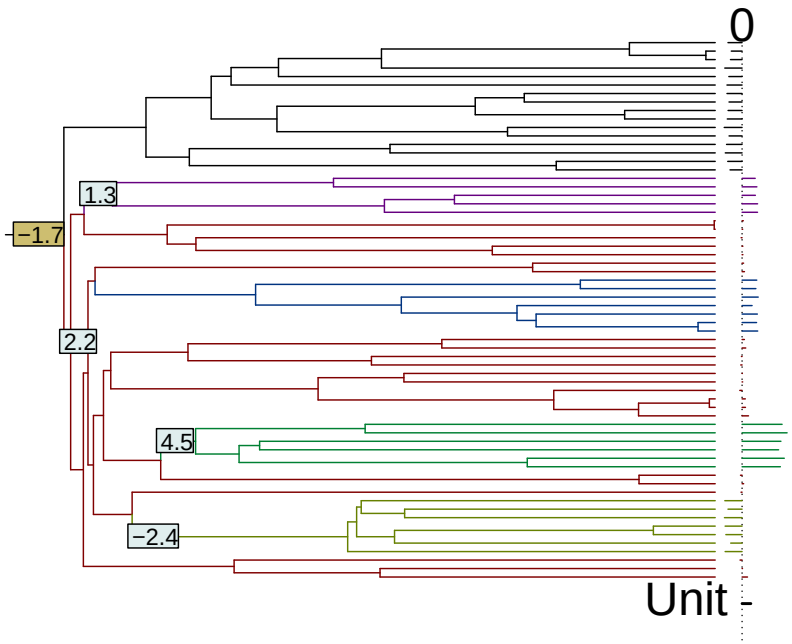

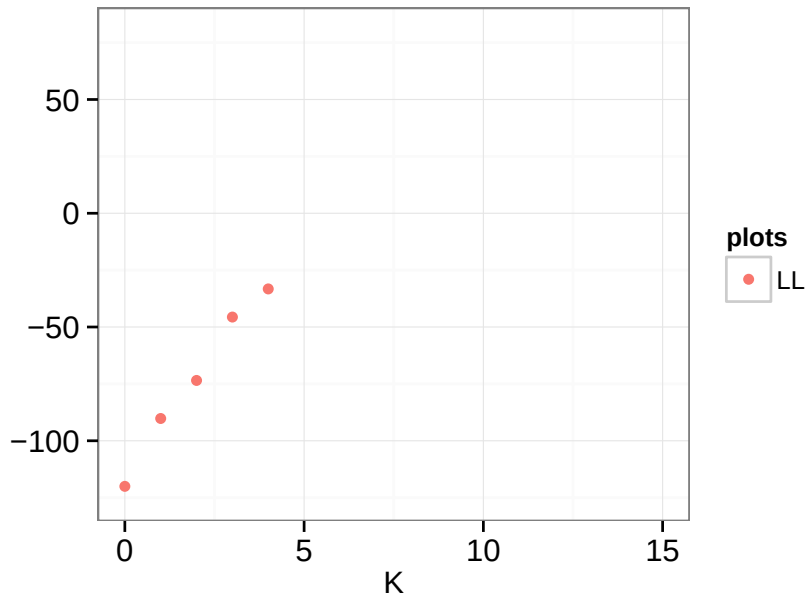

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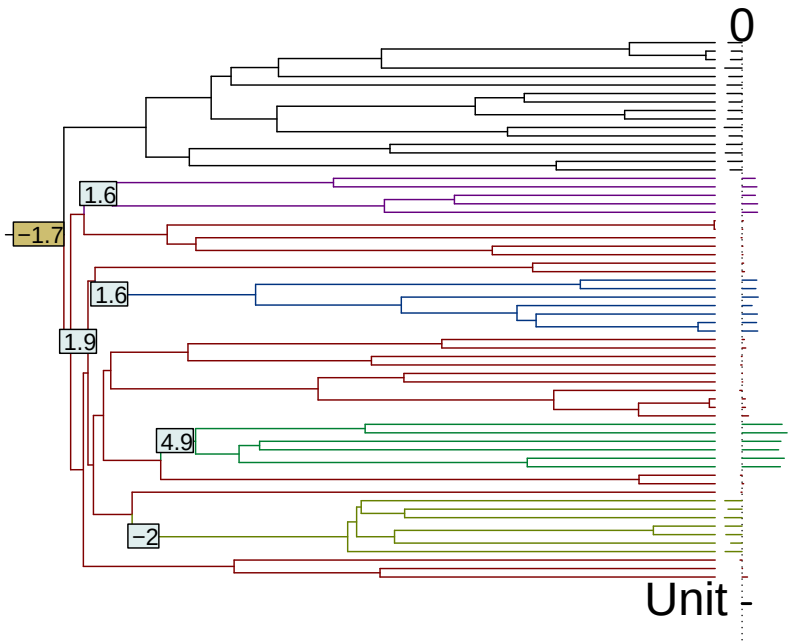
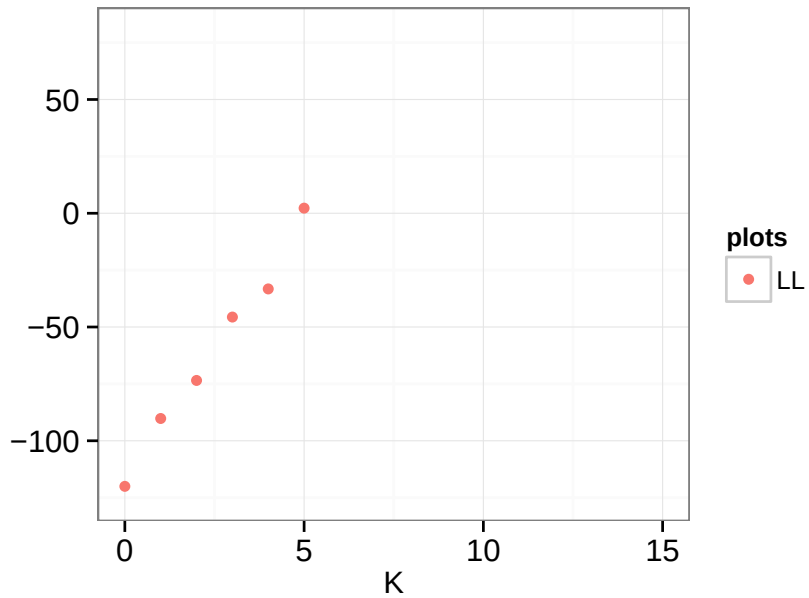
$$LL = -\frac{n}{2} \log \left(\frac{\left\| Y - \hat{Y}_K \right\|_V^2}{n} \right)$$

Model Selection on K





$$\hat{Y}_K = \underset{\eta \in \mathcal{S}_K^{PI}}{\text{argmax}} -\frac{n}{2} \log \left(\frac{\left\| Y - \hat{Y}_\eta \right\|_V^2}{n} \right)$$

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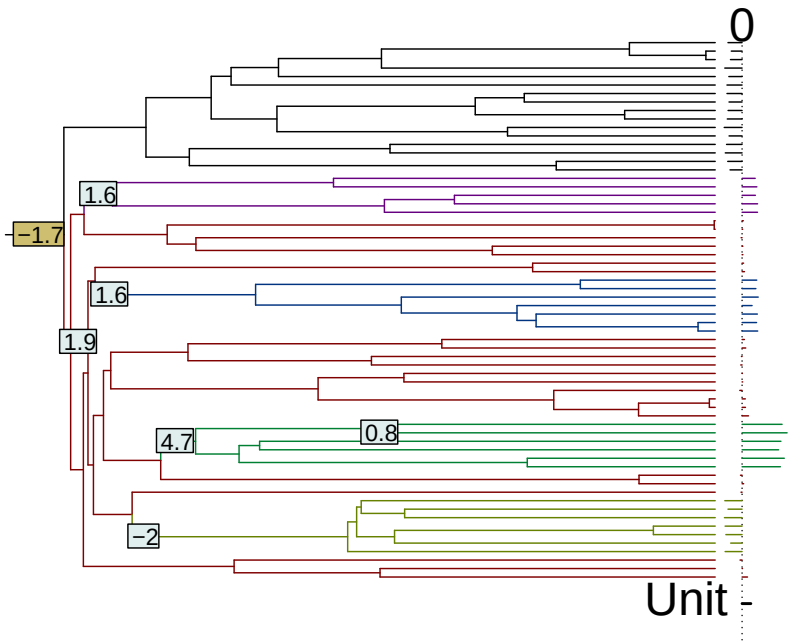
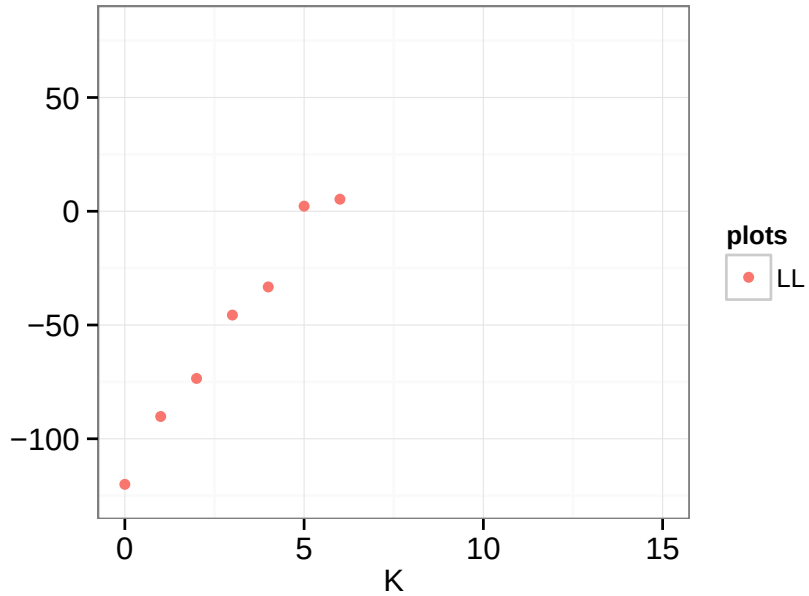
Model Selection on K





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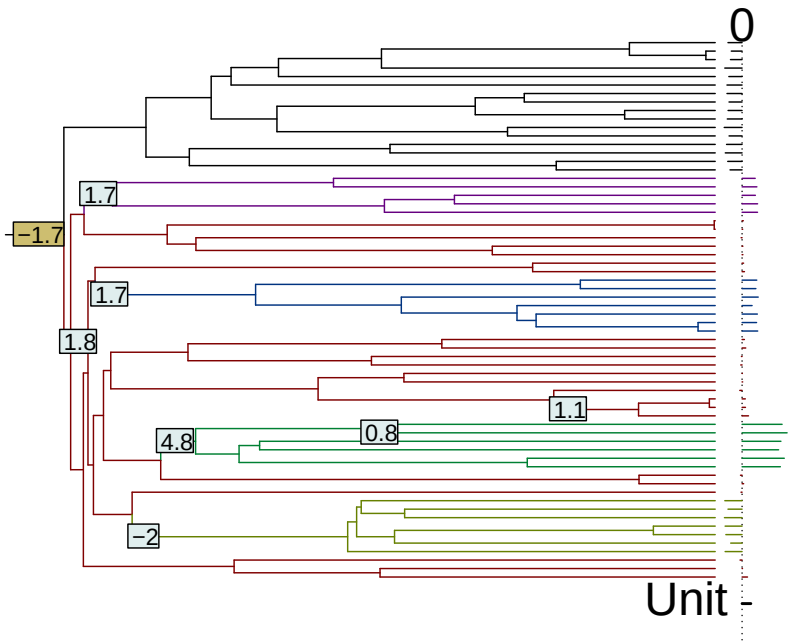

