Shifted stochastic processes evolving on trees: application to models of adaptive evolution.

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Goals and Setting

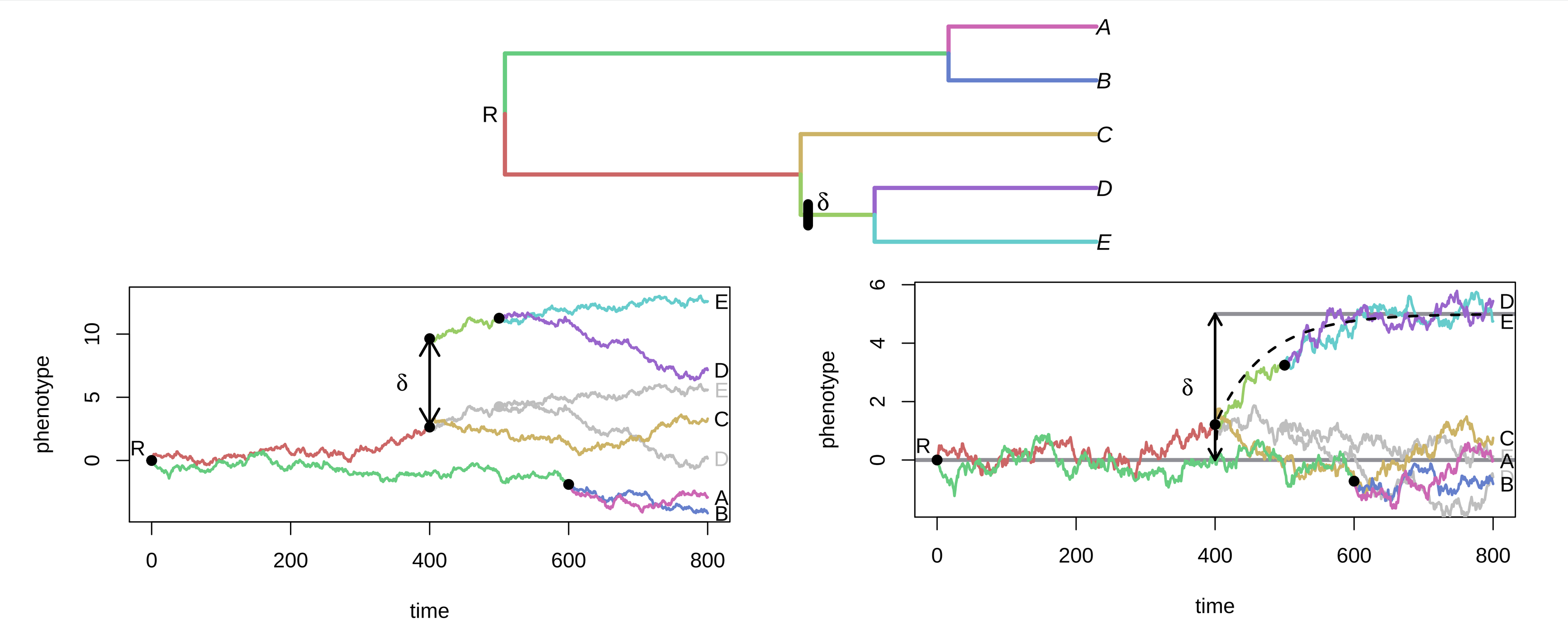
Goals

- **Detect environmental shifts that occurred in the past.**
- Explain the observed trait distribution, while accounting for phylogenetic correlations.

Data

- Measure of one quantitative trait for a set of related extant species.
- A phylogenetic tree, time-calibrated and ultrametric.

Model [2, 4]



$\mathbf{dW(t) = \sigma dB(t)}$

BM Shifts in the **mean**.

