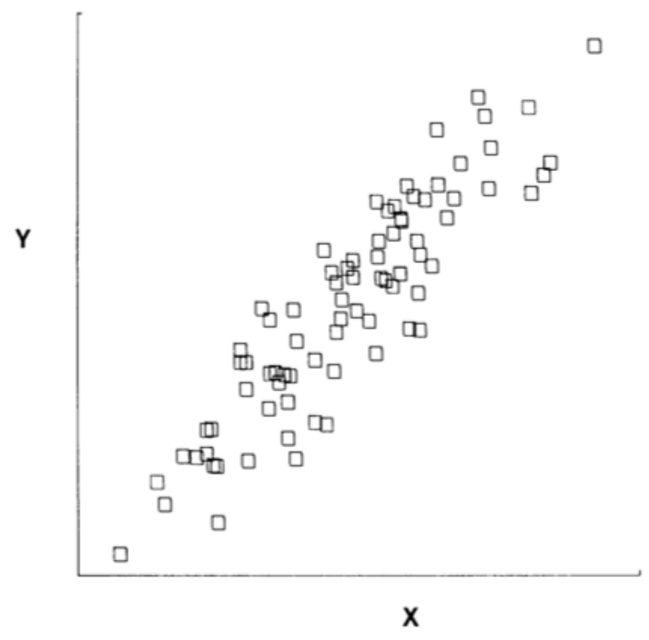
A Brief Introduction to Phylogenetic Diffusion Models

Bodega Bay
Applied Phylogenetics Workshop
May 25 – June 2, 2019

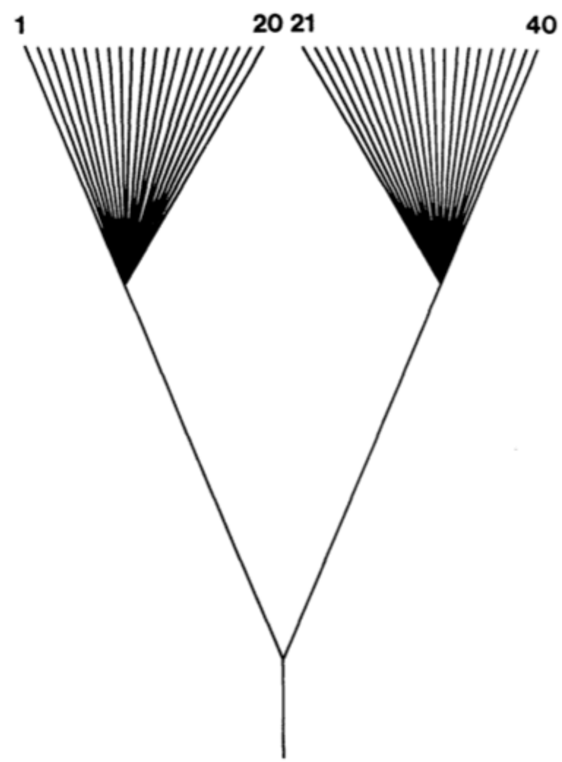
Are traits *X* and *Y* evolutionary correlated?

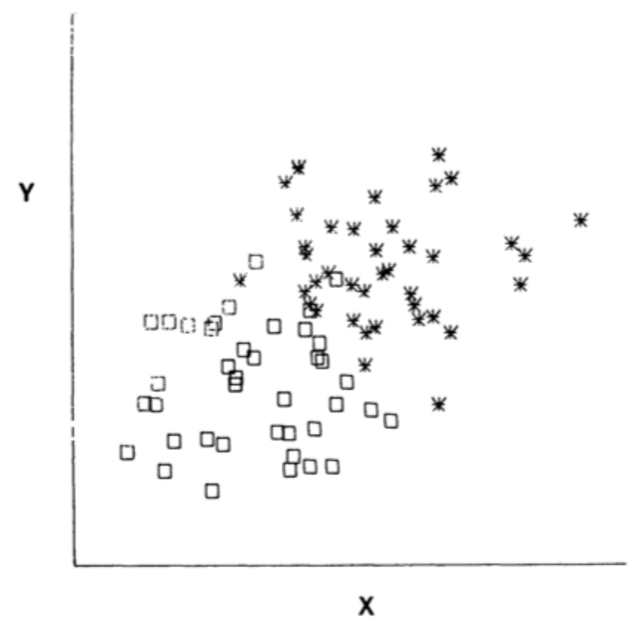
Pattern: *X* and *Y* look correlated!



Are traits *X* and *Y* evolutionary correlated?

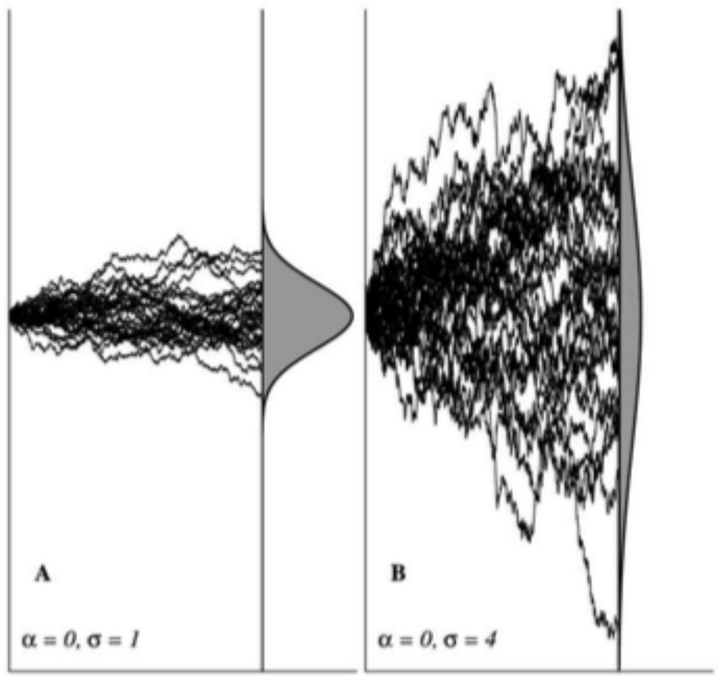
Process: *X* and *Y* evolved on a phylogeny!



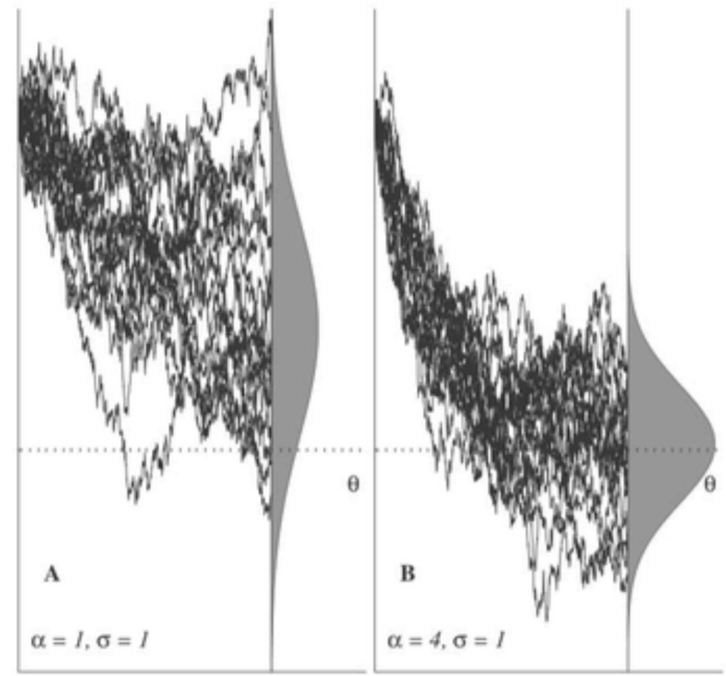


Felsenstein 1985

How is X evolving?

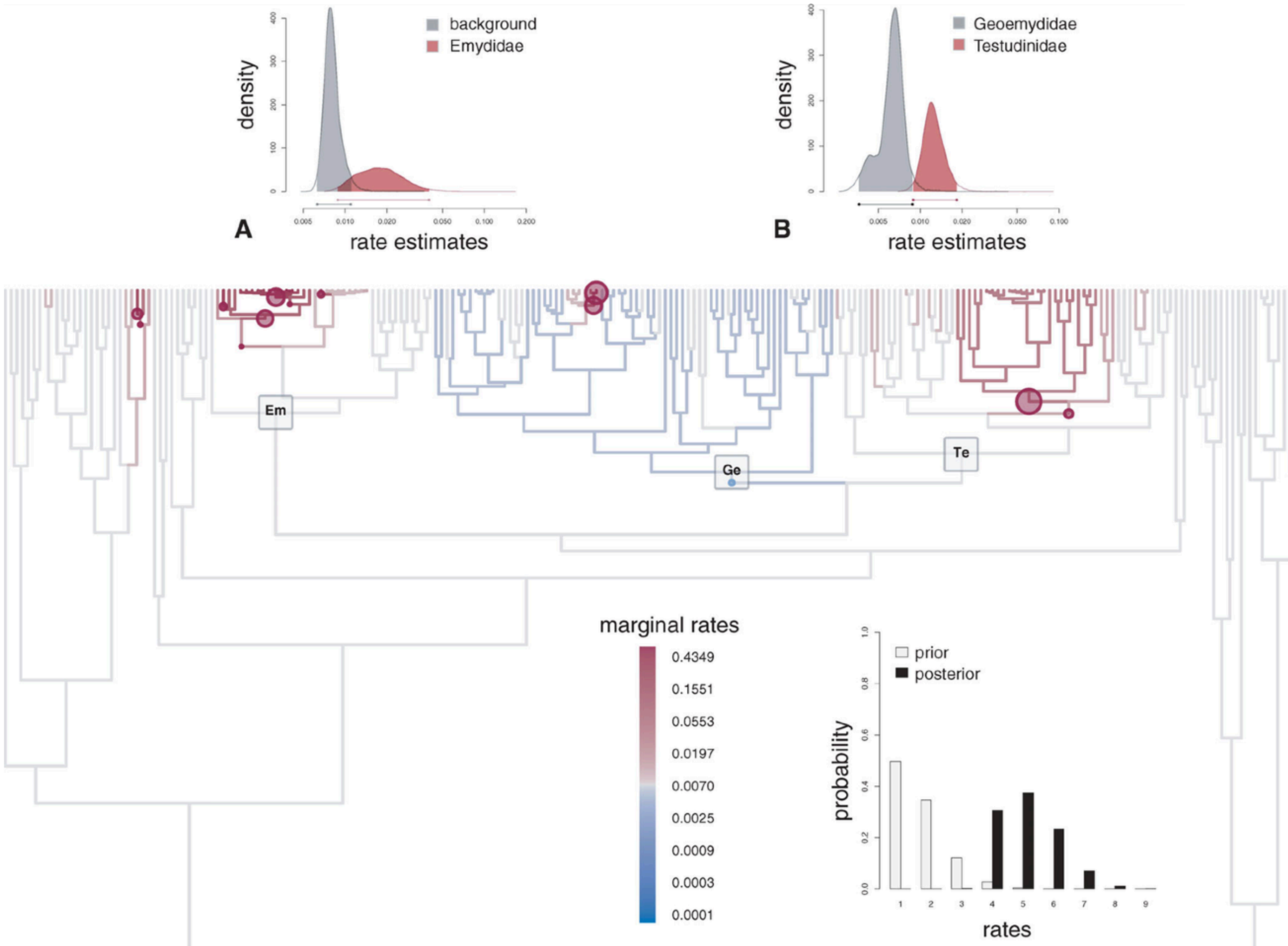


vs.