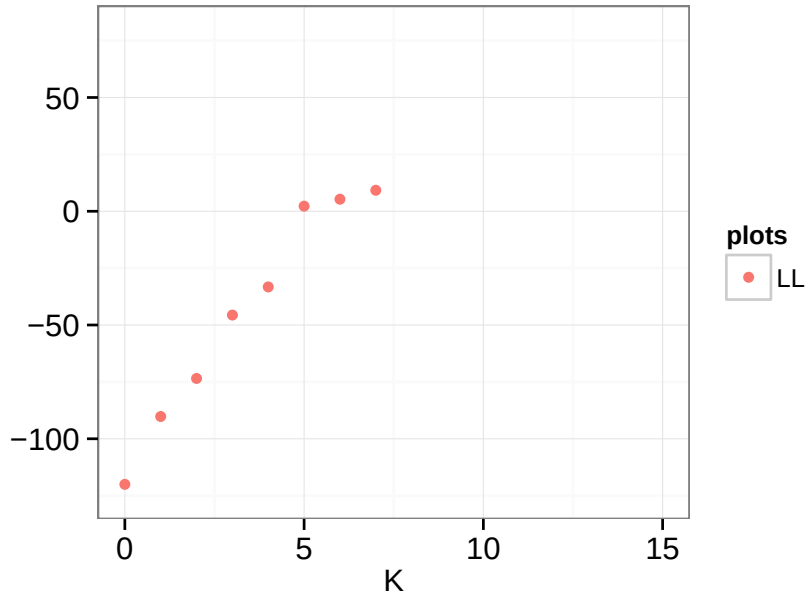

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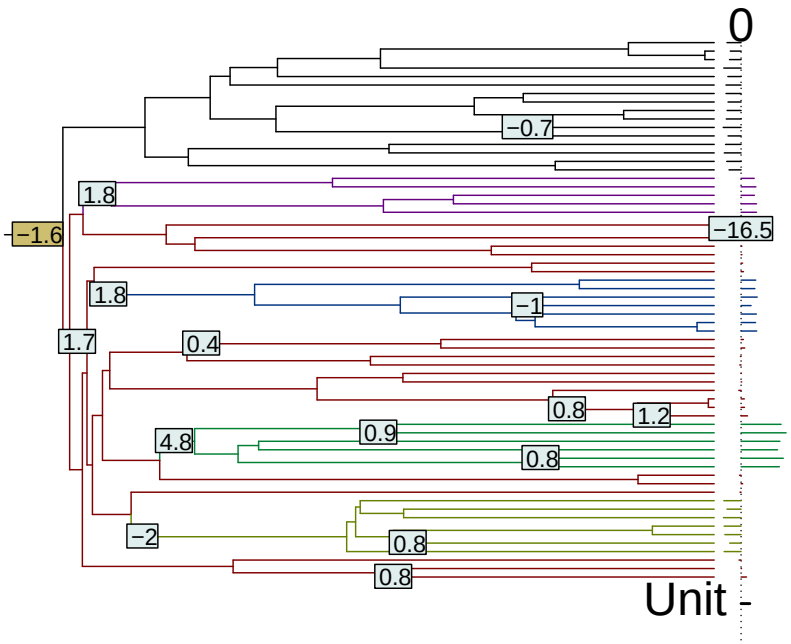

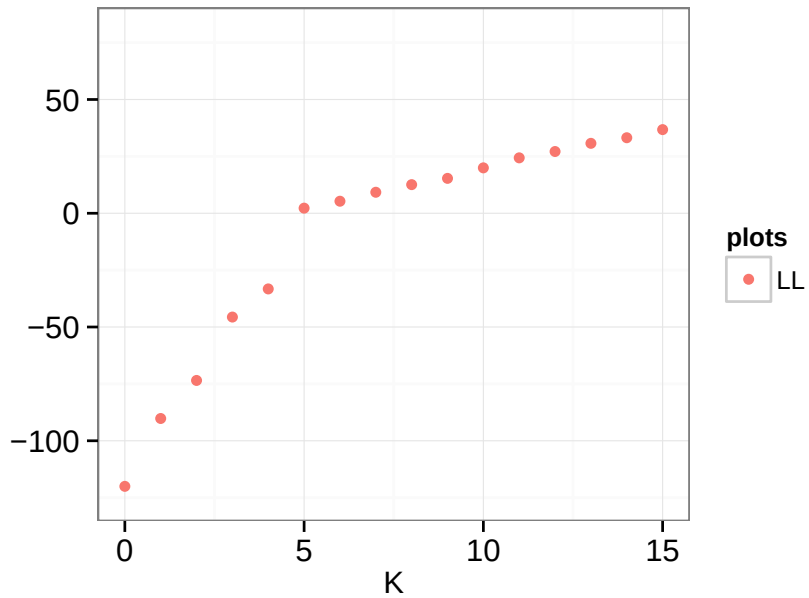

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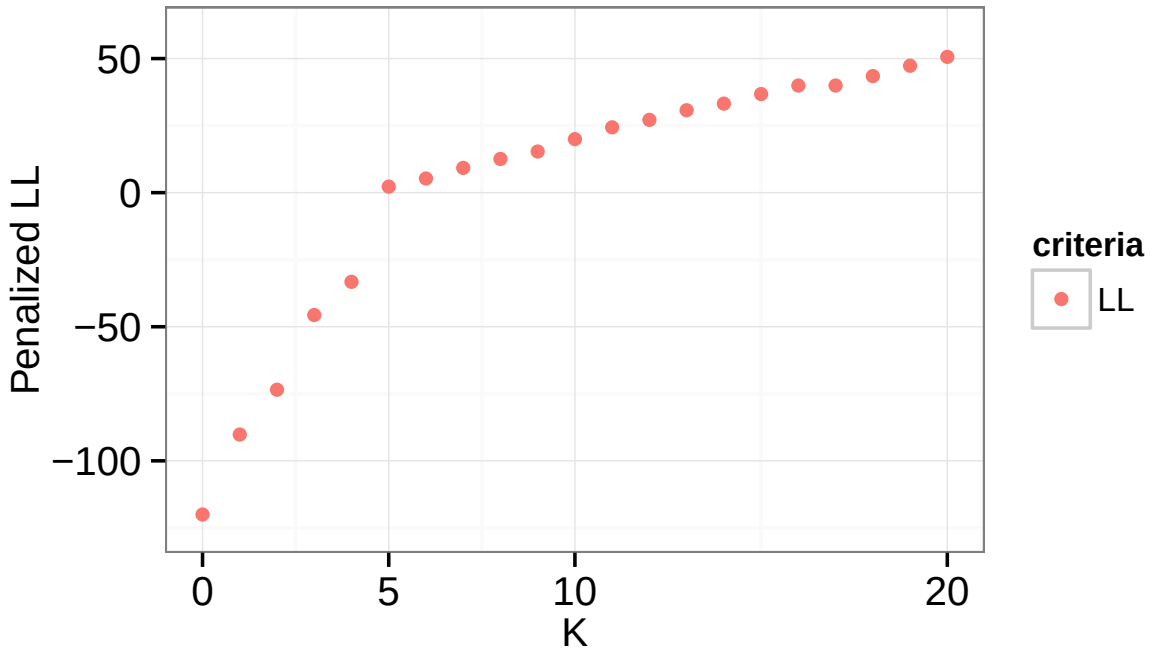
Model Selection: Penalized Likelihood

$$\text{Idea} \quad \hat{K} = - \underset{0 \leq K \leq p-1}{\operatorname{argmin}} \frac{n}{2} \log \left(\frac{\left\| Y - \hat{Y}_K \right\|_V^2}{n} \right) - \frac{1}{2} \operatorname{pen}'(K)$$



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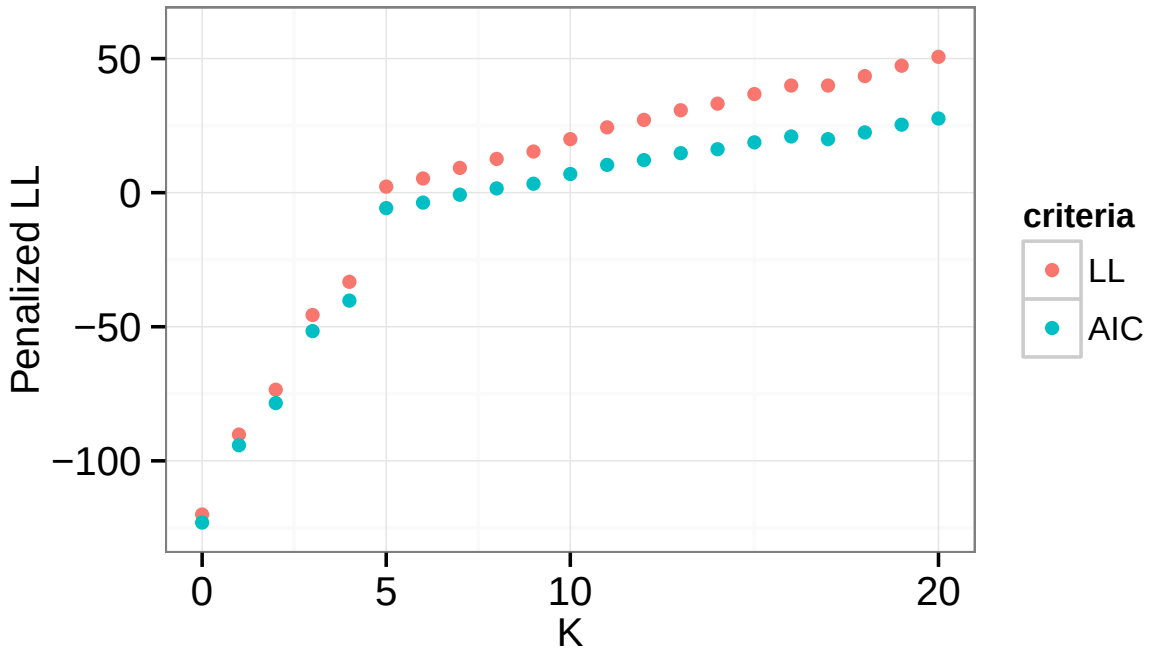

Penalties:

AIC $K + 3$

Model Selection: Penalized Likelihood

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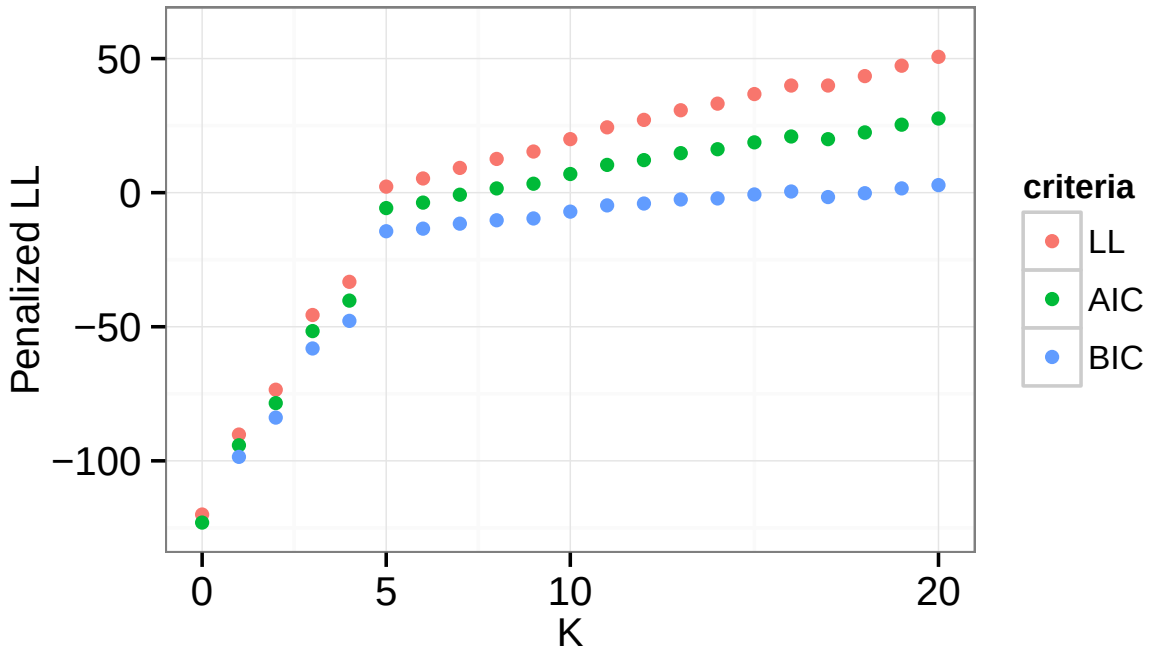


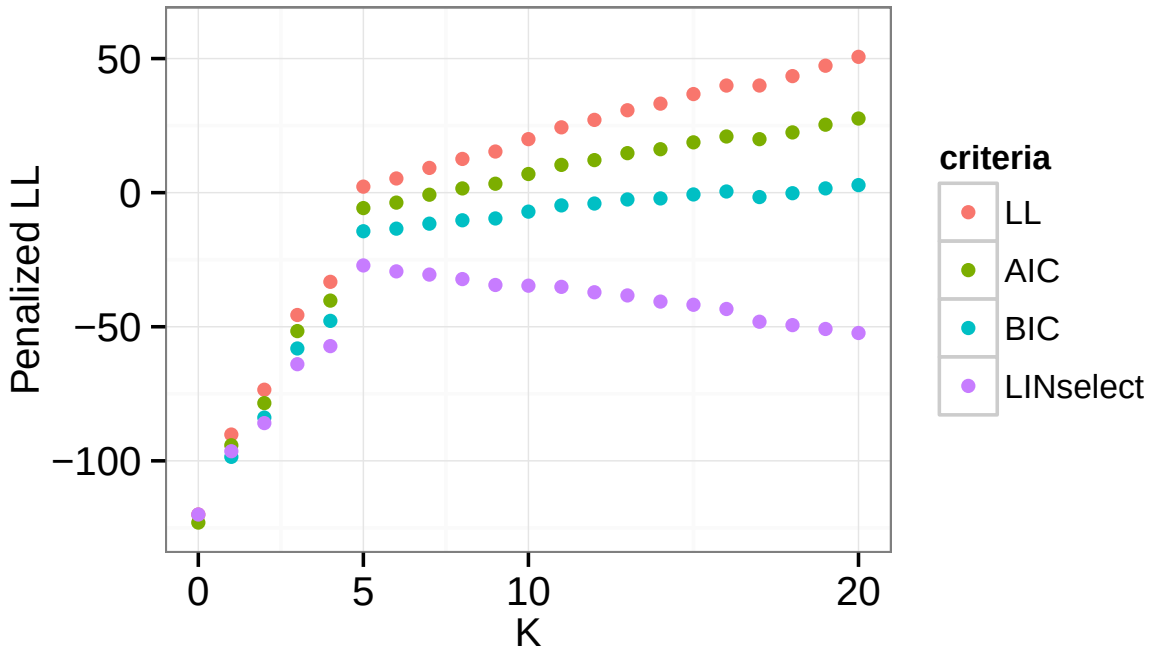
Penalties:

AIC $K + 3$

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

Model Selection: Penalized Likelihood

$$\text{Idea} \quad \hat{K} = - \underset{0 \leq K \leq p-1}{\operatorname{argmin}} \frac{n}{2} \log \left(\frac{\left\| Y - \hat{Y}_K \right\|_V^2}{n} \right) - \frac{1}{2} \operatorname{pen}'(K)$$



Penalties:

AIC $K + 3$

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

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

Proposition: LINselect Penalty

Proposition (Form of the Penalty and guarantees (α known))

Under our setting: $Y = TW(\alpha)\Delta + \gamma E$ *with* $E \sim \mathcal{N}(0, V)$, *define the penalty:*

$$\text{pen}(K) = A\frac{n-K-1}{n-K-2}\,\text{EDkhi}\left[K+2, n-K-2, exp\left(-\log\left|\mathcal{S}_K^{Pl}\right| - 2\log(K+2)\right)\right]$$

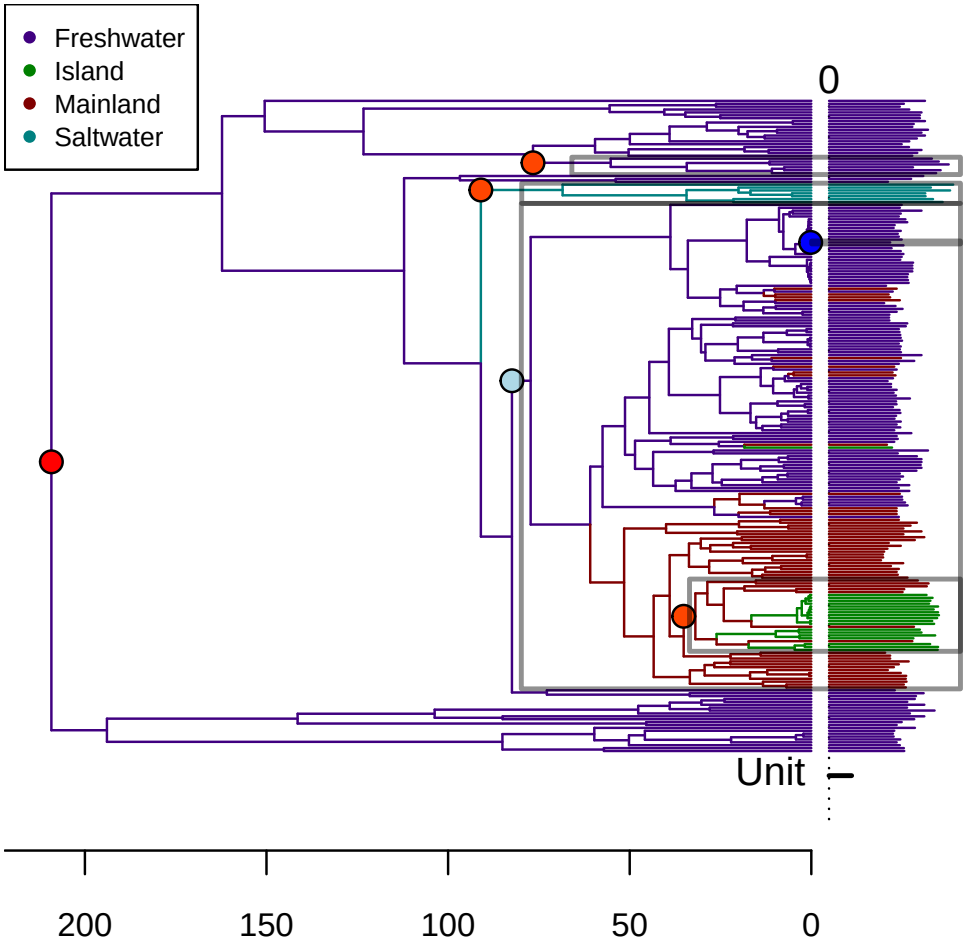
If $\kappa < 1$, *and* $p \leq \min\left(\frac{\kappa n}{2+\log(2)+\log(n)}, n-7\right)$, *we get:*

$$\mathbb{E}\left[\frac{\left\|\mathbb{E}[Y] - \hat{Y}_{\hat{K}}\right\|_V^2}{\gamma^2}\right] \leq C(A,\kappa)\inf_{\eta\in\mathcal{M}}\left\{\frac{\left\|\mathbb{E}[Y] - Y_\eta^*\right\|_V^2}{\gamma^2} + (K_\eta+2)(3+\log(n))\right\}$$

with $C(A,\kappa)$ *a constant depending on* A *and* κ *only.*

Based on Baraud et al. (2009) +

Turtles Dataset

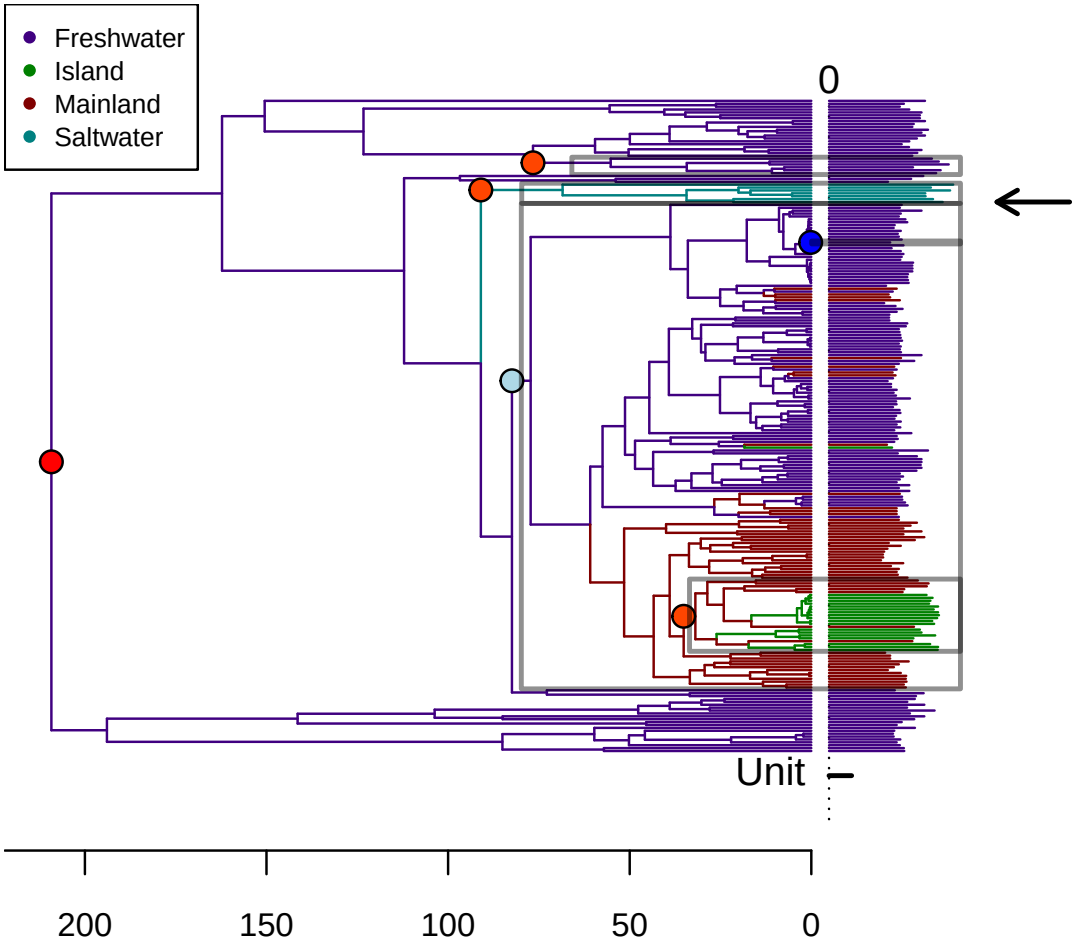


Colors: habitats.
Boxes: selected EM regimes.

	Habitat	EM
No. of shifts	16	5
No. of regimes	4	6
lnL	-133.86	-97.59
$\ln 2/\alpha$ (%)	7.44	5.43
$\sigma^2/2\alpha$	0.33	0.22
CPU t (min)	65.25	134.49

(Jaffe et al., 2011)

Turtles Dataset



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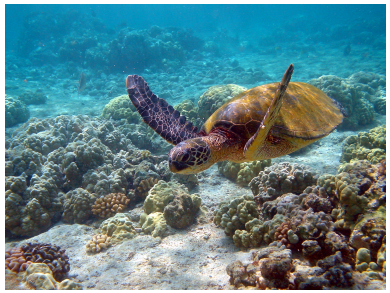
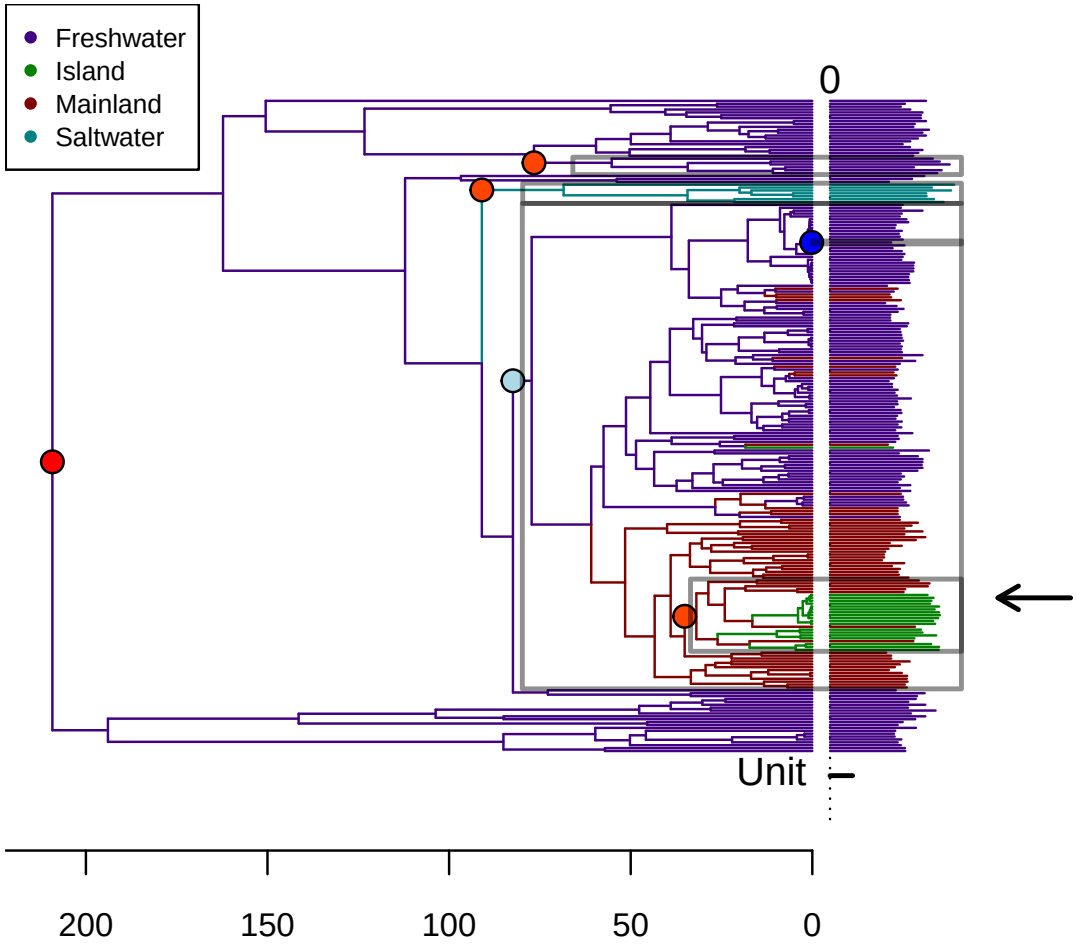