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

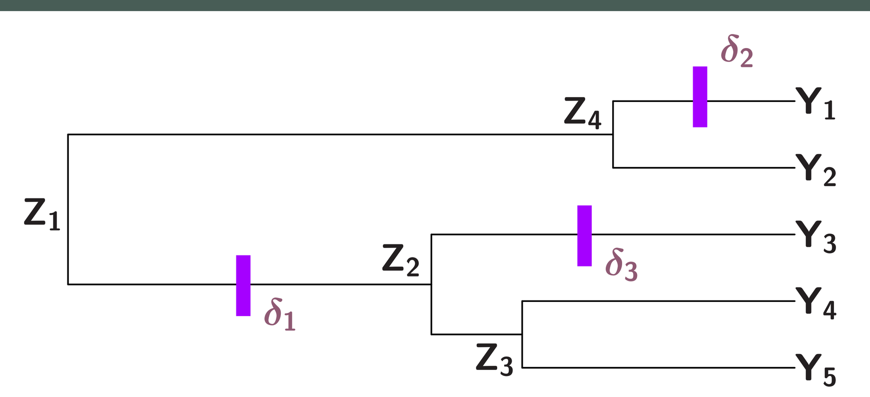
OU Shifts in the **optimal value**.

Incomplete Data Point of View

$$X_j | X_{pa(j)} \sim \mathcal{N}\left(q_j X_{pa(j)} + r_j + s_j \sum_k \mathbb{I}\{\tau_k = b_j\}\delta_k, \sigma_j^2\right)$$

EM Algorithm	Maximize $\mathbb{E}_\theta[\log p_\theta(Z, Y) \mid Y]$.
E step	"Upward-Downward" Algorithm.
M step	OU: increase objective function (GM).
Initialization	LASSO regression.

Linear Regression Point of View



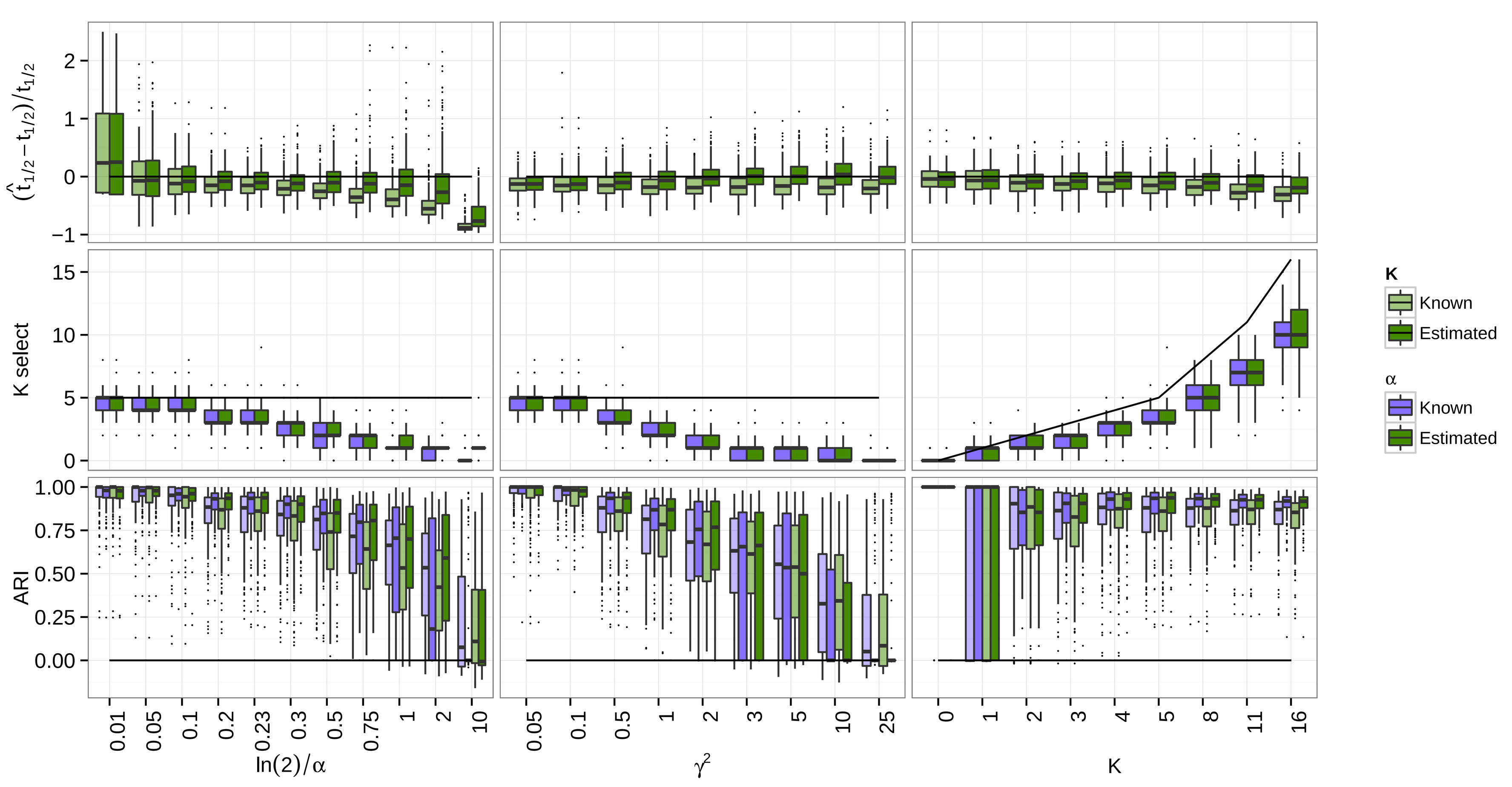
$$\Delta = \begin{pmatrix} \mu \\ \delta_1 \\ 0 \\ 0 \\ \delta_2 \\ 0 \\ \delta_3 \\ 0 \\ 0 \end{pmatrix} \quad T\Delta = \begin{pmatrix} \mu + \delta_2 \\ \mu \\ \mu + \delta_1 + \delta_3 \\ \mu + \delta_1 \\ \mu + \delta_1 \end{pmatrix}$$