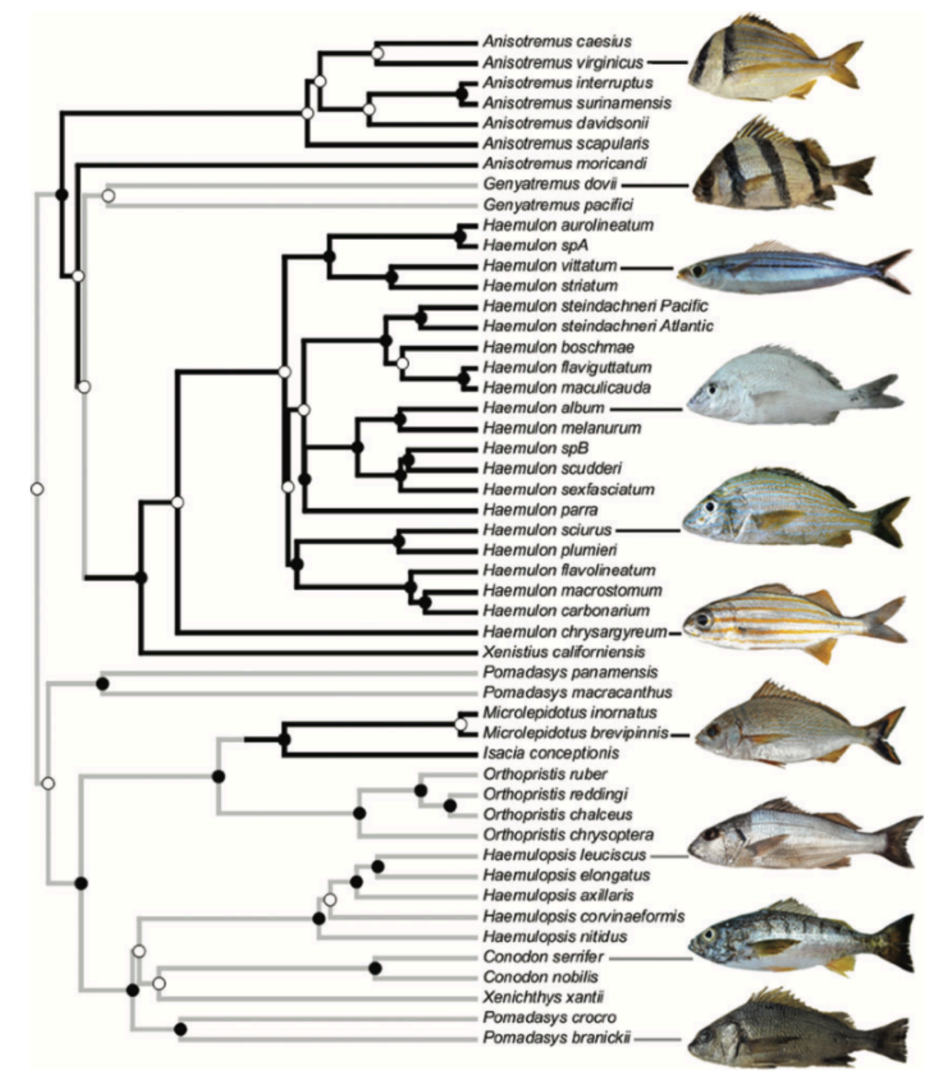
Butler & King 2004

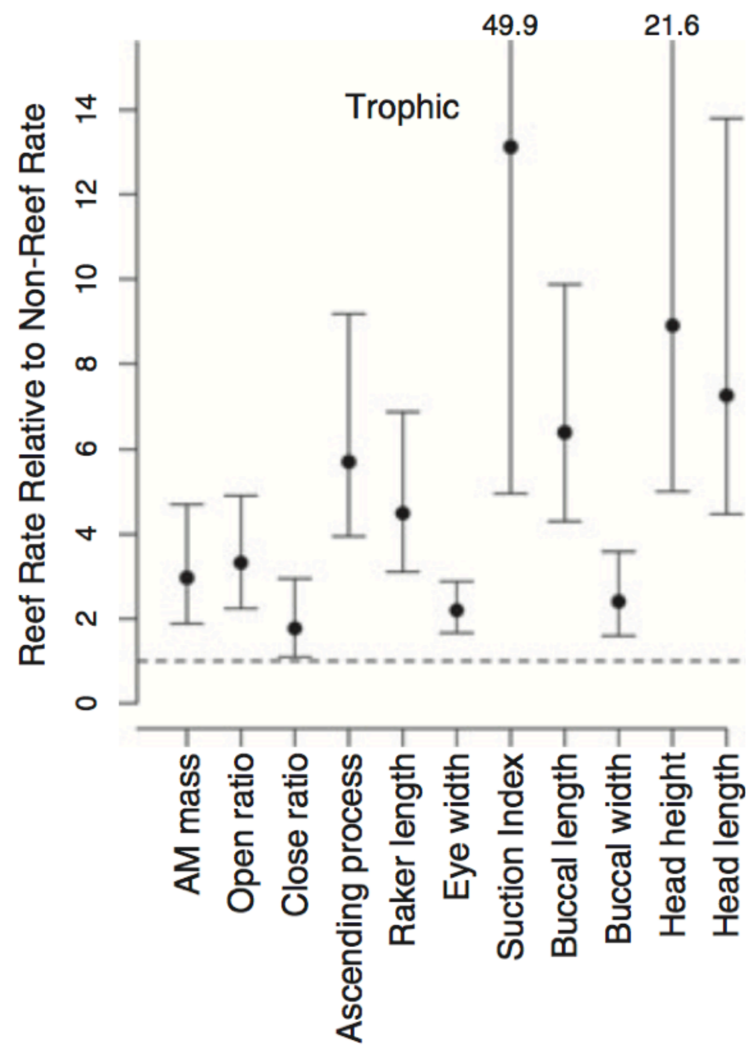
Do rates of evolution vary?



Eastman et al. 2011

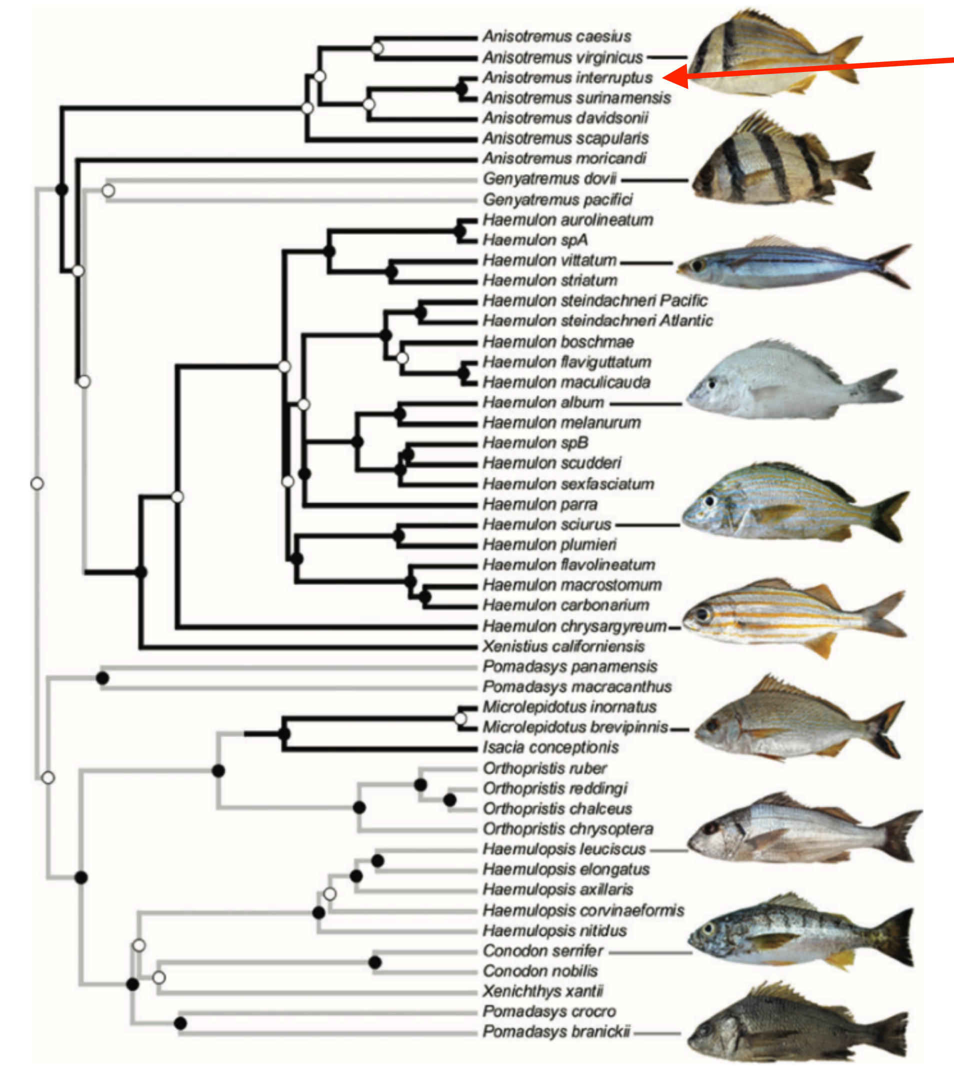
Do rates of continuous-trait evolution depend on a discrete variable?

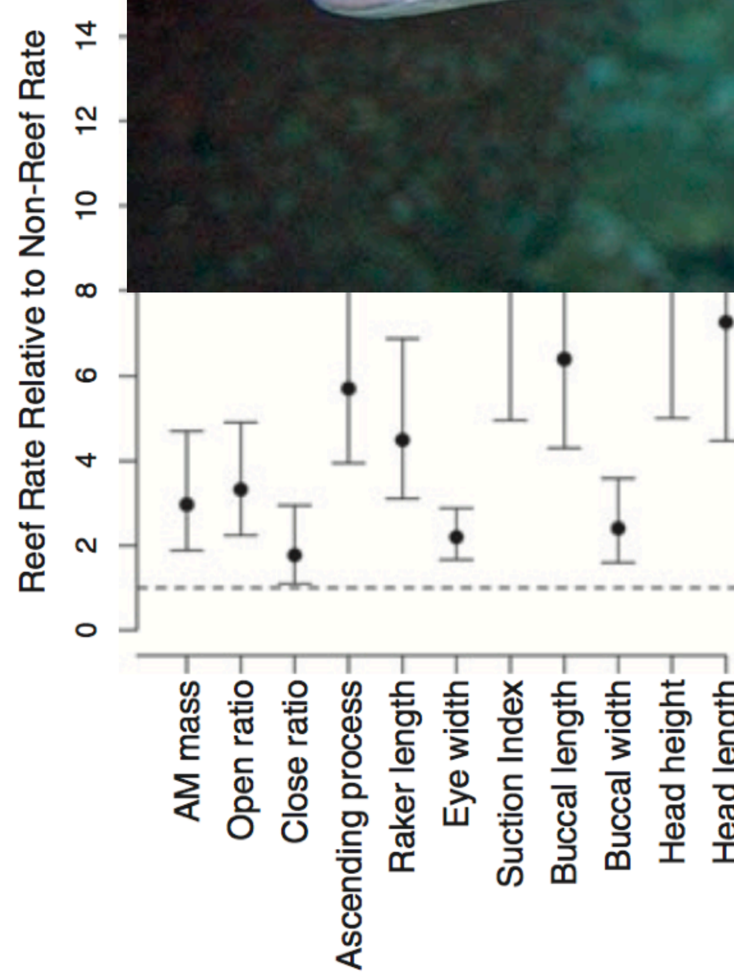




Price et al. 2013

Do rates of continuous-trait evolution depend on a discrete variable?





Price et al. 2013

Outline

I. Calculating likelihoods for continuous traits

- A generic framework for calculating probabilities

II. A simple model of continuous-character evolution

- Brownian motion model
- Multivariate Brownian motion model

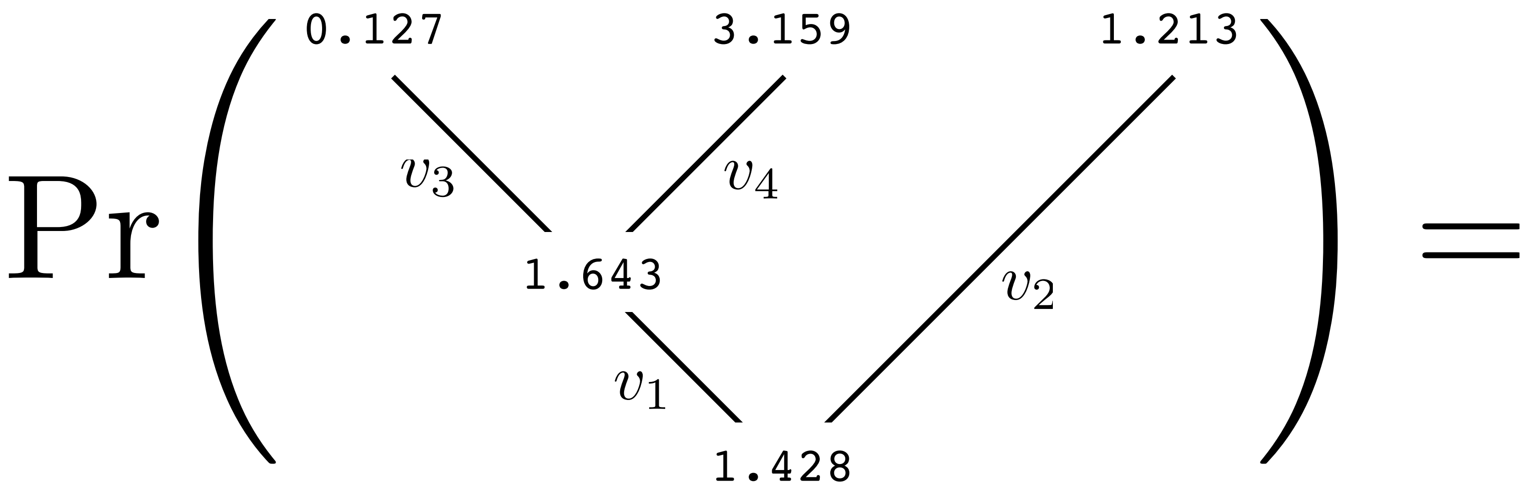
III. Exotic models of continuous-character evolution

- Ornstein-Uhlenbeck model
- Lévy models
- State-dependent models

Likelihoods for Continuous Characters

Species	Character data			
Species I	0.127	1.212	3.882	...
Species II	3.159	2.857	2.460	...
Species III	1.213	3.552	2.811	...