Chelonia mydas

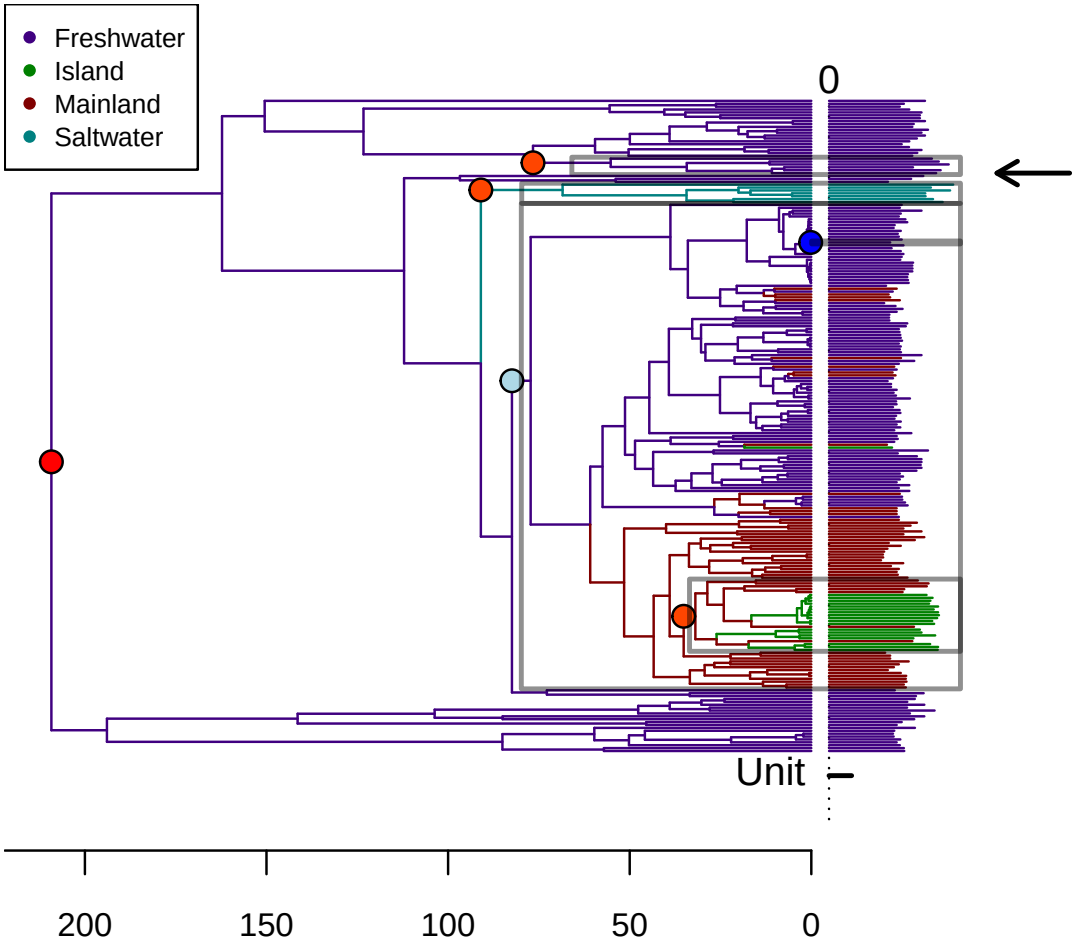
Turtles Dataset



Colors: habitats.
Boxes: selected EM regimes.

Geochelone nigra abingdoni

Turtles Dataset



Colors: habitats.
Boxes: selected EM regimes.

Chitra indica

Conclusion and Perspectives

A general inference framework for trait evolution models.

Conclusions

- Some problems of identifiability arise.
- An EM can be written to maximize likelihood.
- Adaptation of model selection results to non-iid framework.

R codes Available on GitHub:
`https://github.com/pbastide/Phylogenetic-EM`

Perspectives

- Multivariate traits.
- Deal with uncertainty (tree, data).
- Use fossil records.

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- "Florida Box Turtle Digon3a", "Jonathan Zander (Digon3)" derivative work: Materialscientist

Thank you for listening

Appendices

Model Selection with Unknown Variance

Theorem (Baraud et al. (2009))

Under the following setting:

$$Y' = \mathbb{E}\left[Y'\right] + \gamma E' \quad \textit{with} \quad E' \sim \mathcal{N}(0, I_n) \quad \textit{and} \quad \mathcal{S}' = \{S'_\eta, \eta \in \mathcal{M}\}$$

If $D_\eta = \mathrm{Dim}(S'_\eta)$, $N_\eta = n - D_\eta \geq 7$, $\max(L_\eta, D_\eta) \leq \kappa n$, *with* $\kappa < 1$, *and:*

$$\Omega' = \sum_{\eta \in \mathcal{M}} (D_\eta + 1) e^{-L_\eta} < +\infty$$

$$\textit{If:} \quad \hat{\eta} = \underset{\eta \in \mathcal{M}}{\mathrm{argmin}} \left\| Y' - \hat{Y}'_\eta \right\|^2 \left(1 + \frac{\mathrm{pen}(\eta)}{N_\eta}\right)$$

$$\textit{with:} \quad \mathrm{pen}(\eta) = \mathrm{pen}_{A,\mathcal{L}}(\eta) = A \frac{N_\eta}{N_\eta - 1} \mathrm{EDkhi}[D_\eta + 1, N_\eta - 1, e^{-L_\eta}] \quad , \quad A > 1$$

$$\textit{Then:} \ \mathbb{E}\left[\frac{\left\| \mathbb{E}\left[Y'\right] - \hat{Y}'_{\hat{\eta}} \right\|^2}{\gamma^2}\right] \leq C(A, \kappa) \left[\inf_{\eta \in \mathcal{M}} \left\{ \frac{\left\| \mathbb{E}\left[Y'\right] - Y'_\eta \right\|^2}{\gamma^2} + \max(L_\eta, D_\eta) \right\} + \Omega' \right]$$

IID Framework ($\alpha = 0$)

$$\text{Assume} \quad K_\eta = D_\eta - 1 \leq p - 1 \leq n - 8, \quad \forall \eta \in \mathcal{M}$$

Then:

$$\begin{aligned}
\Omega' &= \sum_{\eta \in \mathcal{M}} (D_\eta + 1) e^{-L_\eta} = \sum_{\eta \in \mathcal{M}} (K_\eta + 2) e^{-L_\eta} \\
&= \sum_{K=0}^{p-1} \left| \mathcal{S}_K^{PI} \right| (K+2) e^{-L_K} = \sum_{K=0}^{p-1} \left| \mathcal{S}_K^{PI} \right| (K+2) e^{-(\log \left| \mathcal{S}_K^{PI} \right| + 2\log(K+2))} \\
&= \sum_{K=0}^{p-1} \frac{1}{K+2} \leq \log(p) \leq \log(n)
\end{aligned}$$

And:

$$L_K \leq \log \binom{n+m-1}{K} + 2\log(K+2) \leq K \log(n+m-1) + 2(K+1) \leq p(2 + \log(2n-2))$$

Hence, if $p \leq \min\left(\frac{\kappa n}{2 + \log(2) + \log(n)}, n - 7 \right)$, then $\max(L_\eta, D_\eta) \leq \kappa n$ for any $\eta \in \mathcal{M}$.

Non-IID Framework ($\alpha \neq 0$)

Cholesky decomposition: $V = LL^T \quad Y' = L^{-1}Y \quad s' = L^{-1}s \quad E' = L^{-1}E$

$$Y' = \mathbb{E}\left[Y'\right] + \gamma E', \text{ with: } E' \sim \mathcal{N}(0, I_n)$$

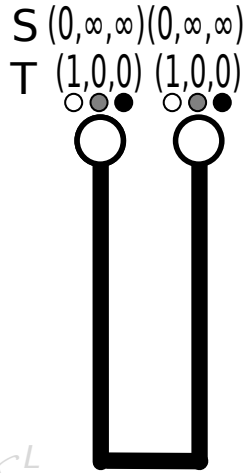
$$S'_\eta = L^{-1}S_\eta, \qquad \hat{Y}'_\eta = \text{Proj}_{S'_\eta} Y' = \underset{a' \in S'_\eta}{\text{argmin}} \left\| Y - La' \right\|_V^2 = L^{-1}\hat{Y}_\eta$$

$$\left\| \mathbb{E}\left[Y\right] - \hat{Y}_{\hat{\eta}} \right\|_V^2 = \left\| \mathbb{E}\left[Y'\right] - \hat{Y}'_{\hat{\eta}} \right\|^2, \qquad \left\| Y - \hat{Y}_\eta \right\|_V^2 = \left\| Y' - \hat{Y}'_\eta \right\|^2$$

$$\text{Crit}_{MC}(\eta) = \left\| Y' - \hat{Y}'_\eta \right\|^2 \left(1 + \frac{\text{pen}_{A,\mathcal{L}}(\eta)}{N_\eta}\right) = \left\| Y - \hat{Y}_\eta \right\|_V^2 \left(1 + \frac{\text{pen}_{A,\mathcal{L}}(\eta)}{N_\eta}\right)$$

back

Cardinal of Equivalence Classes



Initialization For tips

Propagation

$$\mathcal{K}_k^l = \underset{1 \leq p \leq K}{\operatorname{argmin}} \left\{ S_{i_l}(p) + \mathbb{I}\{p \neq k\} \right\}$$

$$S_i(k) = \sum_{l=1}^{L} S_{i_l}(p_l) + \mathbb{I}\{p_l \neq k\} \ , \ \forall (p_1, \dots p_L) \in \mathcal{K}_k^1 \times \dots \times \mathcal{K}_k^L$$

$$T_i(k) = \sum_{(p_1, \dots p_L) \in \mathcal{K}_k^1 \times \dots \times \mathcal{K}_k^L} \prod_{l=1}^{L} T_{i_l}(p_l) = \prod_{l=1}^{L} \sum_{p_l \in \mathcal{K}_k^l} T_{i_l}(p_l)$$

Termination Sum on the root vector

back

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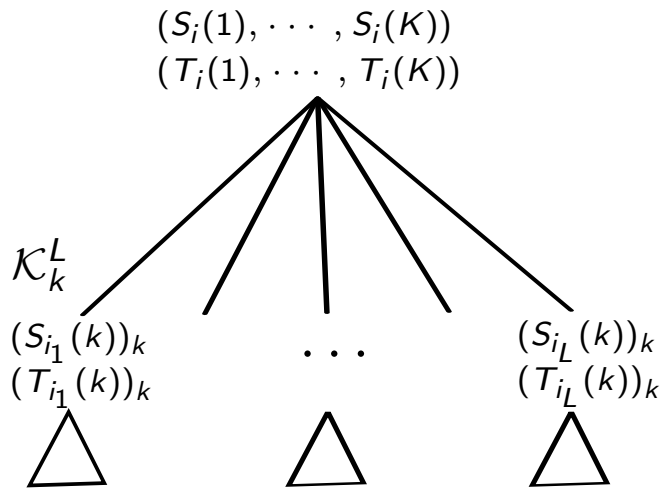

Termination Sum on the root vector

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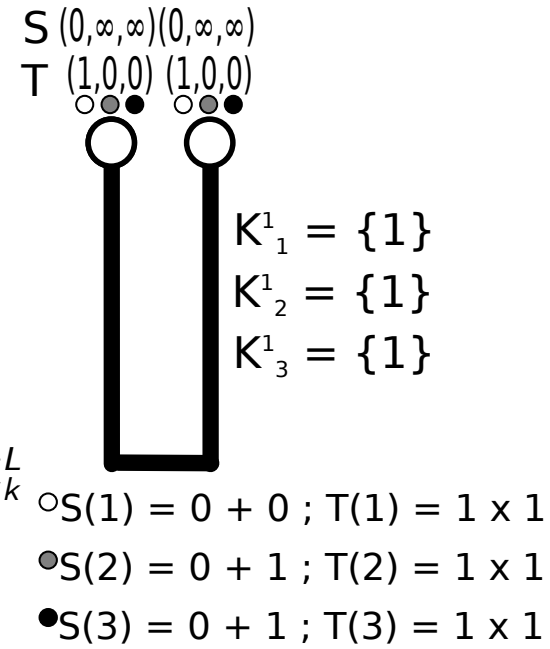

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Termination Sum on the root vector