$$T = \begin{array}{c|cccc|ccccc} & Z_1 & Z_2 & Z_3 & Z_4 & Y_1 & Y_2 & Y_3 & Y_4 & Y_5 \\ \hline Y_1 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 \\ Y_2 & 1 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 \\ Y_3 & 1 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ Y_4 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 1 & 0 \\ Y_5 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 1 \end{array}$$

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

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

Some Simulation Results



Scores for an OU simulated on a fixed random tree with 256 taxa, one parameter varying at a time.

References

[1] Y. Baraud, C. Giraud, and S. Huet. Gaussian model selection with an unknown variance. *Annals of Statistics*, 37(2):630–672, Apr. 2009.

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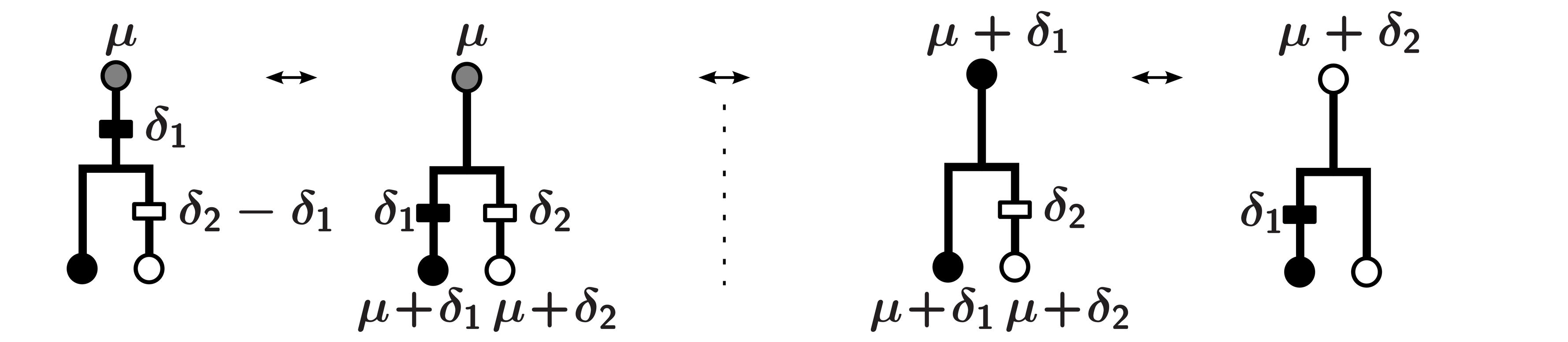
[3] J. Felsenstein. *Inferring Phylogenies*. Sinauer Associates, Suderland, USA, 2004.

[4] T. F. Hansen. Stabilizing selection and the comparative analysis of adaptation. *Evolution*, 51(5):1341–1351, oct 1997.