Likelihoods for Continuous Characters



Likelihoods for Continuous Characters

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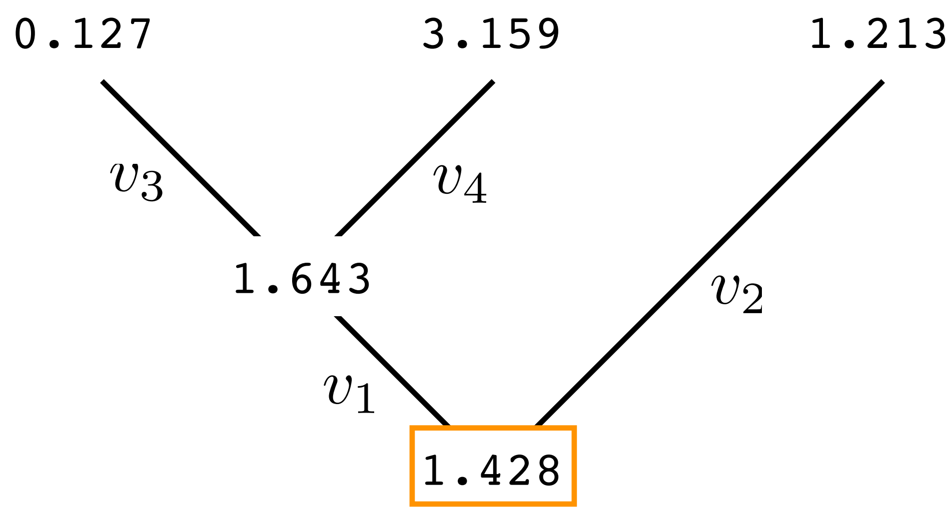

$\Bigg) =$

$p(1.428)$

Likelihoods for Continuous Characters

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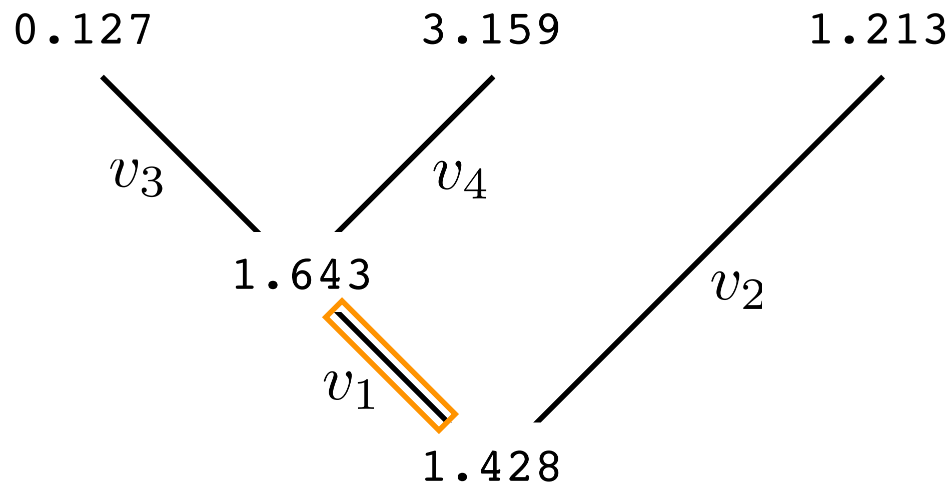

) =

$$p(1.428) \times p(1.428 \rightarrow 1.643 \mid v_1)$$

Likelihoods for Continuous Characters

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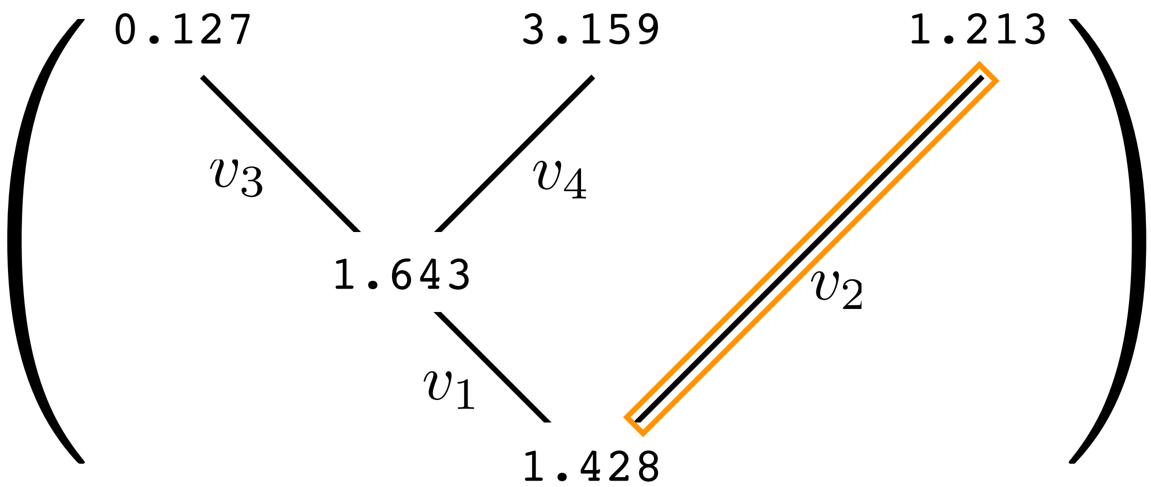

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$$p(1.428) \times p(1.428 \to 1.643 \mid v_1) \times p(1.428 \to 1.213 \mid v_2)$$

Likelihoods for Continuous Characters

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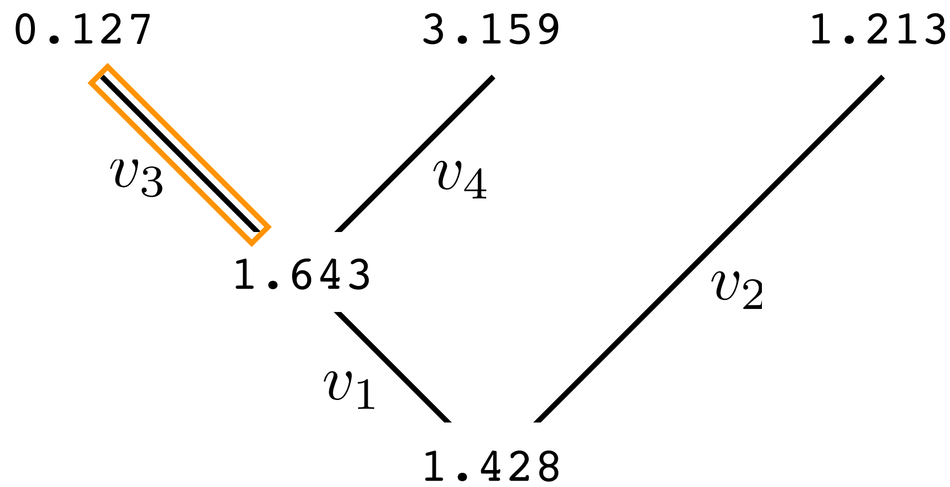
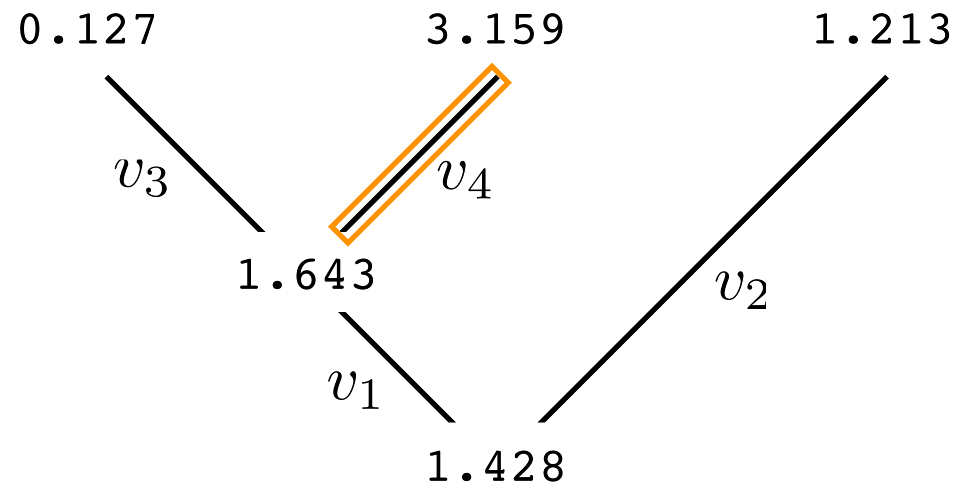


$\Bigg) =$

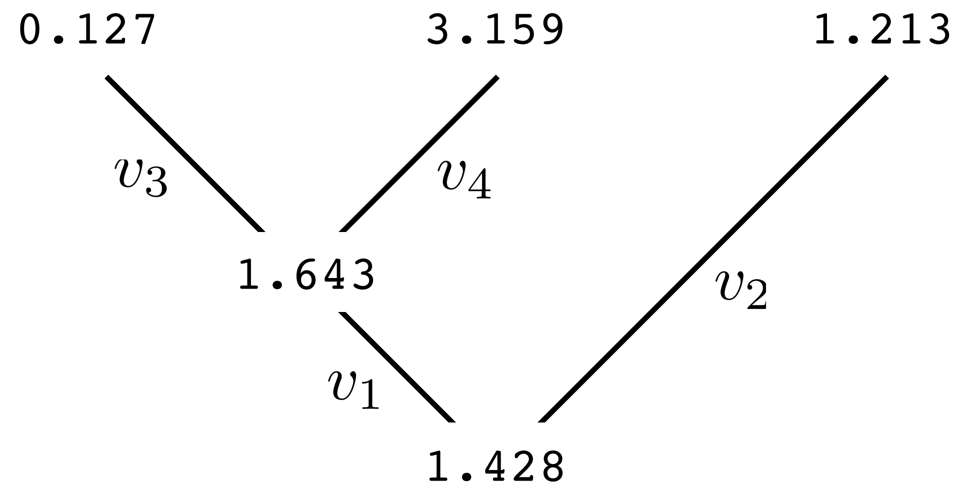
$$p(1.428) \times p(1.428 \to 1.643 \mid v_1) \times p(1.428 \to 1.213 \mid v_2) \times$$
$$p(1.643 \to 0.127 \mid v_3)$$

Likelihoods for Continuous Characters

$\Pr\Bigg($  $\Bigg) =$

$$p(1.428) \times p(1.428 \rightarrow 1.643 \mid v_1) \times p(1.428 \rightarrow 1.213 \mid v_2) \times$$
$$p(1.643 \rightarrow 0.127 \mid v_3) \times p(1.643 \rightarrow 3.159 \mid v_4)$$

Likelihoods for Continuous Characters



$$\Pr\left(\cdots \right) =$$

$$p(1.428) \times p(1.428 \to 1.643 \mid v_1) \times p(1.428 \to 1.213 \mid v_2) \times$$
$$p(1.643 \to 0.127 \mid v_3) \times p(1.643 \to 3.159 \mid v_4)$$

$p(x)$ Prior probabilities (root probabilities)

$p(x_i \to x_j \mid v)$ Transition probabilities

Likelihoods for Continuous Characters

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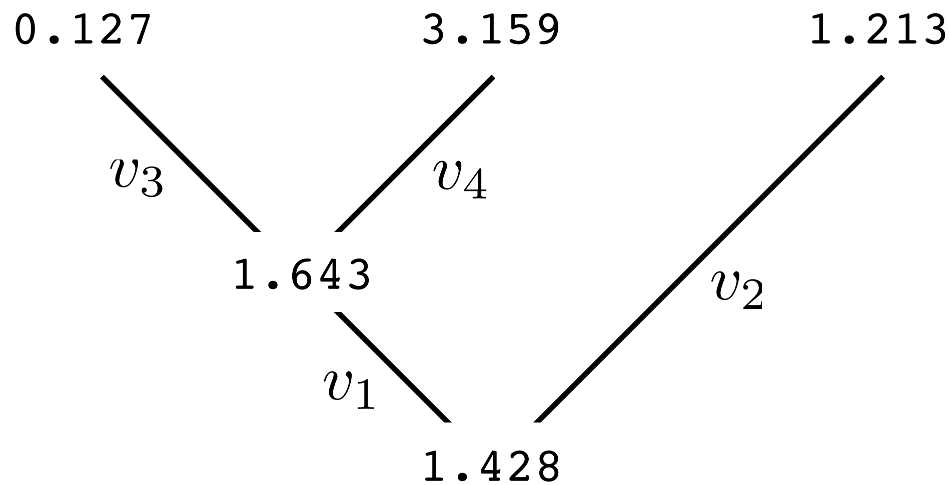

$\Big) +$

Likelihoods for Continuous Characters

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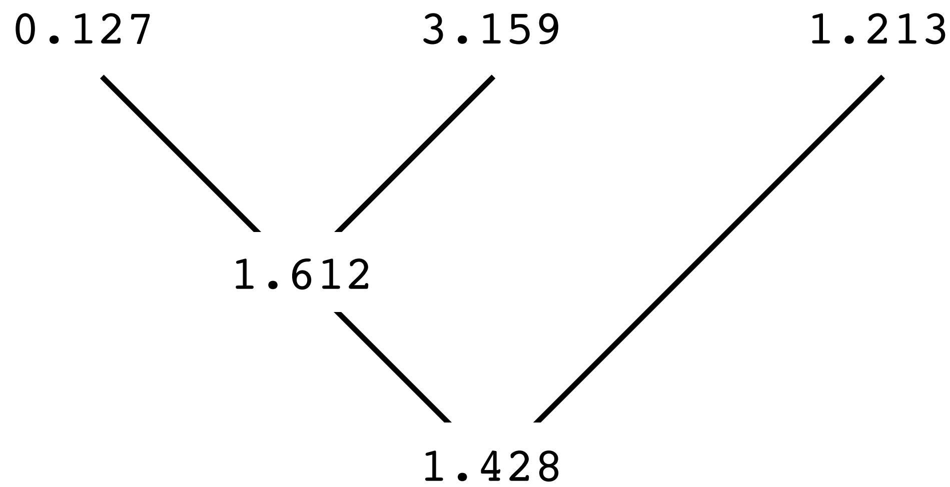

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Likelihoods for Continuous Characters

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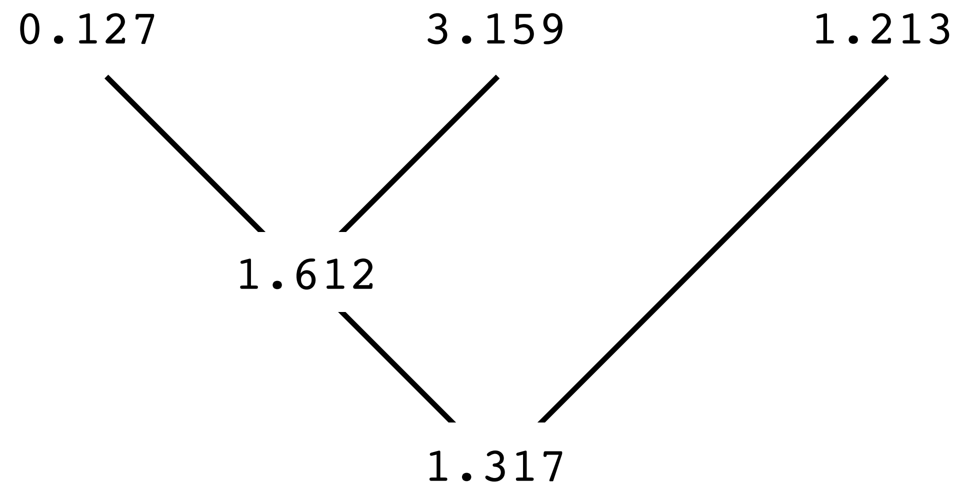