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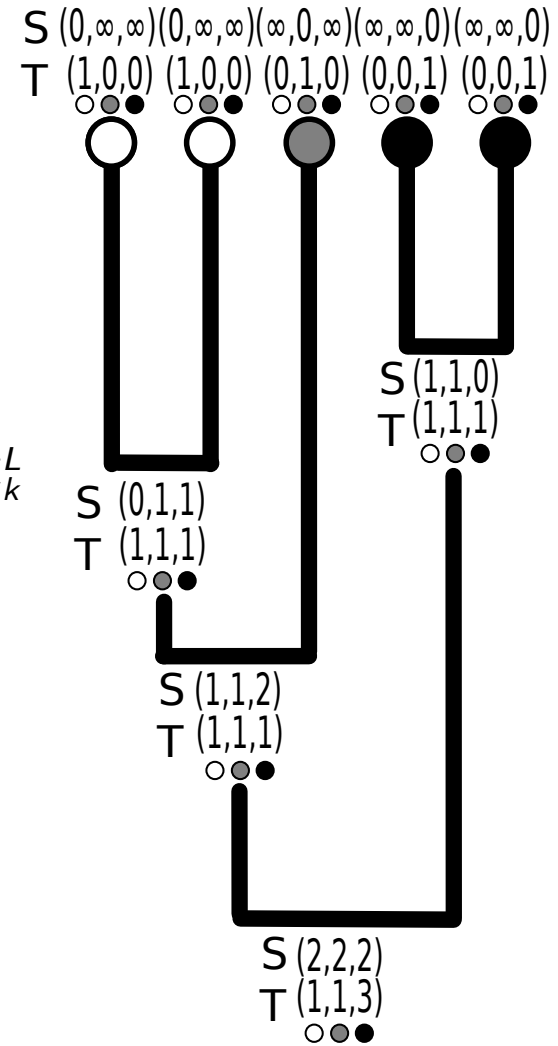


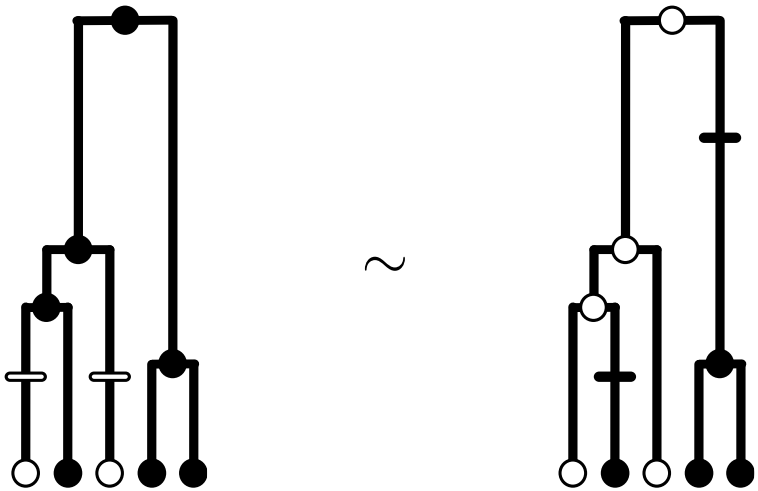
Linking Shifts and Clustering

Assumption "No Homoplasy": 1 shift = 1 new color

Proposition "K shifts $\iff$ $K+1$ clusters"

Linking Shifts and Clustering

Assumption "No Homoplasy": 1 shift = 1 new color



The No Homoplasy hypothesis is not respected.

Proposition "K shifts $\iff$ $K+1$ clusters"

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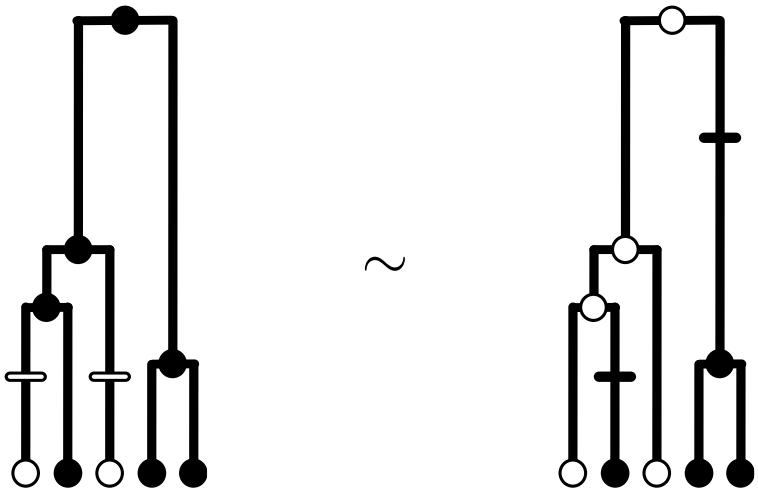
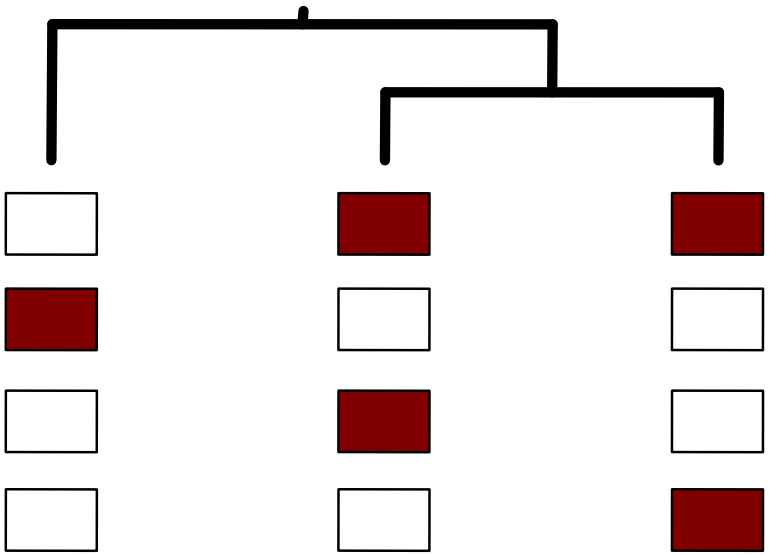


The No Homoplasy hypothesis is not respected.

Proposition "K shifts $\iff$ $K+1$ clusters"

Definitions

- $\mathcal{T}$ a rooted tree with n tips
- $N_K^{(\mathcal{T})} = |\mathcal{C}_K|$ the number of possible partitions of the tips in K clusters
- $A_K^{(\mathcal{T})}$ the number of possible *marked* partitions



Partitions in two groups for a binary tree with 3 tips

Difference between $N_2^{(\mathcal{T}_3)}$ and $A_2^{(\mathcal{T}_3)}$:

- $N_2^{(\mathcal{T}_3)} = 3$: partitions 1 and 2 are equivalent
- $A_2^{(\mathcal{T}_3)} = 4$: one marked color ("white = ancestral state")

General Formula (Binary Case)

If $\mathcal{T}$ is a binary tree, consider T_ℓ and $\mathcal{T}_r$ the left and right sub-trees of $\mathcal{T}$. Then:

$$\begin{cases} N_K^{(\mathcal{T})} = \sum_{k_1+k_2=K} N_{k_1}^{(\mathcal{T}_\ell)} N_{k_2}^{(\mathcal{T}_r)} + \sum_{k_1+k_2=K+1} A_{k_1}^{(\mathcal{T}_\ell)} A_{k_2}^{(\mathcal{T}_r)} \\ A_K^{(\mathcal{T})} = \sum_{k_1+k_2=K} A_{k_1}^{(\mathcal{T}_\ell)} N_{k_2}^{(\mathcal{T}_r)} + N_{k_1}^{(\mathcal{T}_\ell)} A_{k_2}^{(\mathcal{T}_r)} + \sum_{k_1+k_2=K+1} A_{k_1}^{(\mathcal{T}_\ell)} A_{k_2}^{(\mathcal{T}_r)} \end{cases}$$

We get:

$$N_{K+1}^{(\mathcal{T})} = N_{K+1}^{(n)} = \binom{2n-2-K}{K} \quad \text{and} \quad A_{K+1}^{(\mathcal{T})} = A_{K+1}^{(n)} = \binom{2n-1-K}{K}$$

Recursion Formula (General Case)

If we are at a node defining a tree $\mathcal{T}$ that has p daughters, with sub-trees $\mathcal{T}_1, \ldots, \mathcal{T}_p$, then we get the following recursion formulas:

$$\begin{cases} N_K^{(\mathcal{T})} = \displaystyle\sum_{\substack{k_1+\cdots+k_p=K \\ k_1,\ldots,k_p\geq 1}} \prod_{i=1}^{p} N_{k_i}^{(\mathcal{T}_i)} + \sum_{\substack{I\subset[\![1,p]\!] \\ |I|\geq 2}} \sum_{\substack{k_1+\cdots+k_p=K+|I|-1 \\ k_1,\ldots,k_p\geq 1}} \prod_{i\in I} A_{k_i}^{(\mathcal{T}_i)} \prod_{i\notin I} N_{k_i}^{(\mathcal{T}_i)} \\ A_K^{(\mathcal{T})} = \displaystyle\sum_{\substack{I\subset[\![1,p]\!] \\ |I|\geq 1}} \sum_{\substack{k_1+\cdots+k_p=K+|I|-1 \\ k_1,\ldots,k_p\geq 1}} \prod_{i\in I} A_{k_i}^{(\mathcal{T}_i)} \prod_{i\notin I} N_{k_i}^{(\mathcal{T}_i)} \end{cases}$$

No general formula. The result depends on the topology of the tree.

back

Simulations Design

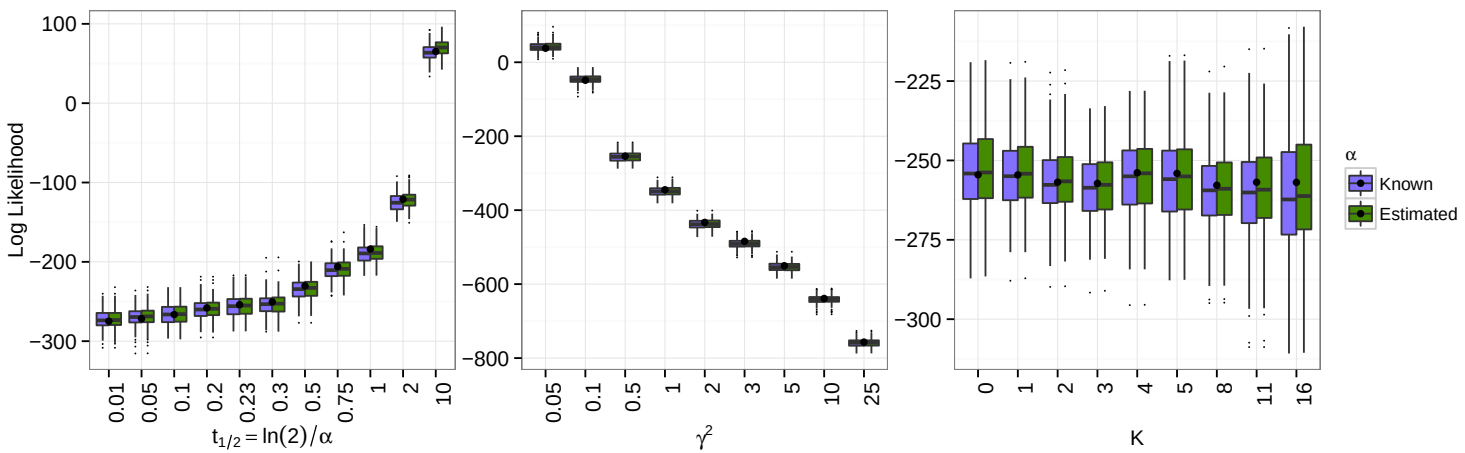
(Uyeda and Harmon, 2014)

- Topology of the tree fixed (unit height, $\lambda = 0.1$, with 64, 128, 256 taxa).
- Initial optimal value fixed: $\beta_0 = 0$
- One "base" scenario $\alpha_b = 3$, $\gamma^2_b = 0.5$, $K_b = 5$.
- $\alpha \in \log(2)/\{0.01, 0.05, 0.1, 0.2, 0.23, 0.3, 0.5, 0.75, 1, 2, 10\}$.
- $\gamma^2 \in \{0.3, 0.6, 3, 6, 12, 18, 30, 60, 150\}/(2\alpha_b)$.
- $K \in \{0, 1, 2, 3, 4, 5, 8, 11, 16\}$.
- Shifts values $\sim \frac{1}{2}\mathcal{N}(4, 1) + \frac{1}{2}\mathcal{N}(-4, 1)$
- Shifts randomly placed at regular intervals separated by 0.1 unit length.
- $n = 200$ repetitions : 16200 configurations.