[5] A. L. Jaffe, G. J. Slater, and M. E. Alfaro. The evolution of island gigantism and body size variation in tortoises and turtles. *Biology letters*, 2011.

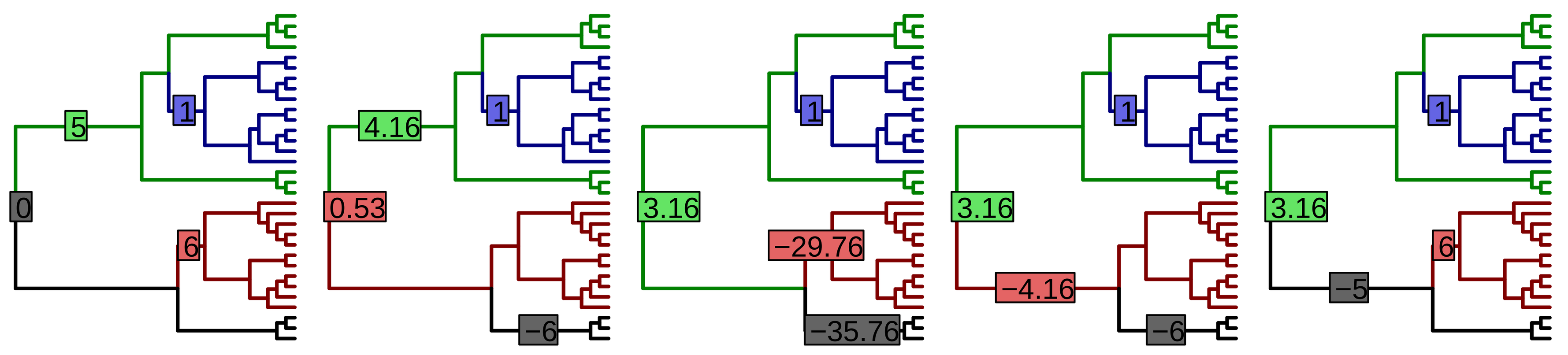
Identifiability Issues



All these shifts allocations give the same tips distribution (under a BM). The two on the right are parsimonious, they are said to be *equivalent*. We discard the two on the left as over-parametrized.

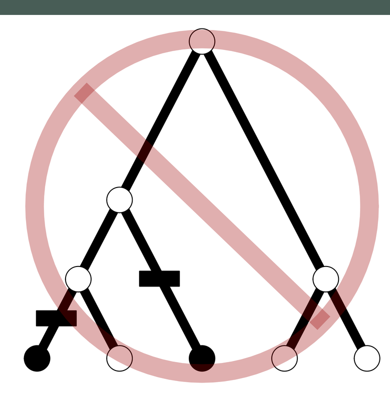
Parsimony and Equivalence Classes

Find one solution: Existing Dynamic Programming algorithms (Fitch, Sankoff) [3].
Enumerate on equivalent class: New recursive algorithm (implemented in R).



These five shifts allocations are equivalent: they are parsimonious and they produce the same tips distribution (under an OU).

Number of Models with K shifts



No Homoplasy: 1 shift = 1 new color.
Proposition: **K** shifts $\iff$ **K + 1** colors.

$$\mathcal{S}_K^{PI} = \{\text{Parsimonious allocations of } \mathbf{K} \text{ shifts}\}/\sim$$
$$\mathcal{S}_K^{PI} \simeq \{\text{Coloring of tips in } \mathbf{K+1} \text{ colors}\}$$