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Likelihoods for Continuous Characters

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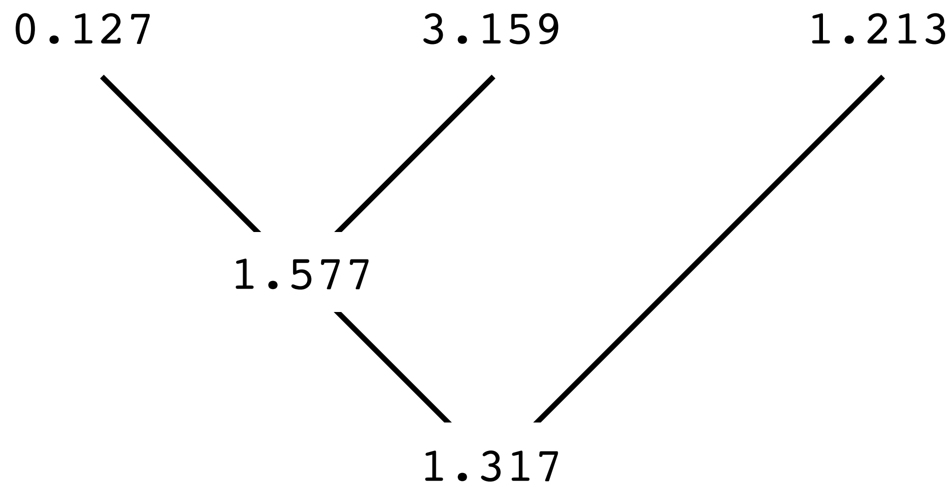

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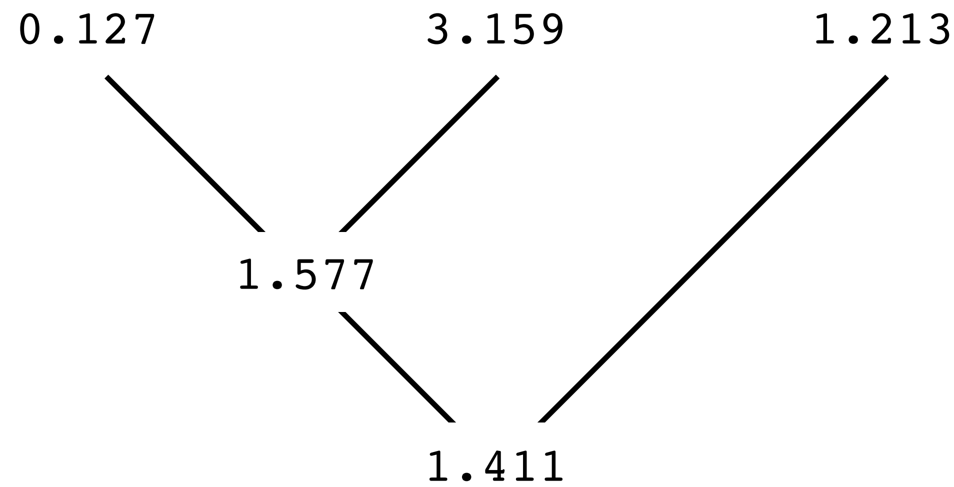
Likelihoods for Continuous Characters

$\Pr\Big($ 

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Likelihoods for Continuous Characters

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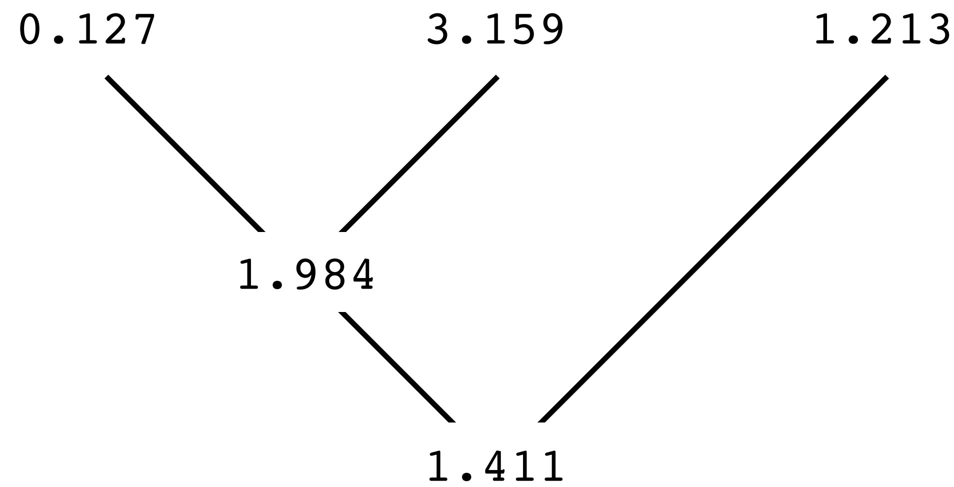

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Likelihoods for Continuous Characters

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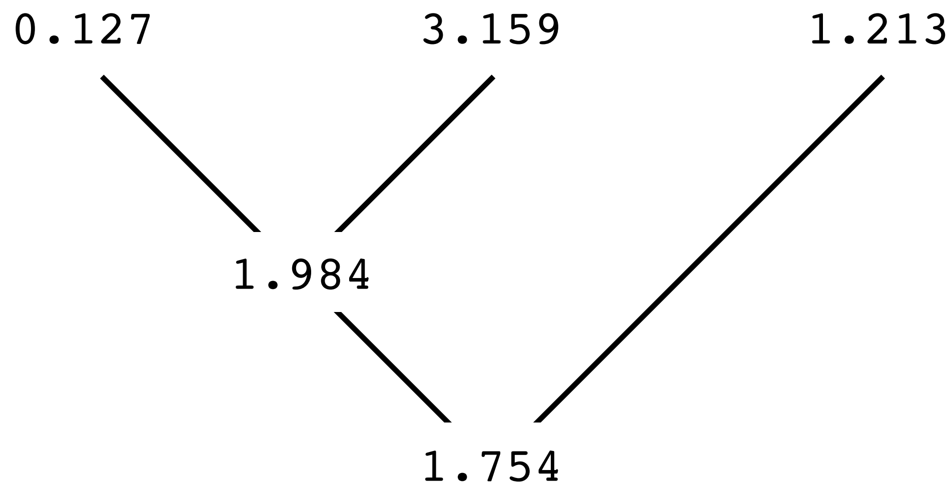

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Likelihoods for Continuous Characters

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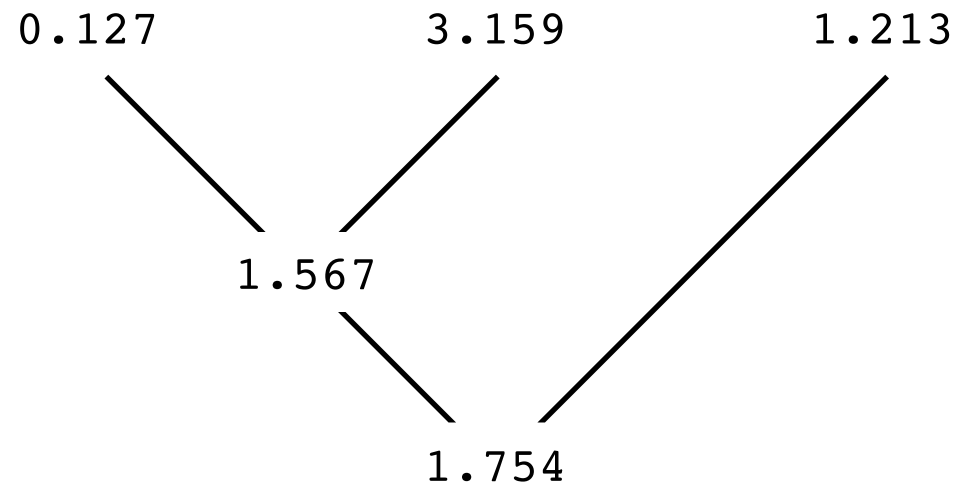

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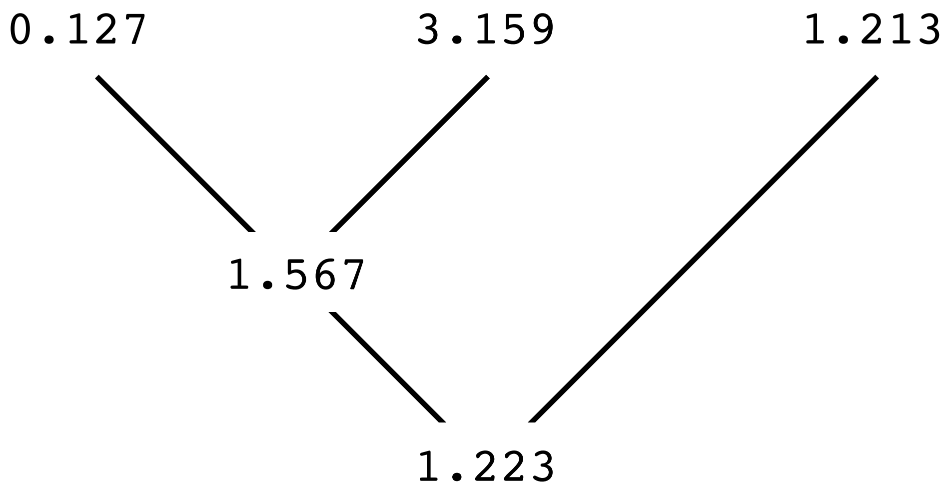
Likelihoods for Continuous Characters

$\Pr($  $) +$

Likelihoods for Continuous Characters

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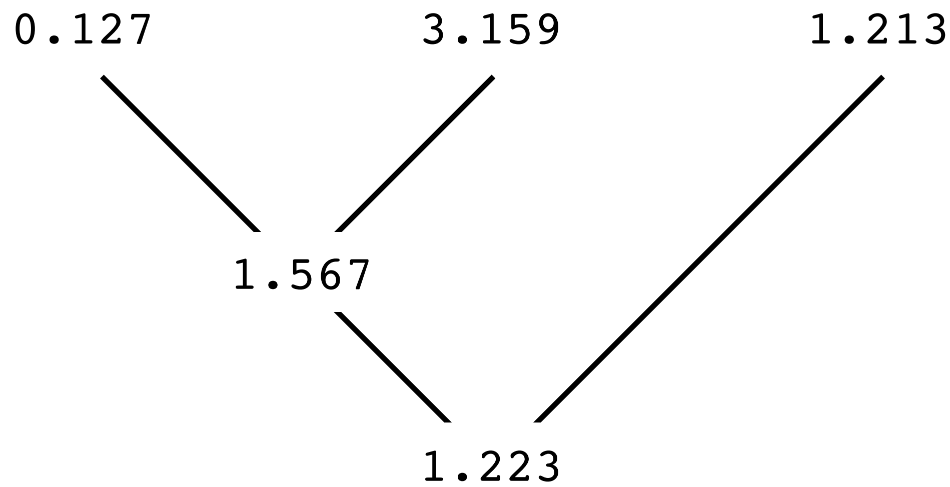


$$\Bigg) + \cdots$$

Likelihoods for Continuous Characters

Calculating transition probabilities and integrating over all ancestral states is the primary challenge of computing likelihoods for continuous characters.

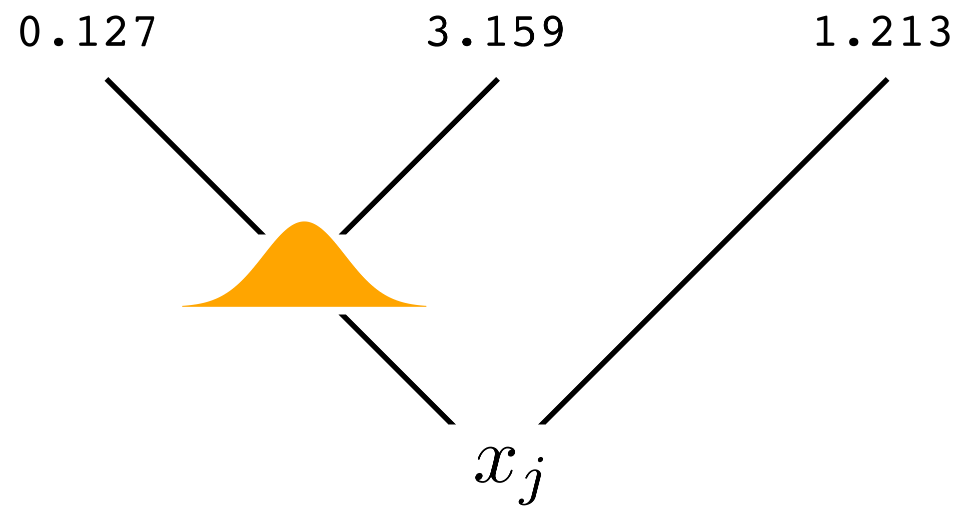
For some models (e.g., Brownian motion and OU), we can use a pruning algorithm (Felsenstein 1985) to efficiently calculate the likelihood.