CPU time on cluster MIGALE (Jouy-en-Josas):

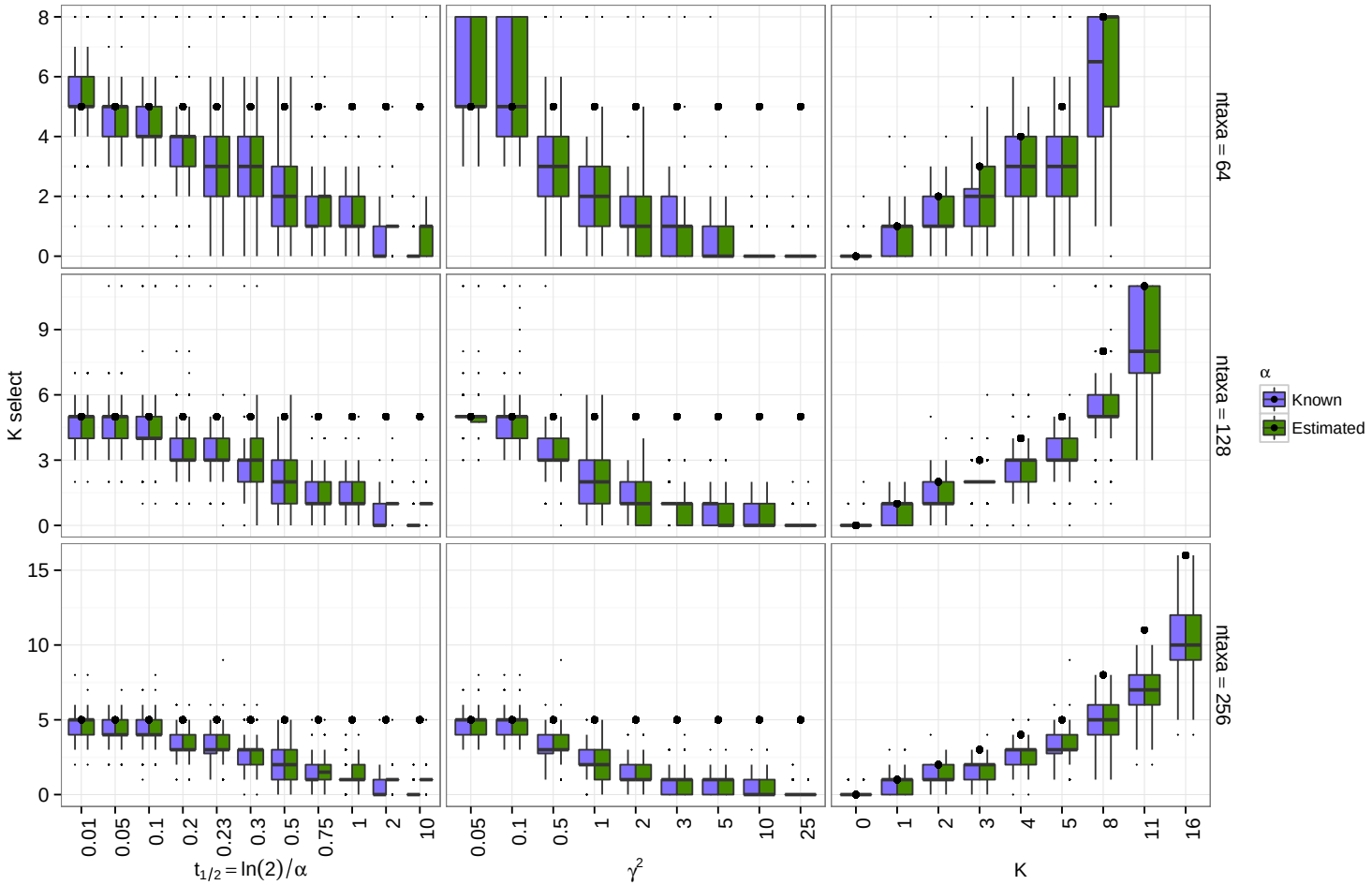
- α known: 6 minutes per estimation (66 days in total).
- α unknown: 52 minutes per estimation (570 days in total).

Log-Likelihood

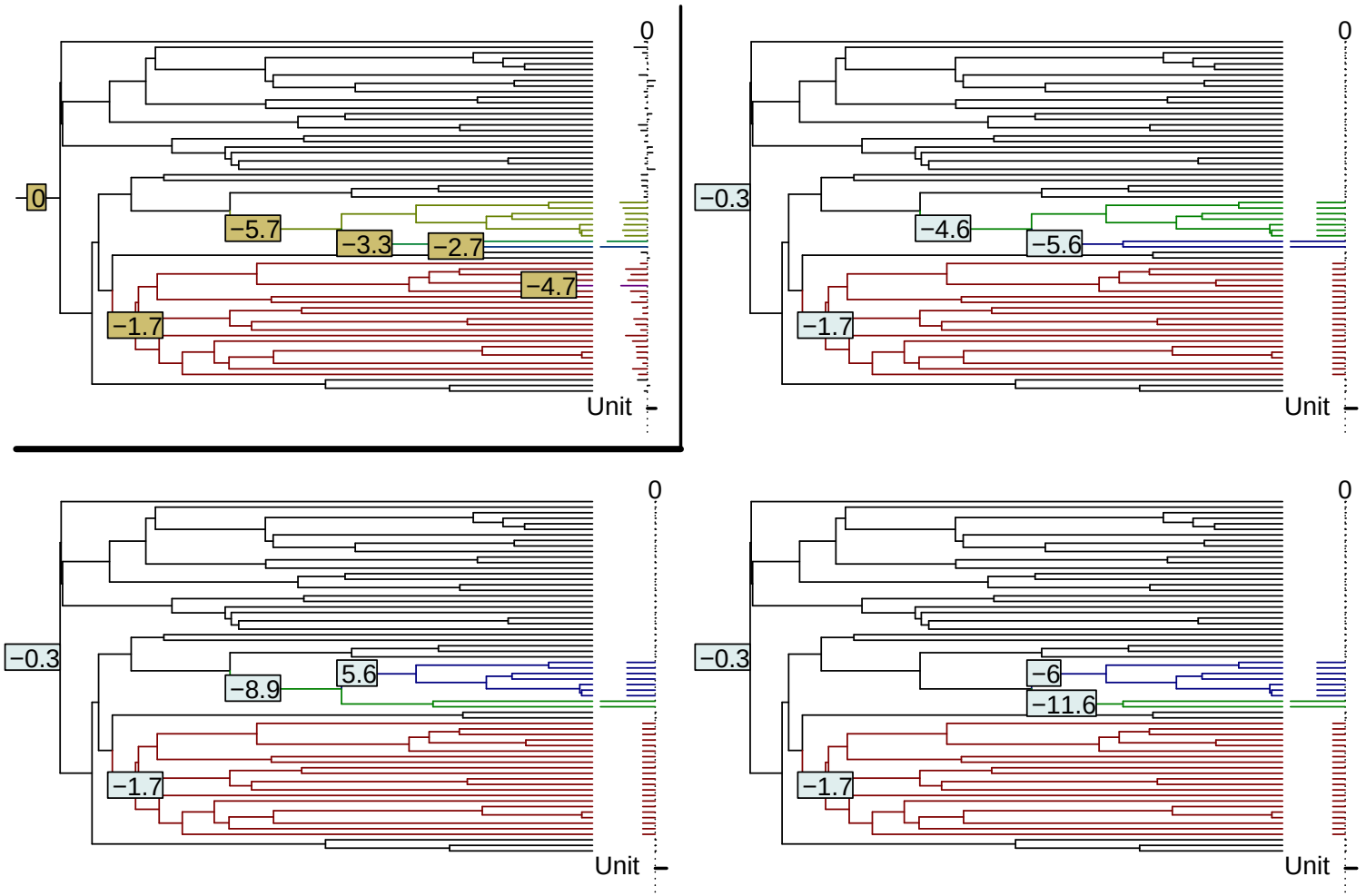


Log likelihood for a tree with 256 tips. Solid black dots are the median of the log likelihood for the true parameters.