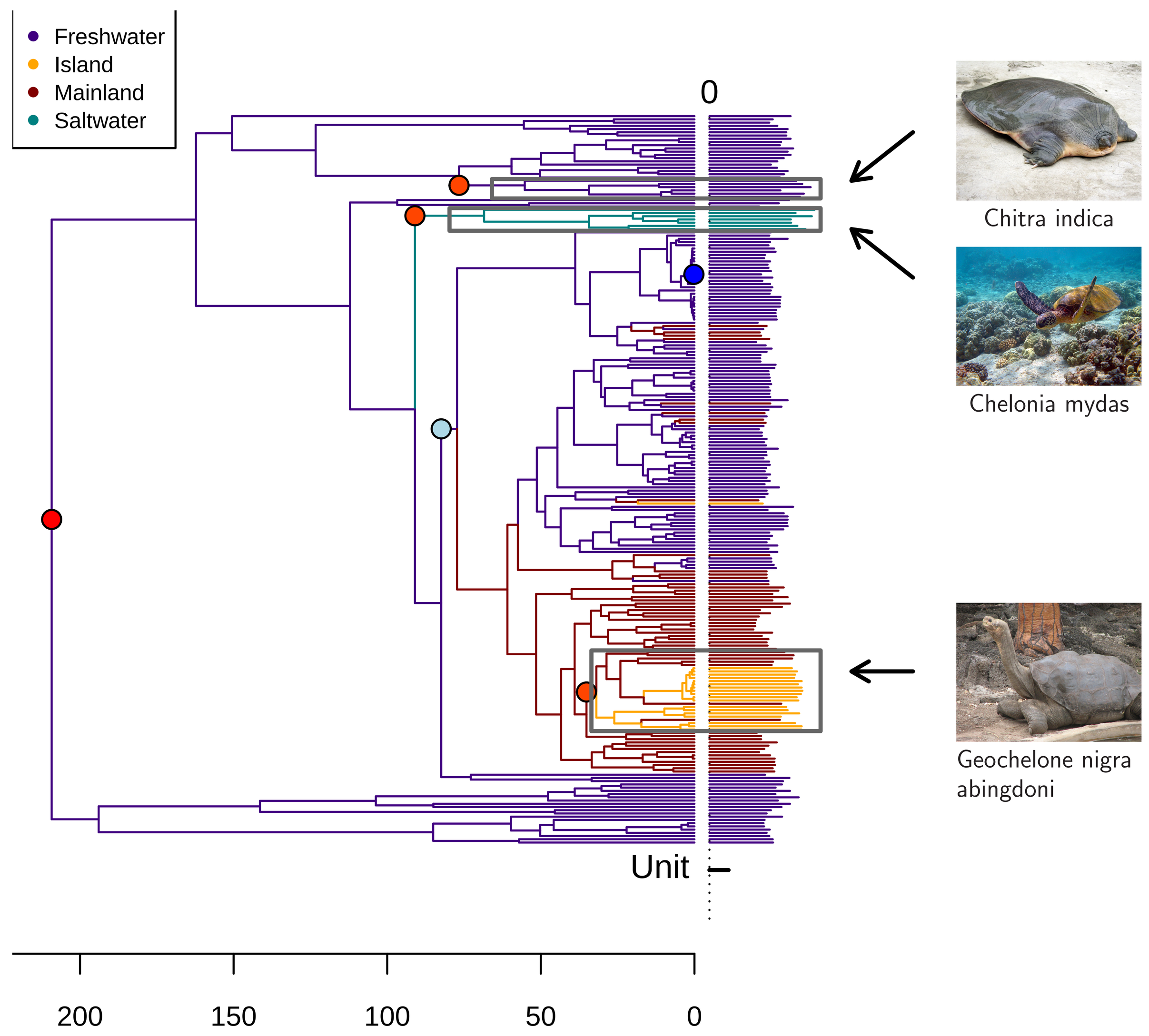
Proposition:

- $|\mathcal{S}_K^{PI}| \leq \binom{m+n-1}{K}$. It depends on the topology of the tree.
- For a binary tree: $|\mathcal{S}_K^{PI}| = \binom{2n-2-K}{K}$.

Model Selection on K (α known) [1]

$$\hat{K} = \underset{K \geq 0}{\text{argmin}} \|Y - \hat{s}_K\|_V^2 \left(1 + \frac{\text{pen}(K)}{n - K - 1}\right)$$

Chelonia Dataset [5]



	Habitat	EM
No. of shifts	16	5
No. of regimes	4	6
lnL	-133.86	-97.59
ln 2 / α (%)	7.44	5.43
γ^2	0.33	0.22
CPU time (min)	65.25	134.49

Colors: habitats. Boxes: selected EM regimes. Positive selected shifts are shown in red, and negative in blue.

Conclusion and Perspectives

A general statistical framework for trait evolution models with unconstrained shifts on ultrametric trees.

- R codes available on GitHub.
- Perspectives:
  - Handle multivariate (correlated) traits.
  - Deal with uncertainty (tree, data).
  - Use fossil records (non-ultrametric tree).