Likelihoods for Continuous Characters

Felsenstein's Other Pruning Algorithm

Likelihoods for Continuous Characters

Felsenstein's Other Pruning Algorithm



Likelihoods for Continuous Characters

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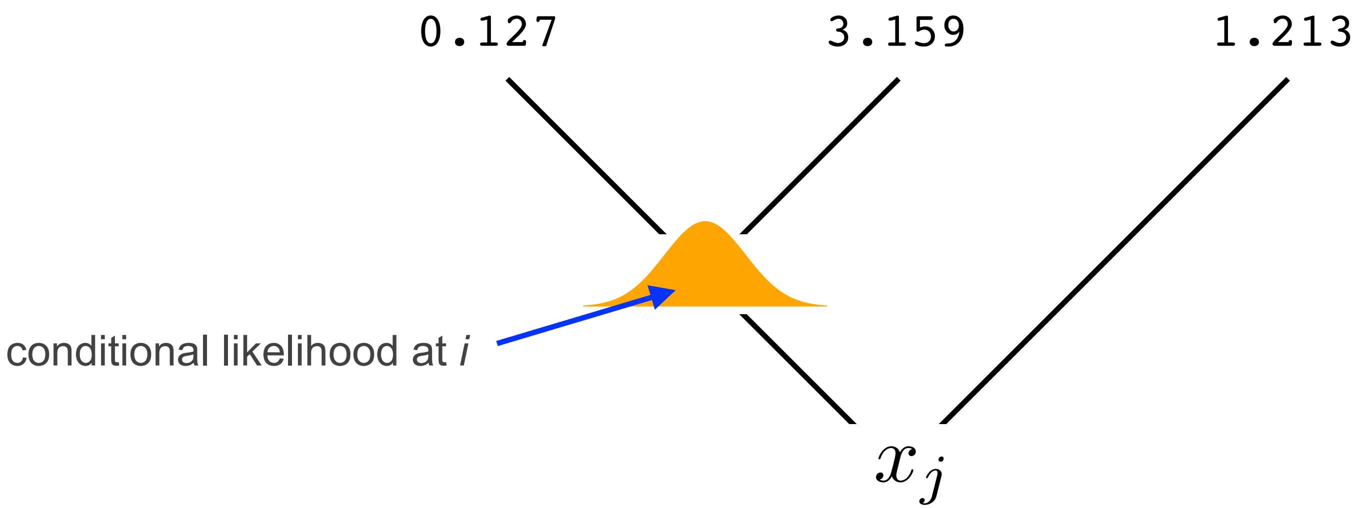

Likelihoods for Continuous Characters

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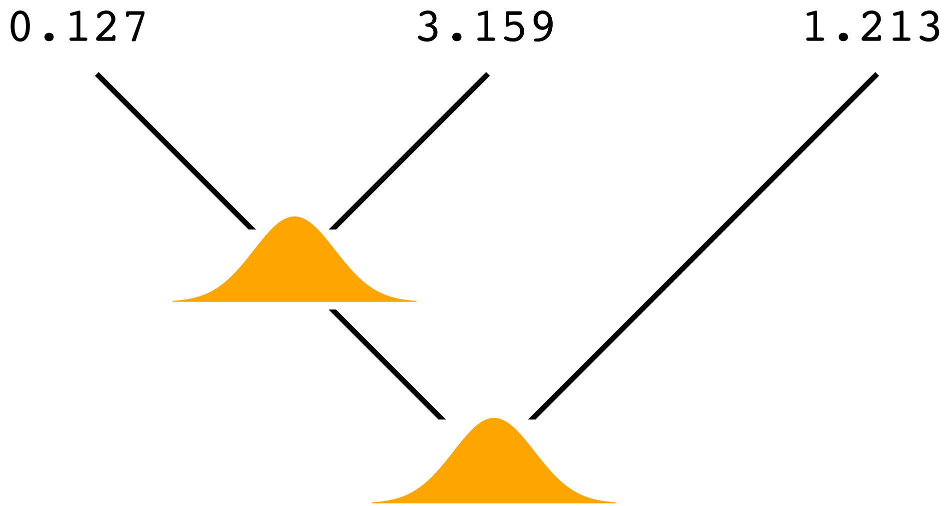
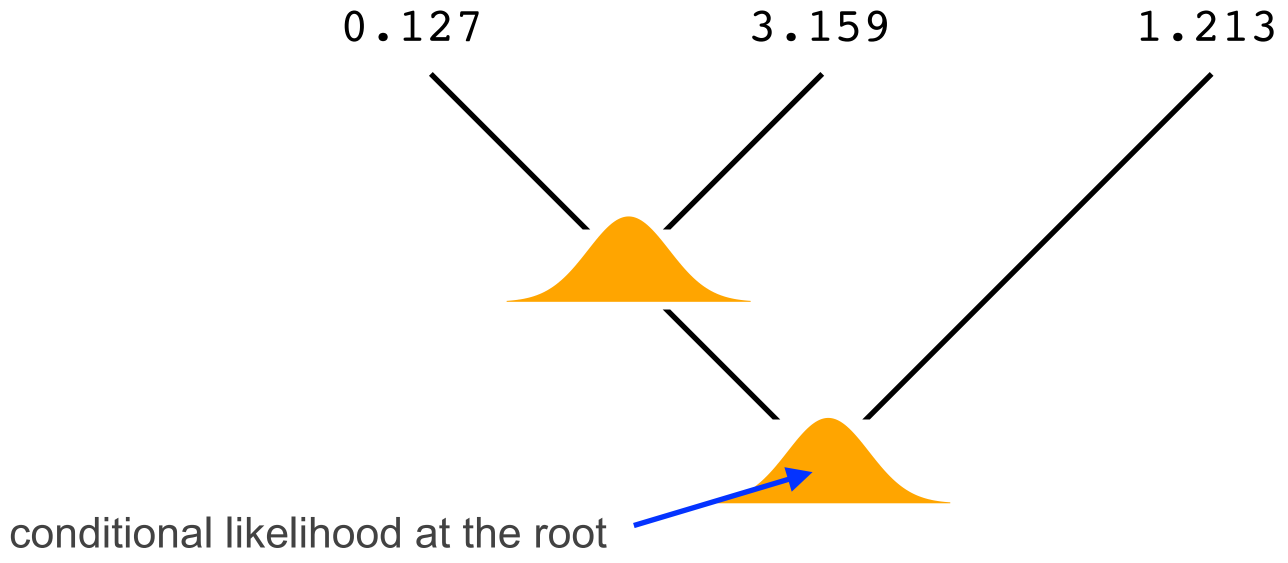


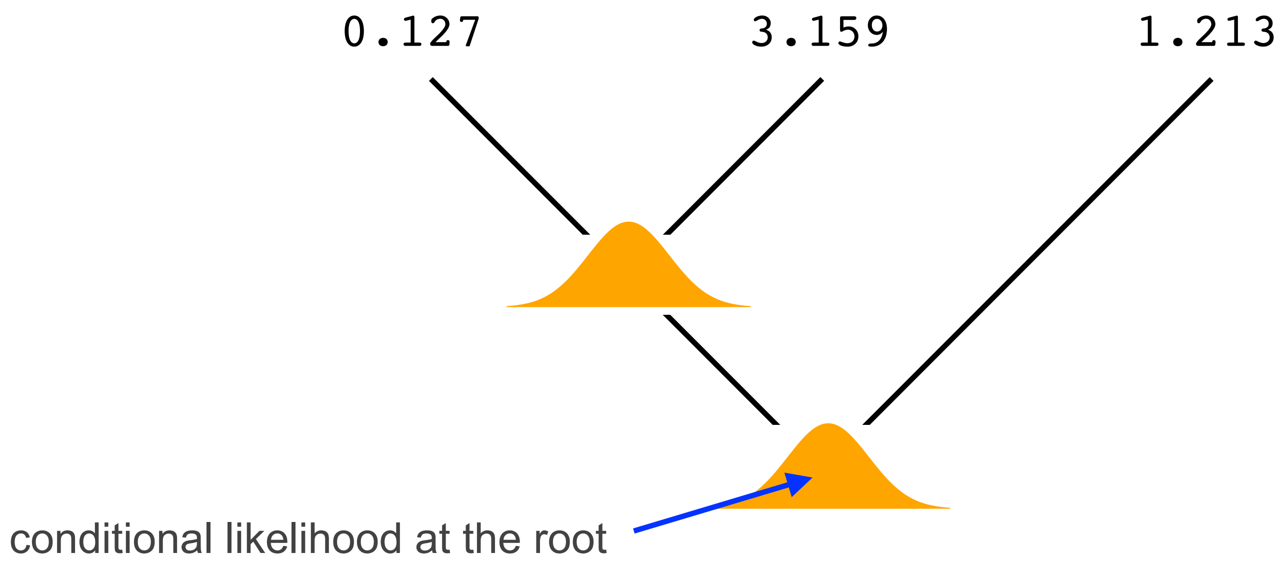
Likelihoods for Continuous Characters

Felsenstein’s Other Pruning Algorithm



Likelihoods for Continuous Characters

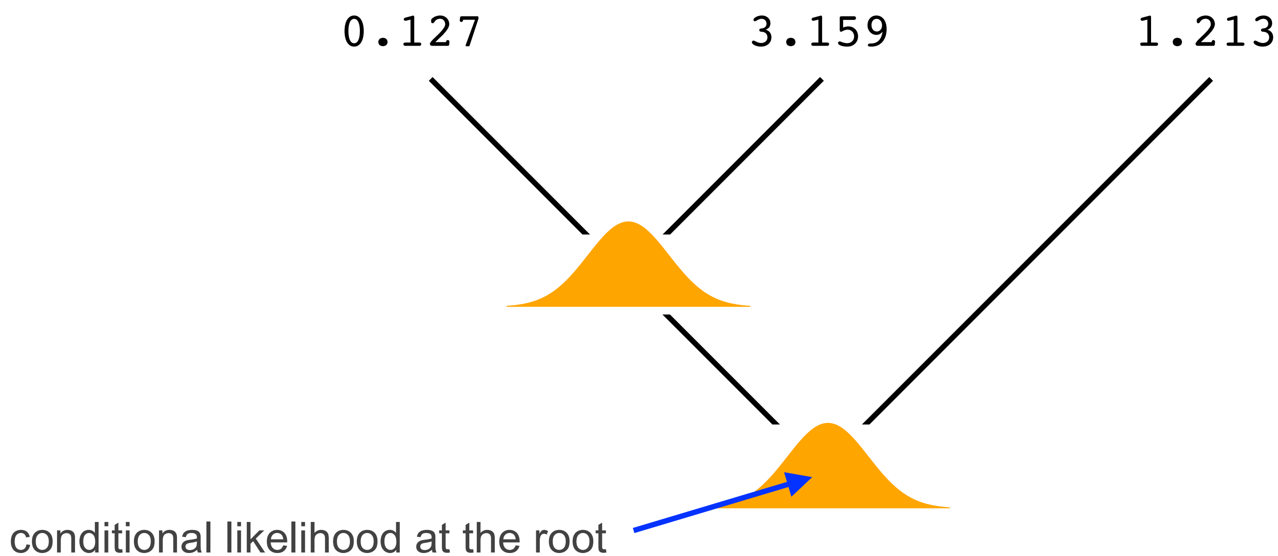
Felsenstein's Other Pruning Algorithm



$$\mathbf{P}(\mathrm{TTGT}) = \pi_{\mathrm{A}}\mathscr{L}_{\mathrm{A}}^{(root)} + \pi_{\mathrm{C}}\mathscr{L}_{\mathrm{C}}^{(root)} + \pi_{\mathrm{G}}\mathscr{L}_{\mathrm{G}}^{(root)} + \pi_{\mathrm{T}}\mathscr{L}_{\mathrm{T}}^{(root)}$$

Likelihoods for Continuous Characters

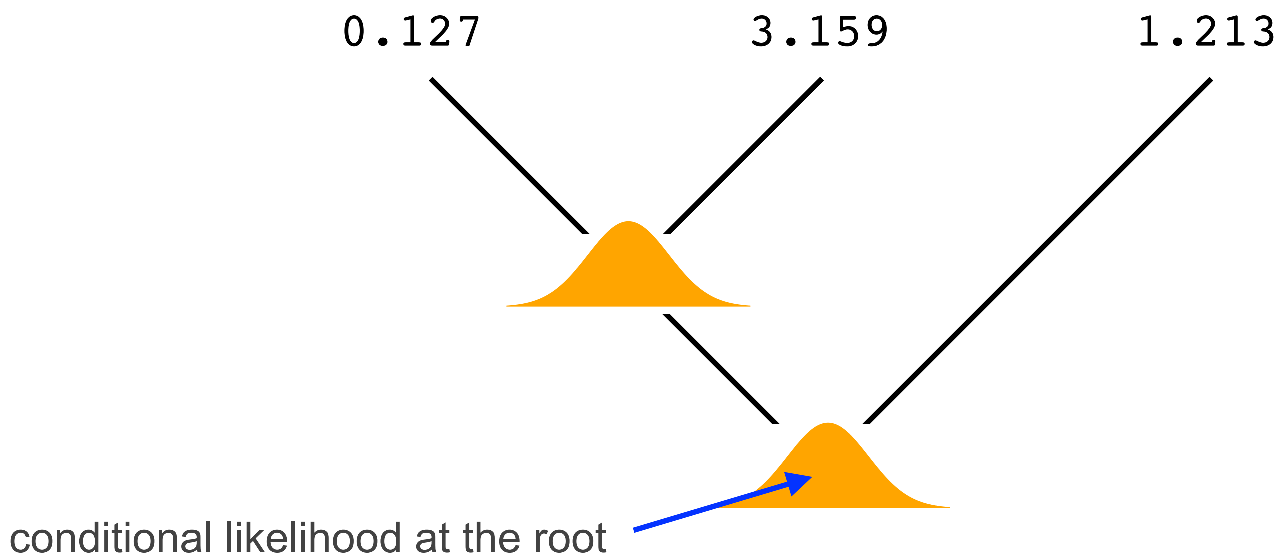
Felsenstein's Other Pruning Algorithm



$$\mathbf{P}(\mathrm{TTGT}) = \sum_{i \in \mathrm{A,C,G,T}} \pi_i \mathcal{L}_i^{(\mathrm{root})}$$