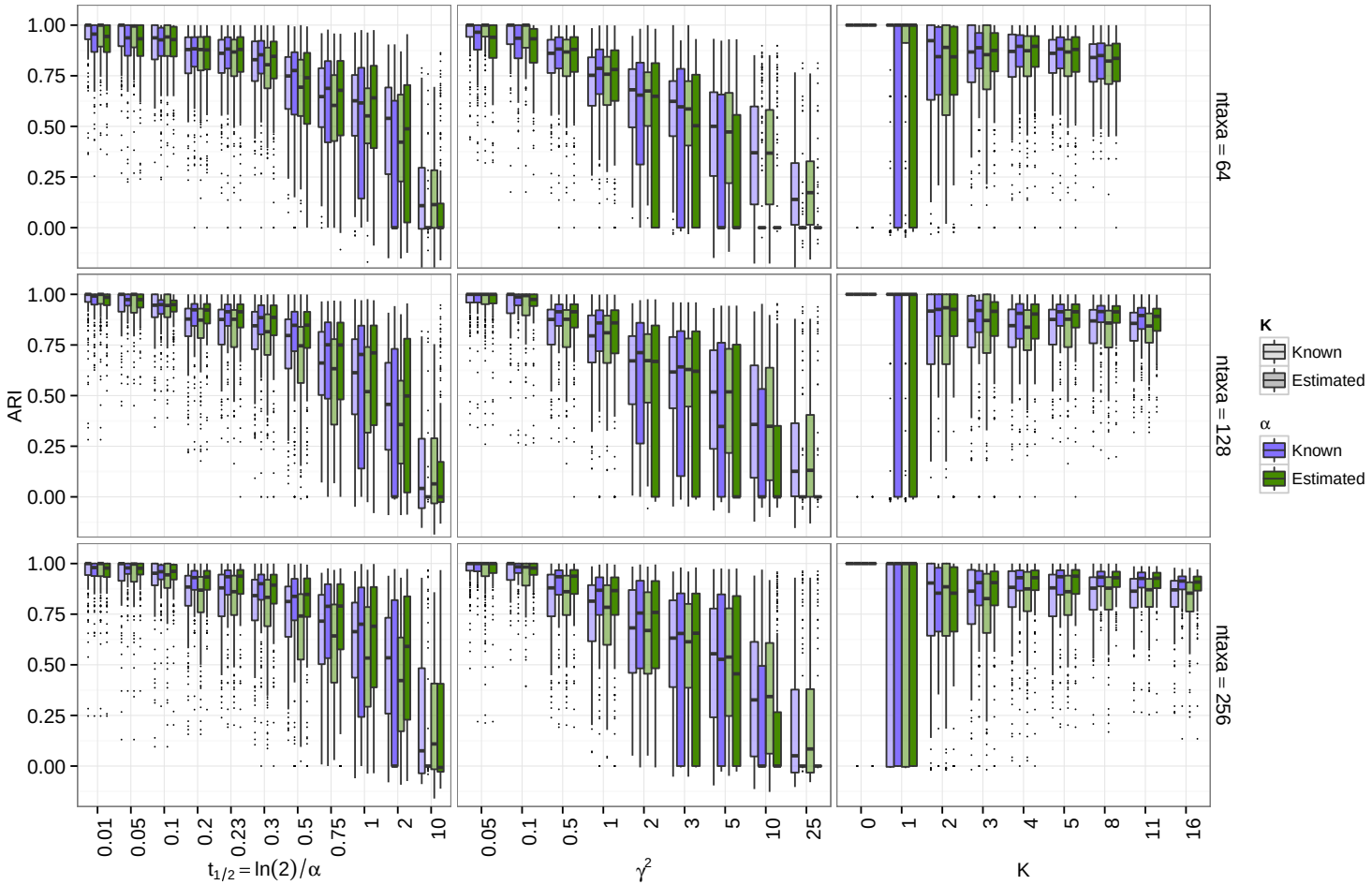
Number of Shifts



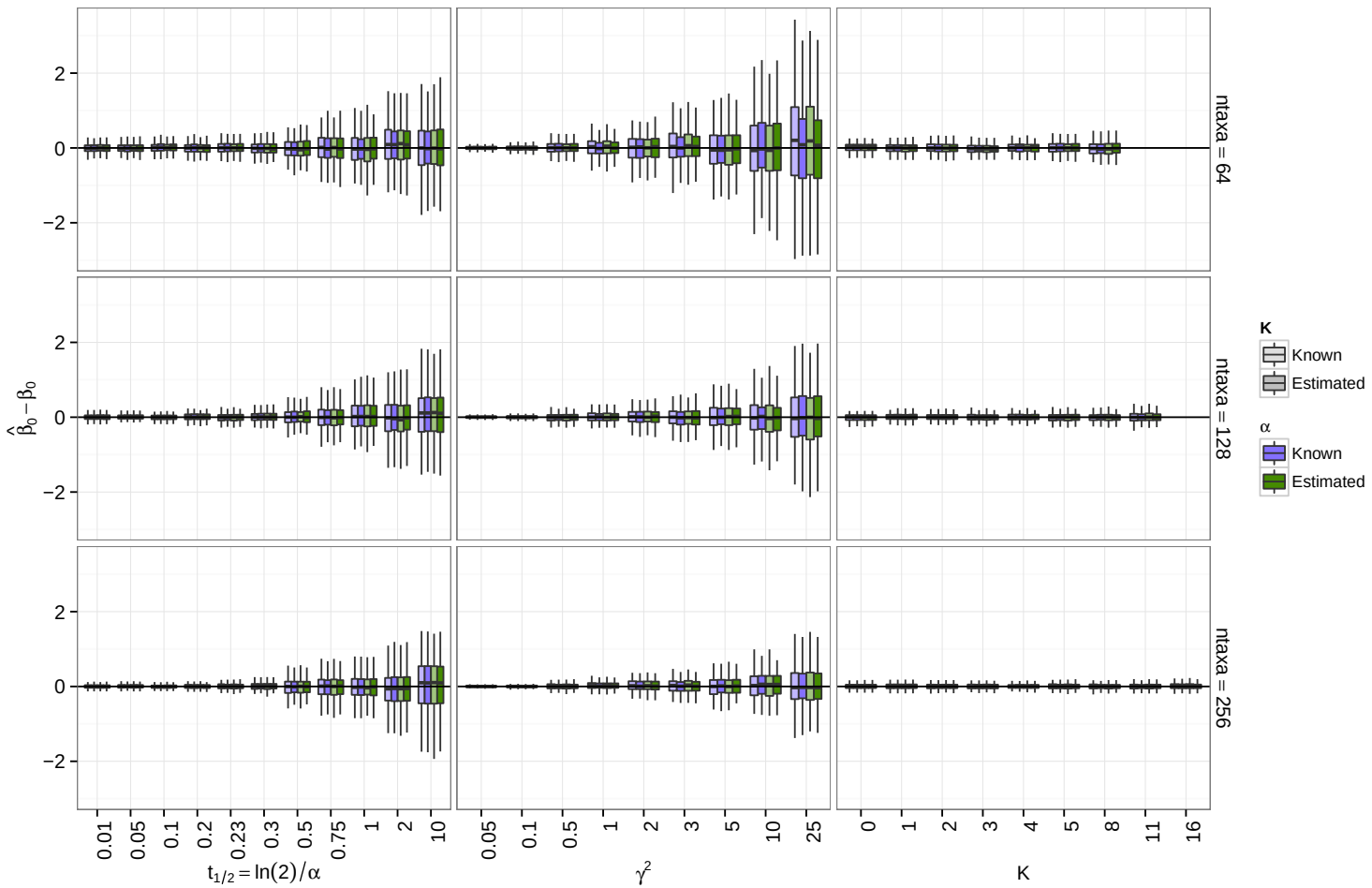
One Example


0
−5.7
−3.3
−2.7
−4.7
−1.7
Unit
0
−0.3
−4.6
−5.6
−1.7
Unit
0
−0.3
−8.9
5.6
−1.7
Unit
0
−0.3
−6
−11.6
−1.7
Unit

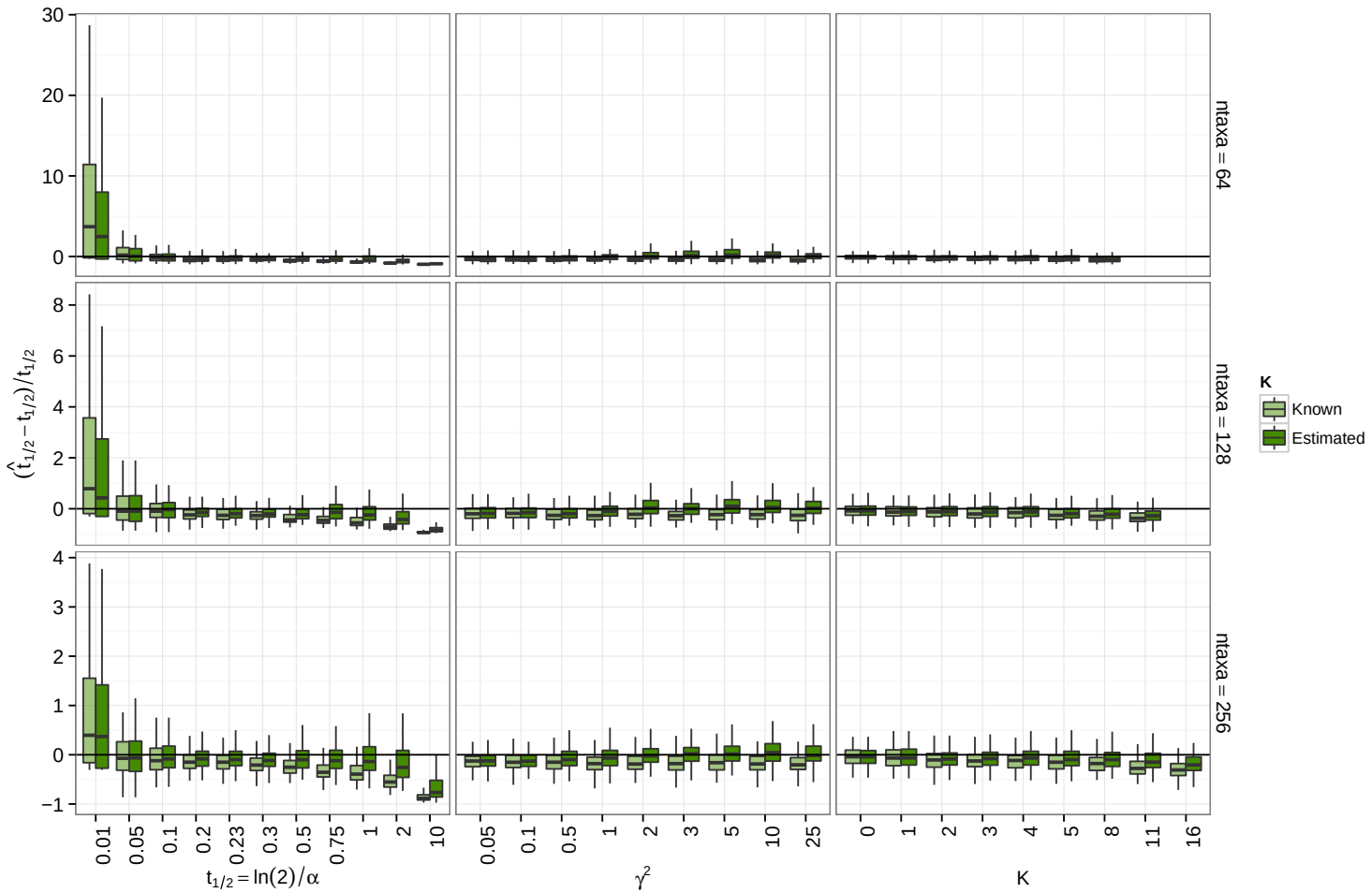
Adjusted Rand Index



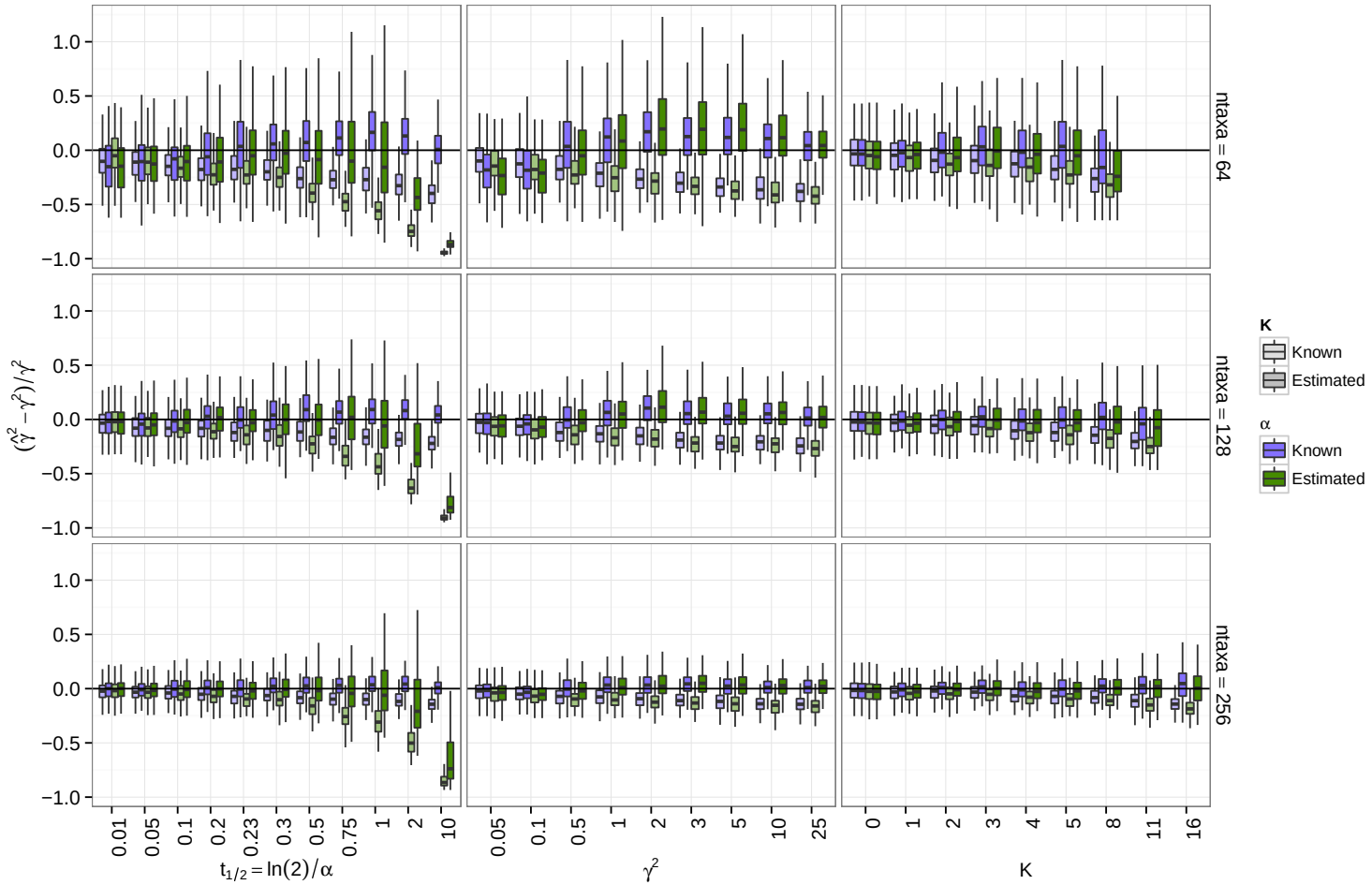
Parameters: β_0



Parameters: α



Parameters: γ^2



BM Model

Data n *vectors* of p traits at the tips: $\mathbf{Y}_i = \begin{pmatrix} Y_{i1} \\ \vdots \\ Y_{ip} \end{pmatrix}$

SDE $d\mathbf{W}(t) = \mathbf{\Sigma} d\mathbf{B}_t$, rate matrix $\mathbf{R} = \mathbf{\Sigma}\mathbf{\Sigma}^T$ $(p \times p)$

Covariances $\mathbb{C}\text{ov}\left[Y_{il}; Y_{jq}\right] = t_{ij} R_{lq}$ for i, j tips, and l, q characters

$$\mathbb{V}\text{ar}\left[\text{vec}(\mathbf{Y})\right] = \mathbf{C}_n \otimes \mathbf{R}$$

Shifts K shifts $\boldsymbol{\delta}_1, \cdots, \boldsymbol{\delta}_K$ *vectors* size p

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

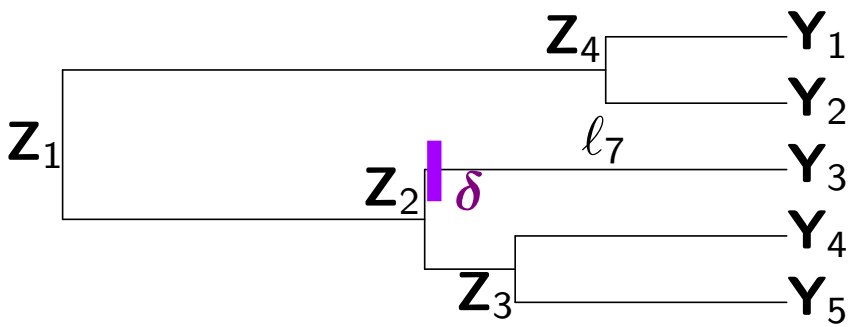
BM Model

Linear Model Representation

$$\text{vec}(\mathbf{Y}) = \text{vec}(\mathbf{\Delta T}^T) + \mathbf{E} \text{ with } \mathbf{E} \sim \mathcal{N}(0, \mathbf{V} = \mathbf{C}_n \otimes \mathbf{R})$$

Incomplete Data Representation

$$\mathbf{Y}_3 \mid \mathbf{Z}_2 \sim \mathcal{N}\Big(\mathbf{Z}_2 + \boldsymbol{\delta},\ \ell_7 \mathbf{R}\Big)$$



OU Model: General Case

Data n *vectors* of p traits at the tips: $\mathbf{Y}_i = \begin{pmatrix} Y_{i1} \\ \vdots \\ Y_{ip} \end{pmatrix}$

SDE $\mathbf{A}$ $(p \times p)$ "selection strength"

$$d\mathbf{W}(t) = -\mathbf{A}(\mathbf{W}(t) - \beta(t))dt + \mathbf{\Sigma} d\mathbf{B}_t$$

Covariances

$$\mathbb{C}\text{ov}\left[\mathbf{X}_i; \mathbf{X}_j\right] = e^{-\mathbf{A}t_i}\mathbf{\Gamma} e^{-\mathbf{A}^T t_j} + e^{-\mathbf{A}(t_i - t_{ij})}\left(\int_0^{t_{ij}} e^{-\mathbf{A}v}\mathbf{\Sigma}\mathbf{\Sigma}^T e^{-\mathbf{A}^T v} dv\right) e^{-\mathbf{A}^T(t_j - t_{ij})}$$

Shifts K shifts $\boldsymbol{\delta}_1, \cdots, \boldsymbol{\delta}_K$ *vectors* size p

$\mapsto$ On the optimal values

OU Model: **A** scalar

Assumption $\mathbf{A} = \alpha \mathbf{I}_p$ "scalar"

Stationnary State $\mathbf{S} = \frac{1}{2\alpha}\mathbf{R}$

Fixed Root For i, j tips and l, q characters:

$$\mathbb{C}\text{ov}\left[Y_{il}; Y_{jq}\right] = \frac{1}{2\alpha} e^{-2\alpha h} \left(e^{2\alpha t_{ij}} - 1\right) R_{lq}$$

$\mapsto$ Can be reduced to a BM on a re-scaled tree

EM algorithm

BM Natural generalization of the univariate case.