Likelihoods for Continuous Characters

Felsenstein's Other Pruning Algorithm

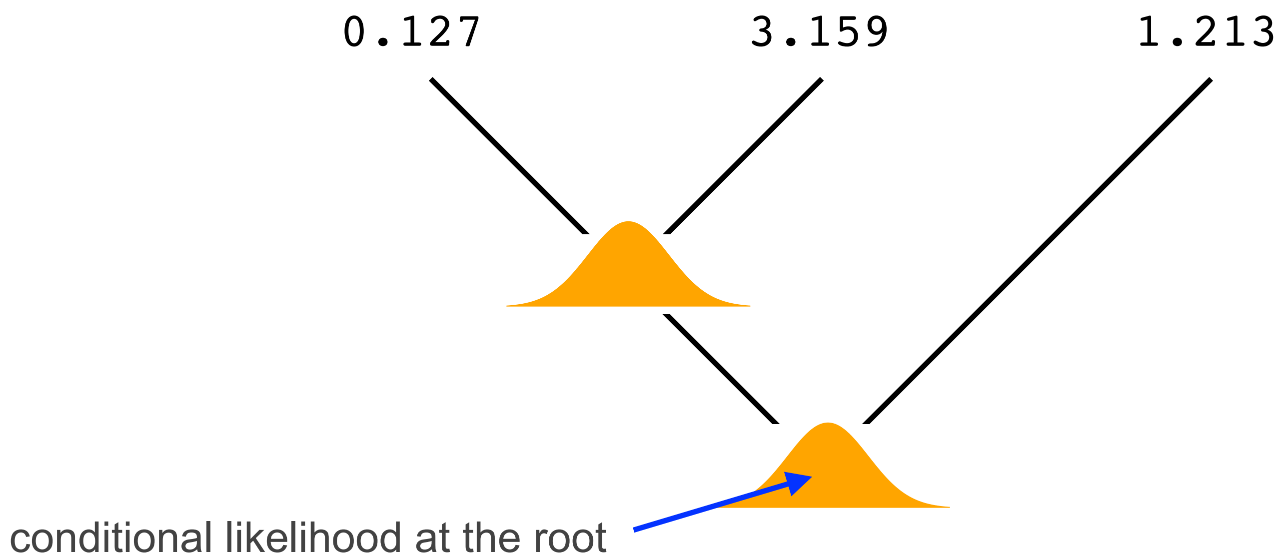


$$\mathbf{P}(\mathrm{TTGT}) = \sum_{i \in \mathrm{A,C,G,T}} \boxed{\pi_i} \mathcal{L}_i^{(\mathrm{root})}$$

prior probability

Likelihoods for Continuous Characters

Felsenstein's Other Pruning Algorithm

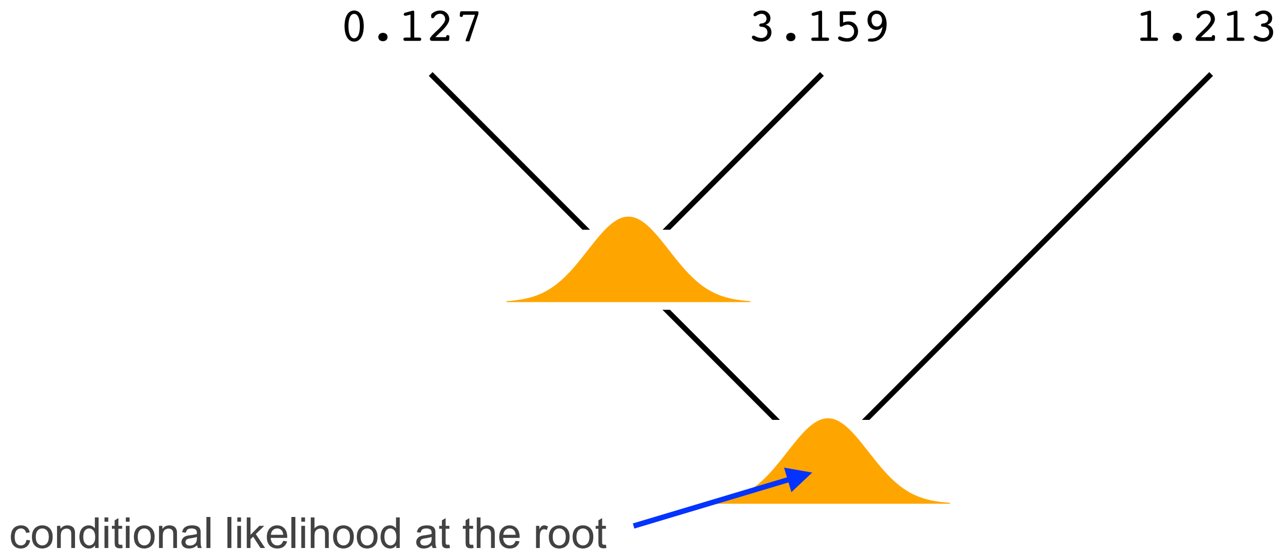


$$\mathbf{P}(\text{TTGT}) = \sum_{i \in \text{A,C,G,T}} \pi_i \boxed{\mathcal{L}_i^{(\text{root})}}$$

conditional likelihood

Likelihoods for Continuous Characters

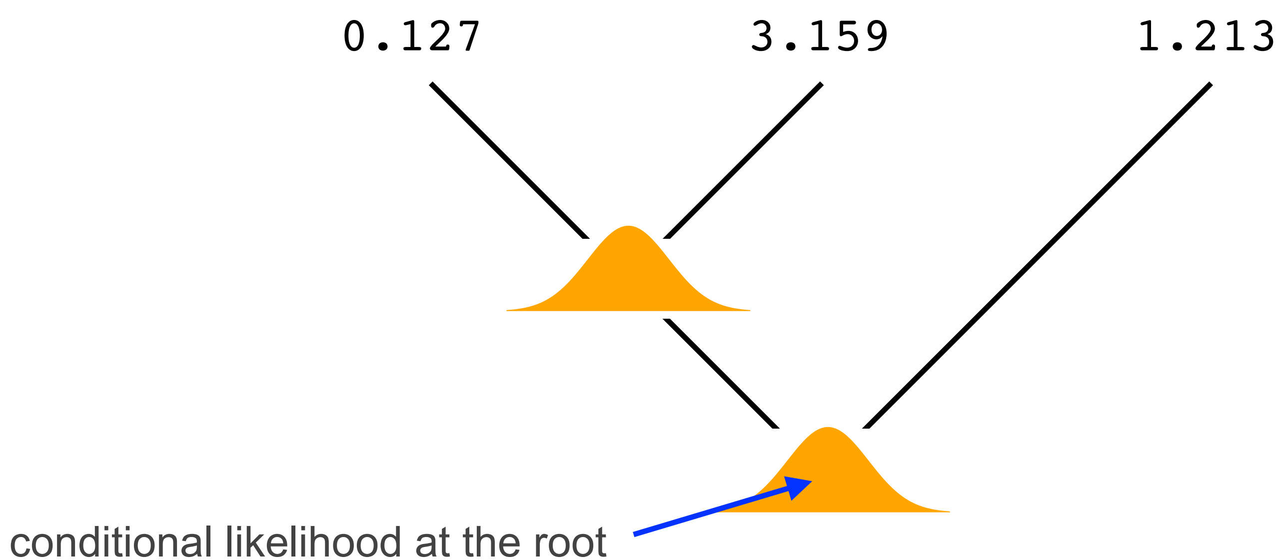
Felsenstein's Other Pruning Algorithm



$$P(0.127, 3.159, 1.213) = \int p(x_i) \mathcal{L}_i^{(\text{root})} \mathrm{d}x_i$$

Likelihoods for Continuous Characters

Felsenstein's Other Pruning Algorithm



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prior probability

Likelihoods for Continuous Characters

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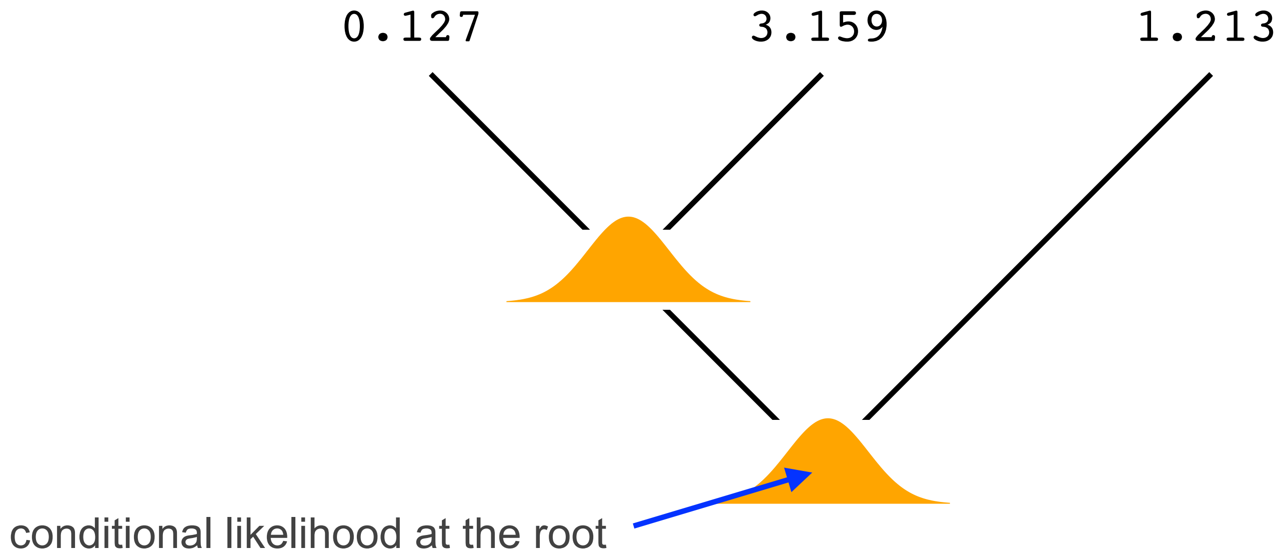


$$P(0.127, 3.159, 1.213) = \int p(x_i) \mathcal{L}_i^{(\text{root})} \mathrm{d}x_i$$

conditional likelihood

Outline

I. Calculating likelihoods for continuous traits

A generic framework for calculating probabilities

II. A simple model of continuous-character evolution

Brownian motion model

Multivariate Brownian motion model

A Simple Model of Continuous-Character Evolution

Brownian motion

Brownian motion was first used to describe the motion of microscopic particles moving in fluid.

Felsenstein proposed Brownian motion as a simple model of continuous-character evolution.

A Simple Model of Continuous-Character Evolution

Brownian motion

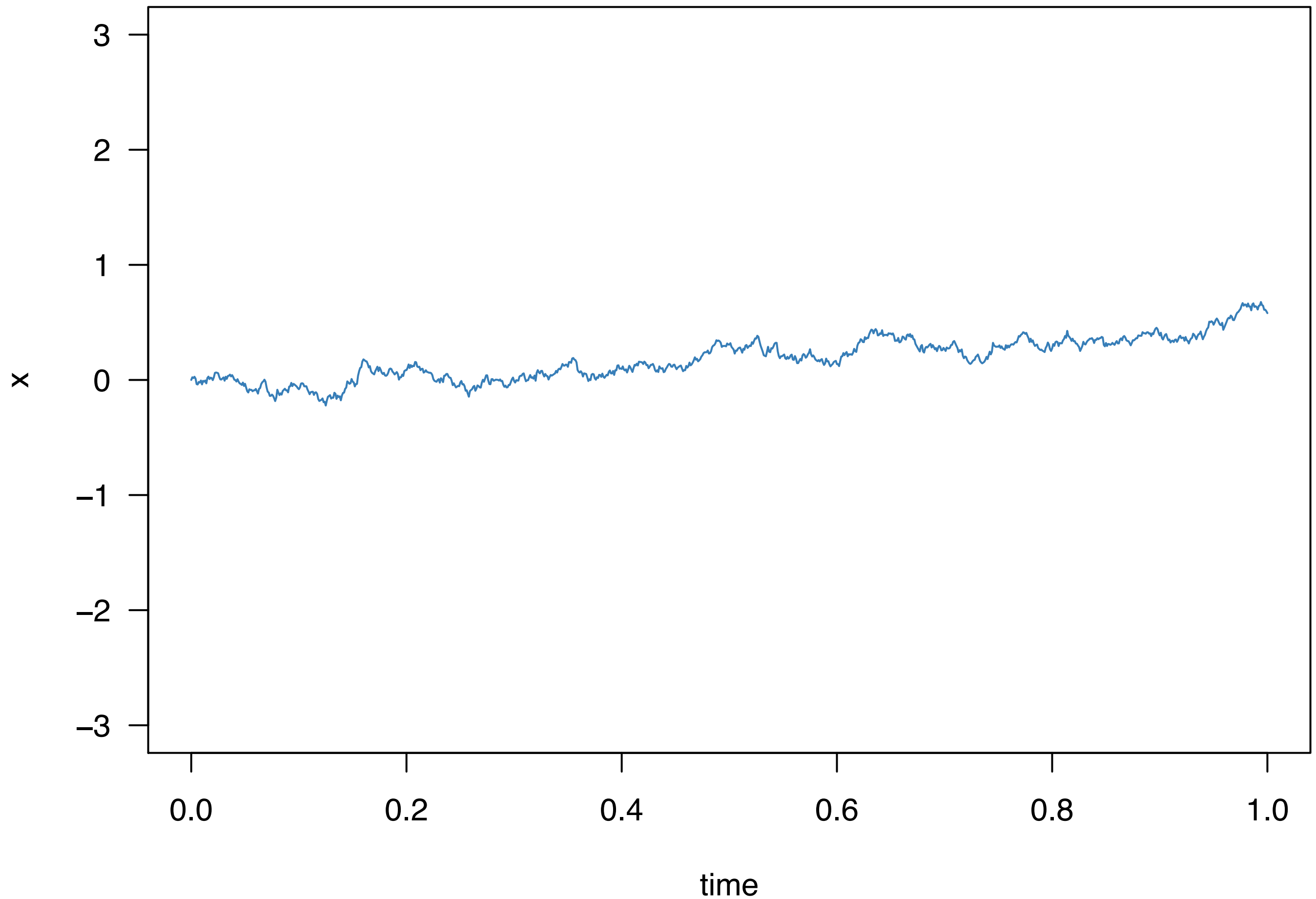
Brownian motion is defined by a single parameter, σ^2, which represents the *rate* of evolution.

The expected amount of character change is zero, but the opportunity for evolution is proportional to the rate of evolution and time.

A Simple Model of Continuous-Character Evolution

Brownian motion

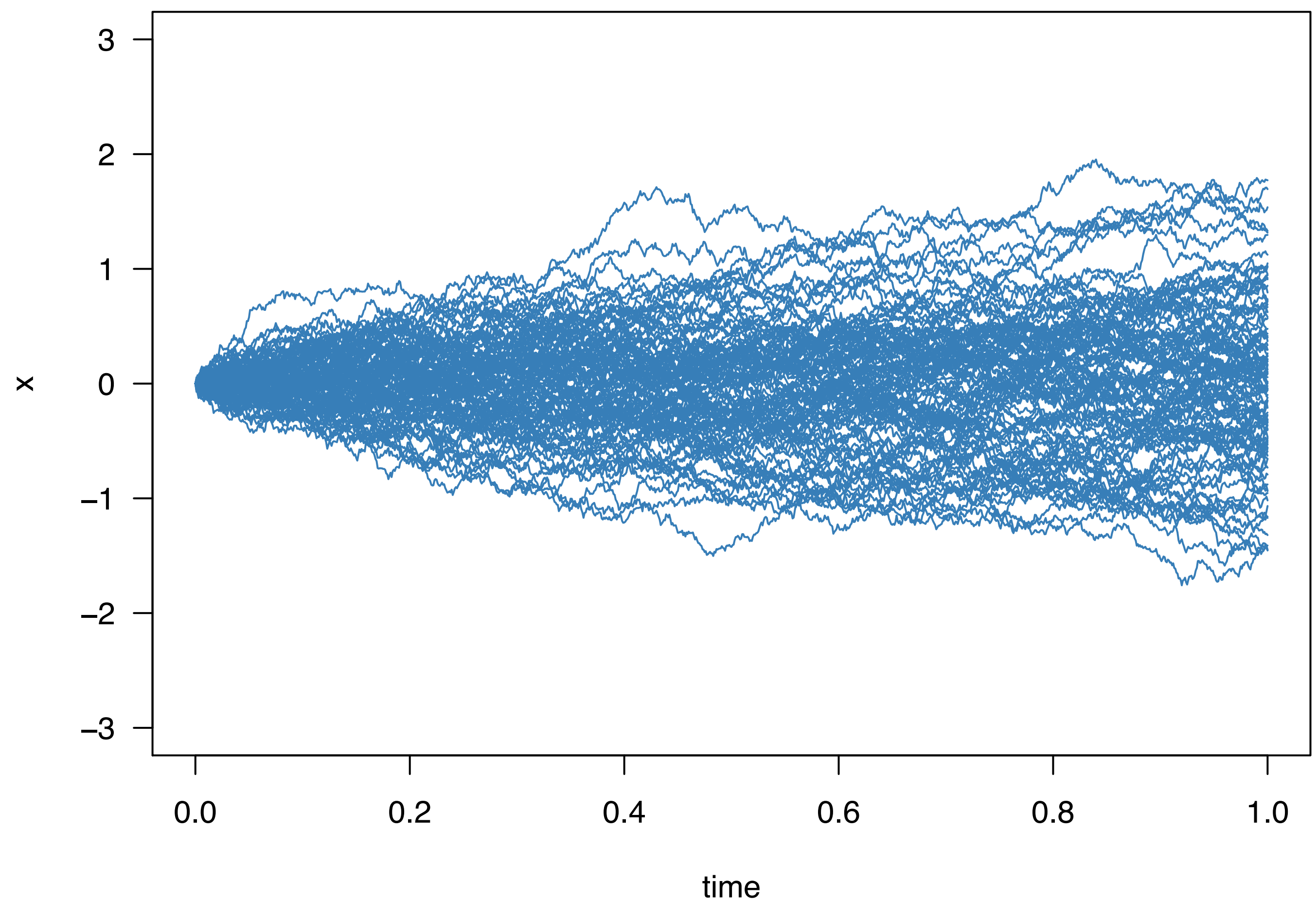
A single sample path under Brownian motion



A Simple Model of Continuous-Character Evolution

Brownian motion

Many sample paths under Brownian motion

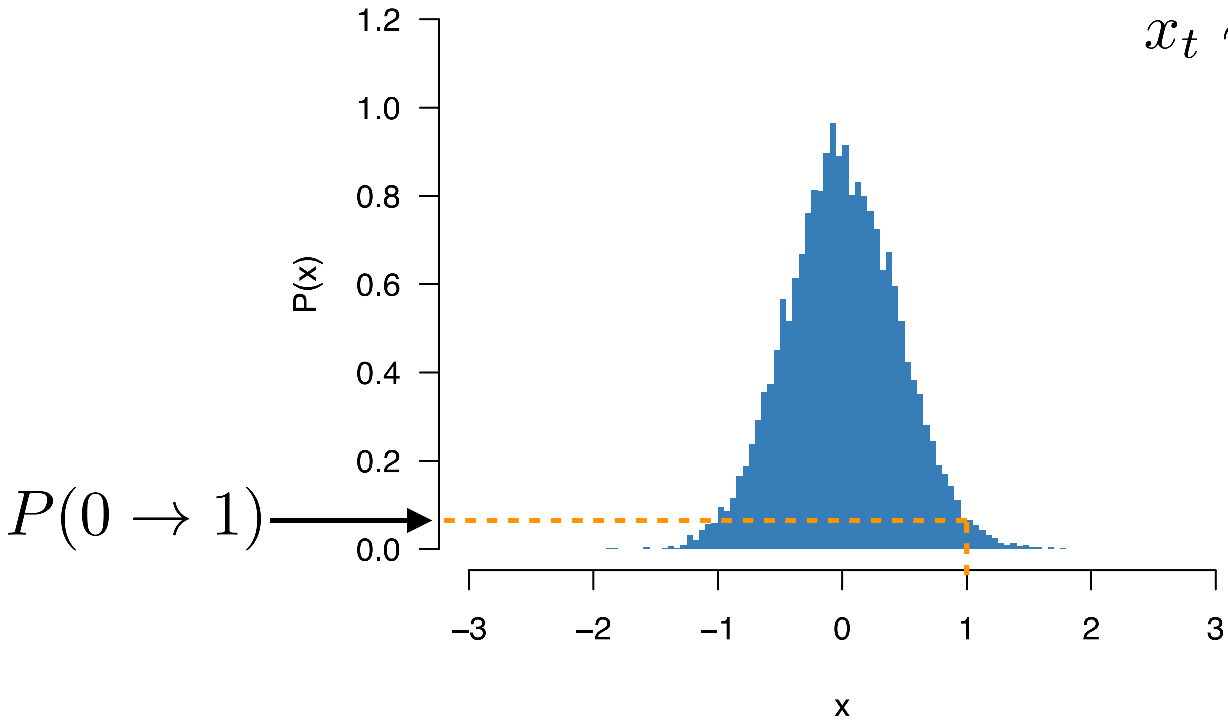


A Simple Model of Continuous-Character Evolution

Brownian motion

The transition probability under Brownian motion

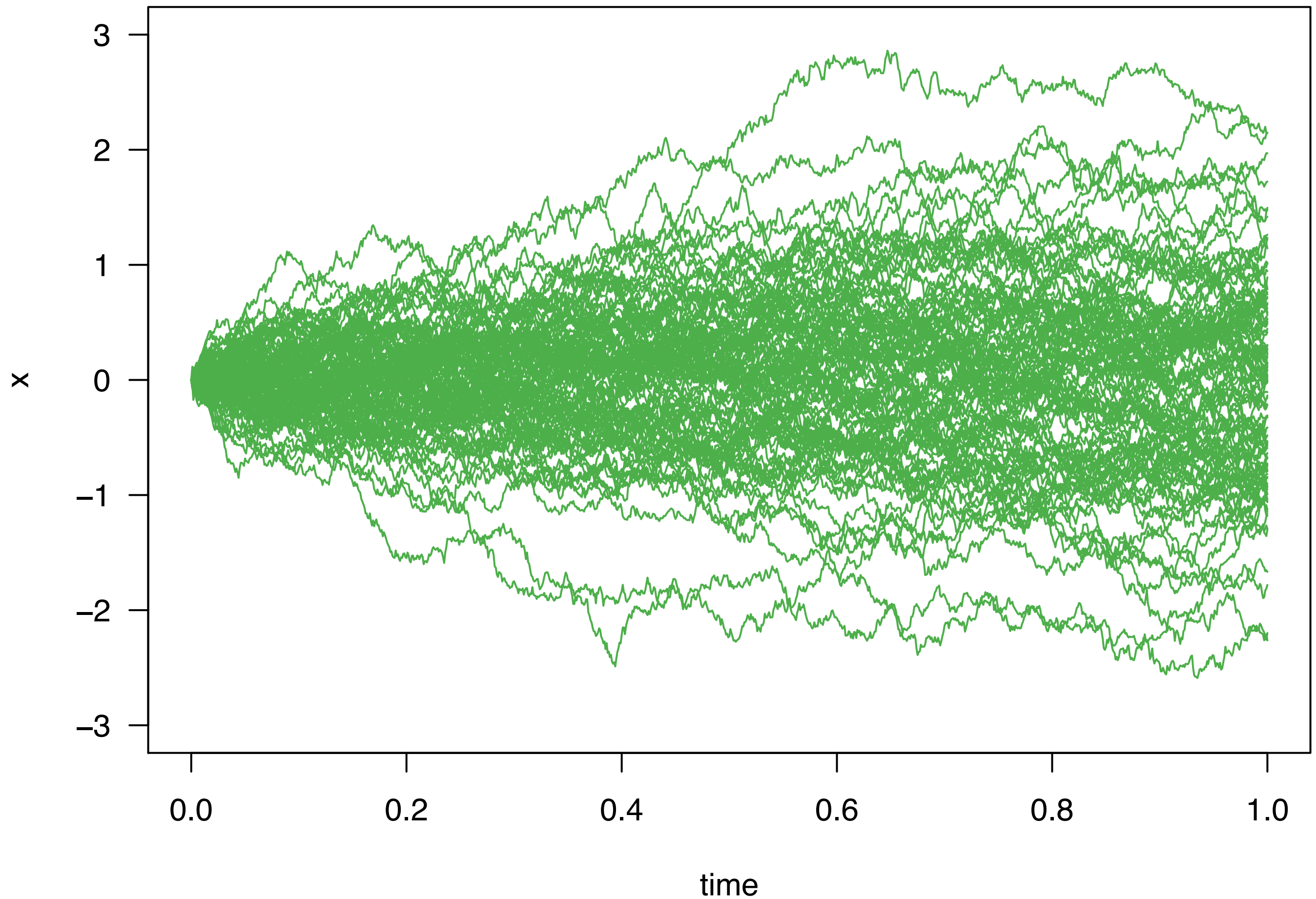
$$x_t \sim \mathrm{Normal}(x_0, t\sigma^2)$$



A Simple Model of Continuous-Character Evolution

Brownian motion

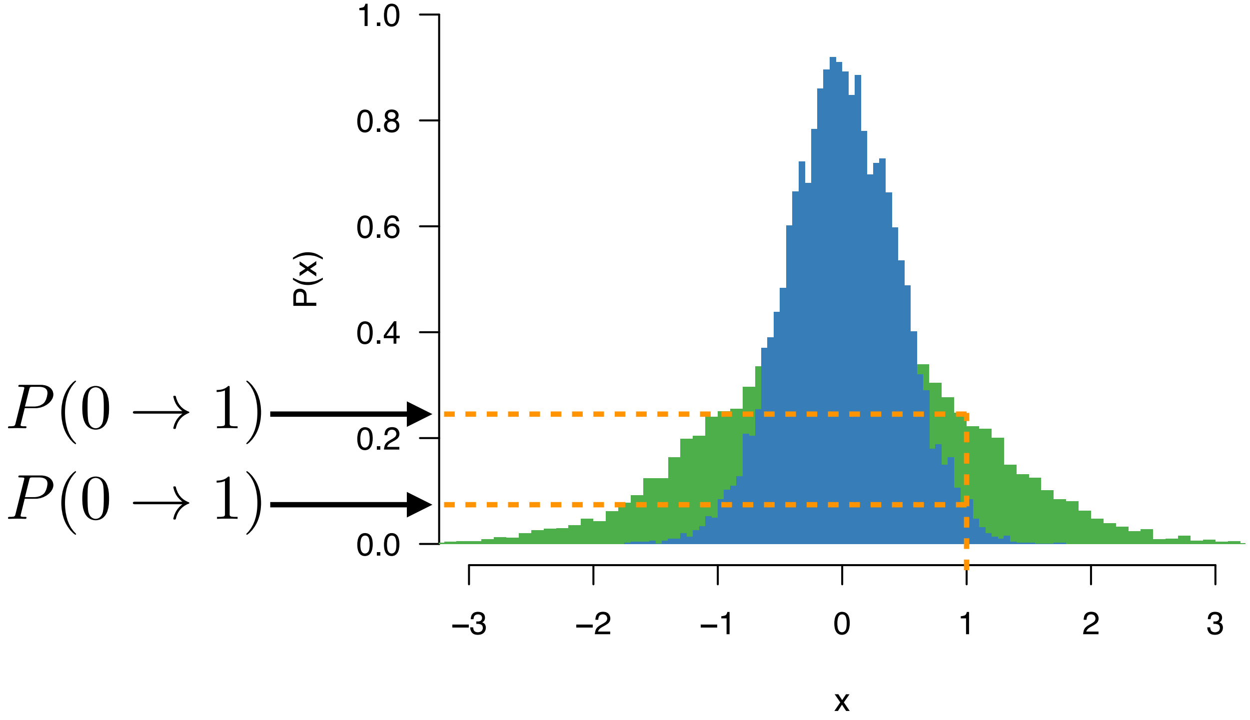
What if we turn up the rate parameter?