OU M step intractable in general.

Incomplete Data Model: Can readily handle missing data.

Model Selection

- Previous criterion cannot be applied
- Solution: "Slope Heuristic"-based method
  - Massart (2007)
    - oracle inequality with known variance
    - penalty up to a multiplicative constant
  - Baudry et al. (2012)
    - Slope-heuristic method to calibrate the constant
    - Implemented in capushe (Brault et al., 2012)

Model Selection: Toy Example

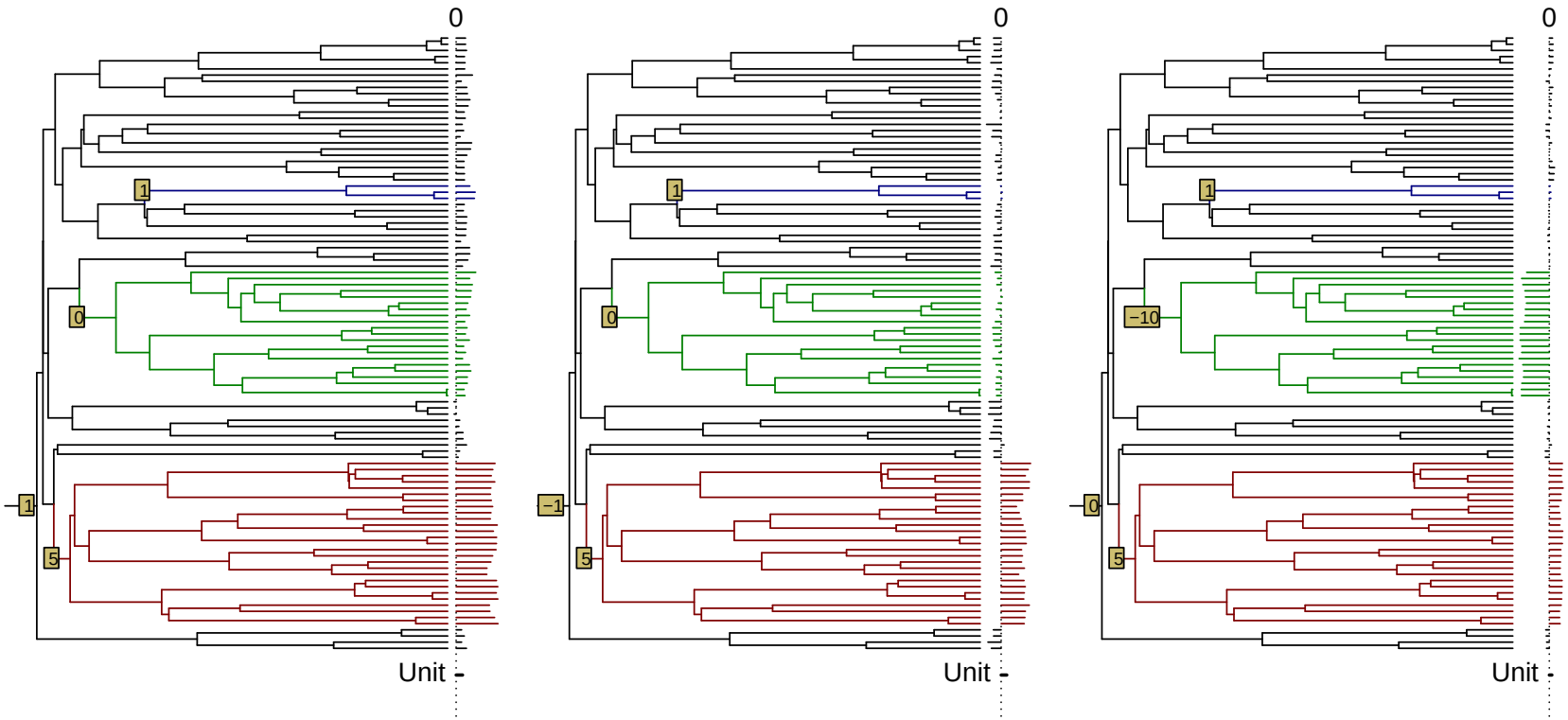


Figure: *Simulated Process.*

Model Selection: Toy Example

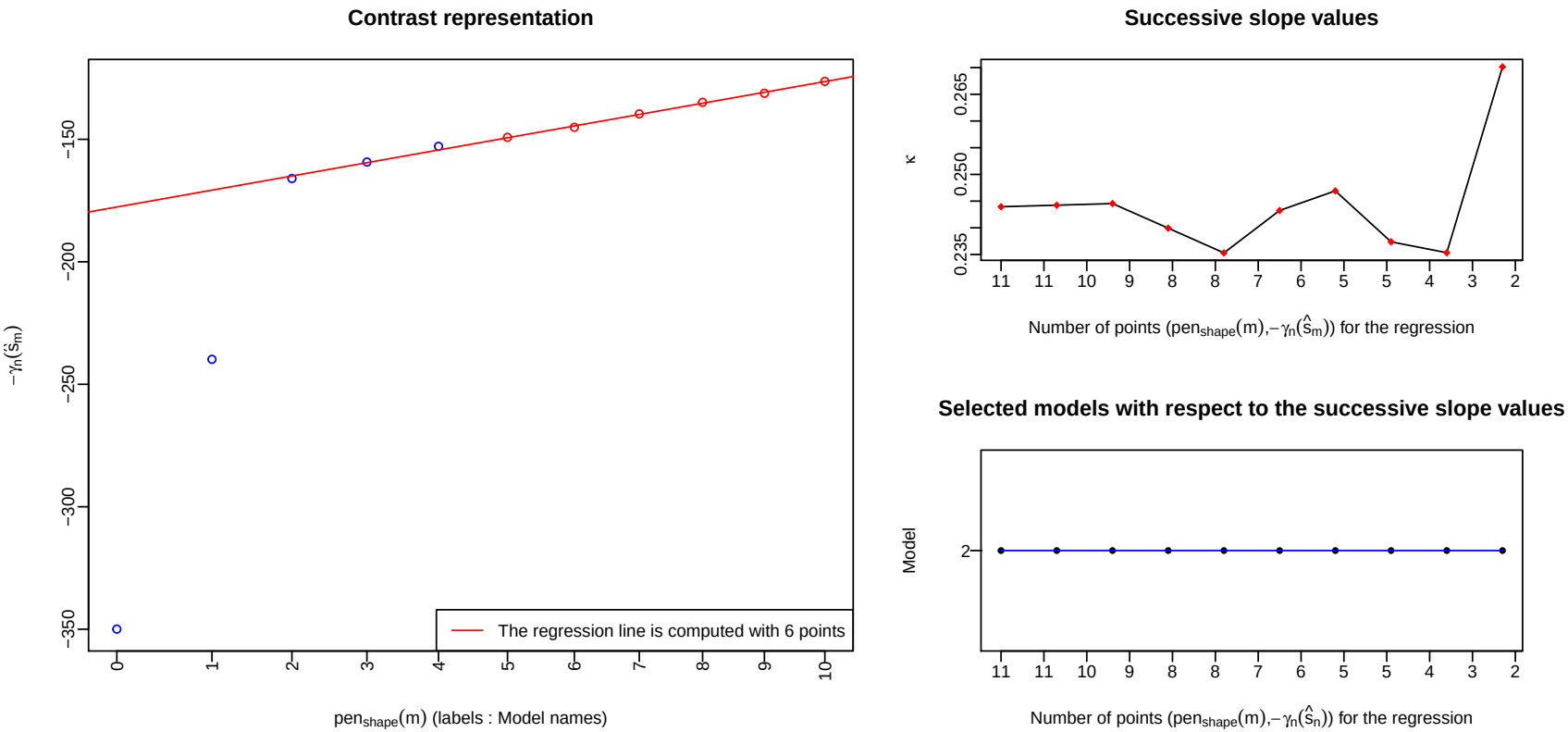


Figure: capushe *output for penalized log-likelihood.*

Model Selection: Toy Example

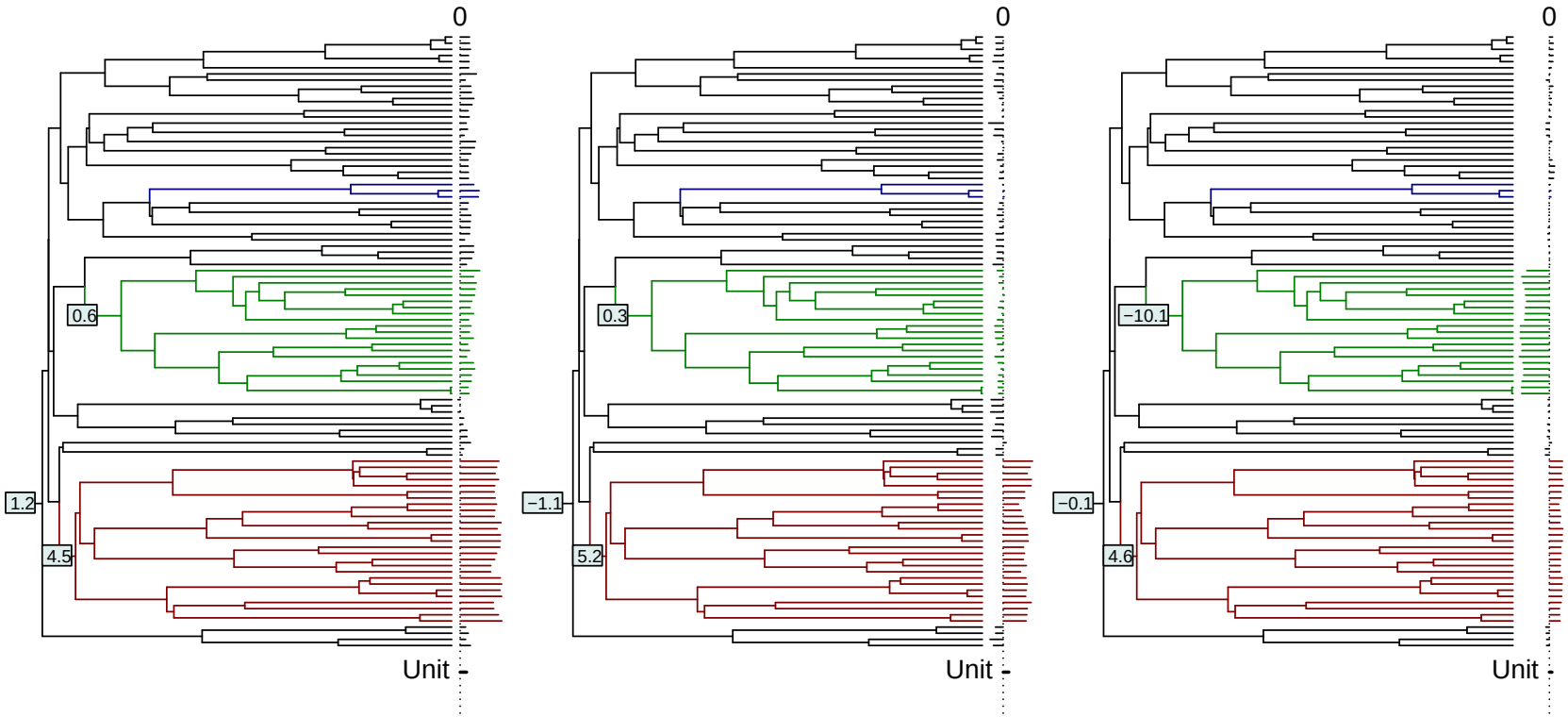


Figure: *Reconstructed Process.*