A Simple Model of Continuous-Character Evolution

Brownian motion

When the rate is higher, the process is more likely to evolve more.



A Simple Model of Continuous-Character Evolution

Brownian motion

We can use these transition probabilities to calculate the likelihood of a single character.

If we have multiple characters, we can make the same assumption that we did for molecular data: that the characters are independent.

$$P(X \mid \sigma^2) = \prod_i P(X_i \mid \sigma^2)$$

A Simple Model of Continuous-Character Evolution

Brownian motion

We can use the likelihood function to estimate the rate parameter!

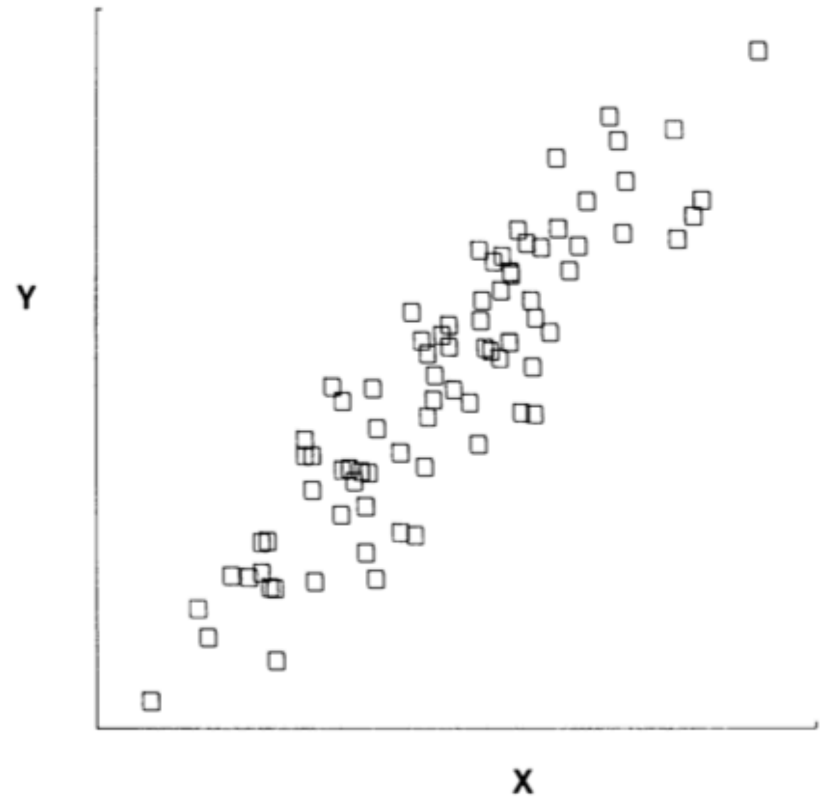
What if we don't want to assume that the characters are independent?

$$\boxed{P(\sigma^2 \mid X)} \propto P(X \mid \sigma^2) P(\sigma^2)$$

posterior

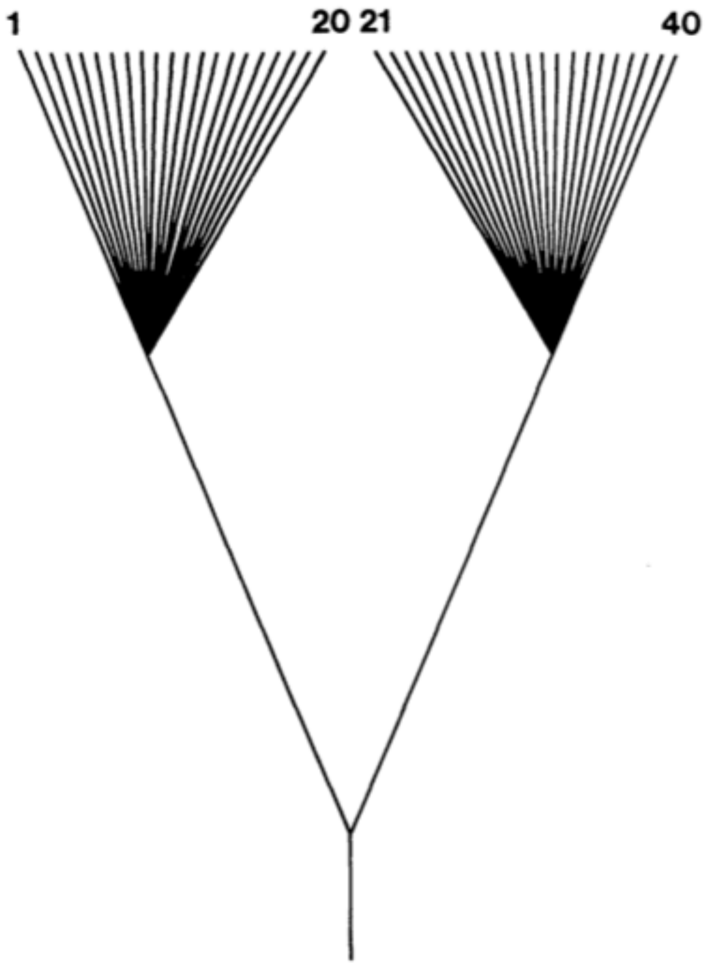
A Simple Model of Continuous-Character Evolution

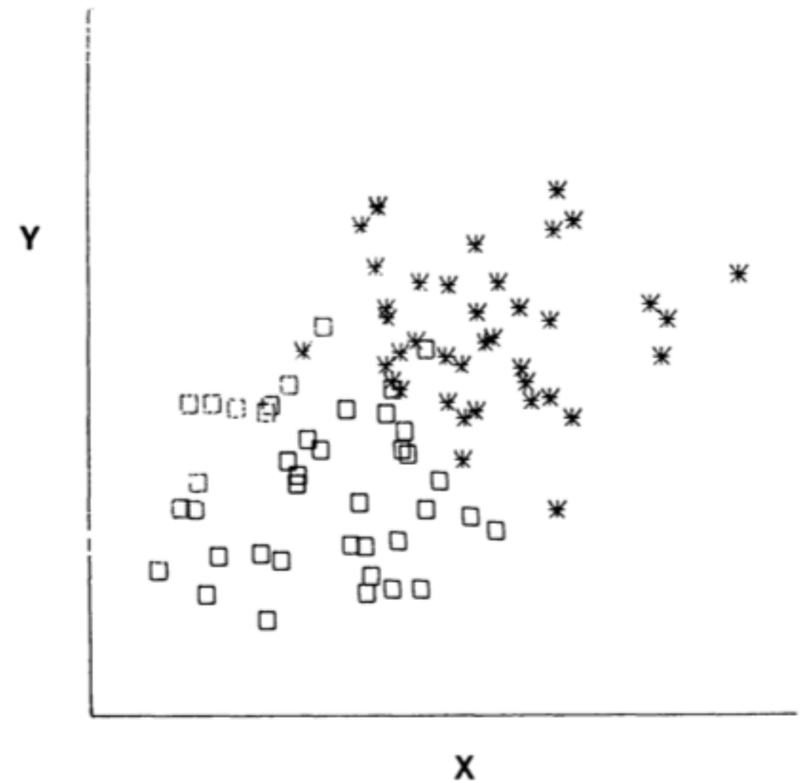
Are characters *X* and *Y* evolutionarily correlated?



A Simple Model of Continuous-Character Evolution

Are characters *X* and *Y* evolutionarily correlated?





A Simple Model of Continuous-Character Evolution

Multivariate Brownian motion

Multivariate Brownian motion is the multivariate generalization of Brownian motion (when there are multiple continuous traits).

Rather than a single diffusion rate, there is one rate for each of *c* traits, as well as a correlation parameter for each pair of traits.

$$\sigma^2 = \sigma_1^2, \sigma_2^2, \ldots, \sigma_c^2$$

evolutionary rates for each character

$$R = \begin{pmatrix} 1 & \rho_{12} & \cdots & \rho_{1c} \\ \rho_{12} & 1 & \cdots & \rho_{2c} \\ \vdots & \vdots & \ddots & \vdots \\ \rho_{1c} & \rho_{2c} & \cdots & 1 \end{pmatrix}$$

evolutionary correlations between each pair of characters

A Simple Model of Continuous-Character Evolution

Multivariate Brownian motion

Multivariate Brownian motion is the multivariate generalization of Brownian motion (when there are multiple continuous traits).

Rather than a single diffusion rate, there is one rate for each of *c* traits, as well as a correlation parameter for each pair of traits.

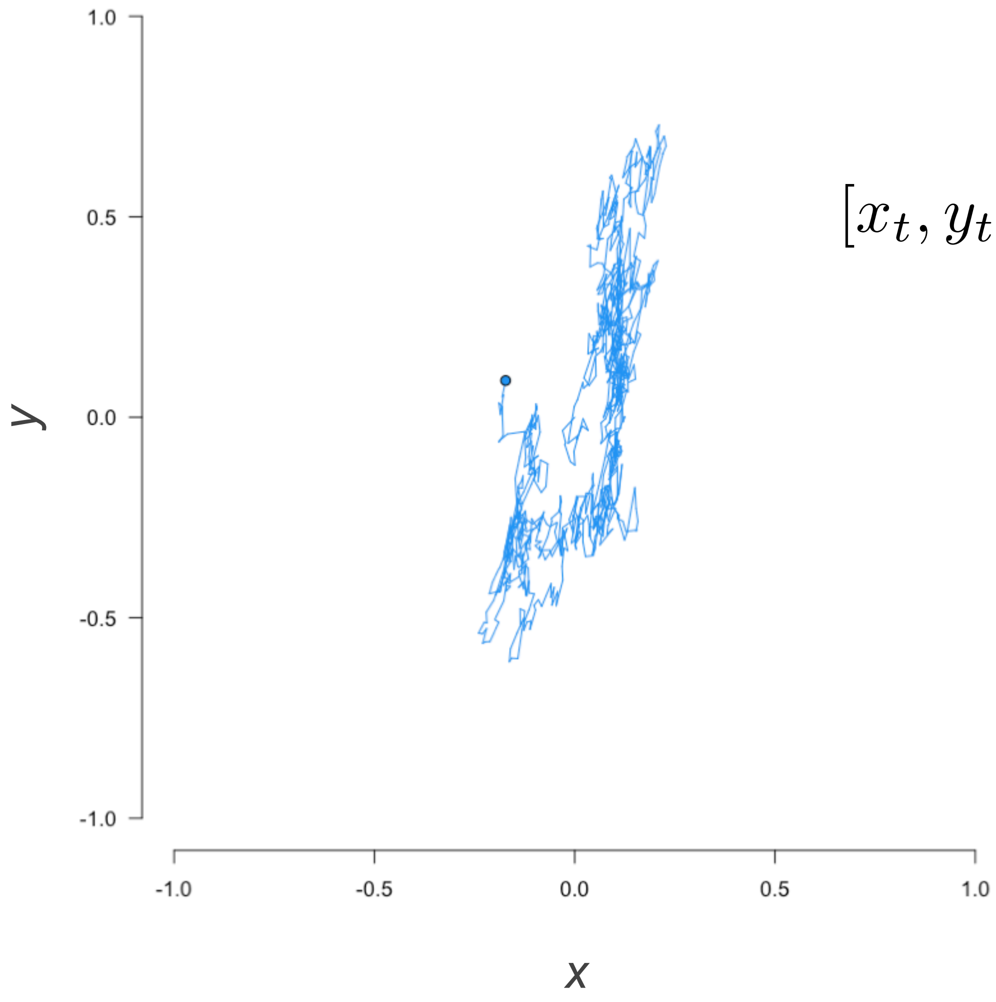
$$\Sigma = \begin{pmatrix} \sigma_1^2 & \sigma_1\sigma_2\rho_{12} & \cdots & \sigma_1\sigma_c\rho_{1c} \\ \sigma_1\sigma_2\rho_{12} & \sigma_2^2 & \cdots & \sigma_2\sigma_c\rho_{2c} \\ \vdots & \vdots & \ddots & \vdots \\ \sigma_1\sigma_c\rho_{1c} & \sigma_2\sigma_c\rho_{2c} & \cdots & \sigma_c^2 \end{pmatrix}$$

evolutionary variance-covariance matrix

A Simple Model of Continuous-Character Evolution

Multivariate Brownian motion

The transition probability density is a multivariate normal density.



$$[x_t, y_t] \sim \mathrm{MVN}([x_0, y_0], t\Sigma)$$

A Simple Model of Continuous-Character Evolution

Multivariate Brownian motion

We estimate the variance-covariance matrix using the likelihood function (and appropriately chosen priors).

$$\underbrace{P(\Sigma \mid X) \propto P(X \mid \Sigma) P(\Sigma)}_{\text{multivariate normal posterior}}$$

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Ornstein-Uhlenbeck model

Lévy models

State-dependent models

Exotic Diffusion Models

Ornstein-Uhlenbeck (OU) model

The Ornstein-Uhlenbeck process describes diffusion toward (and around) an optimal value.

It is commonly used to model stabilizing selection.

There are three parameters:

σ^2 — rate of evolution

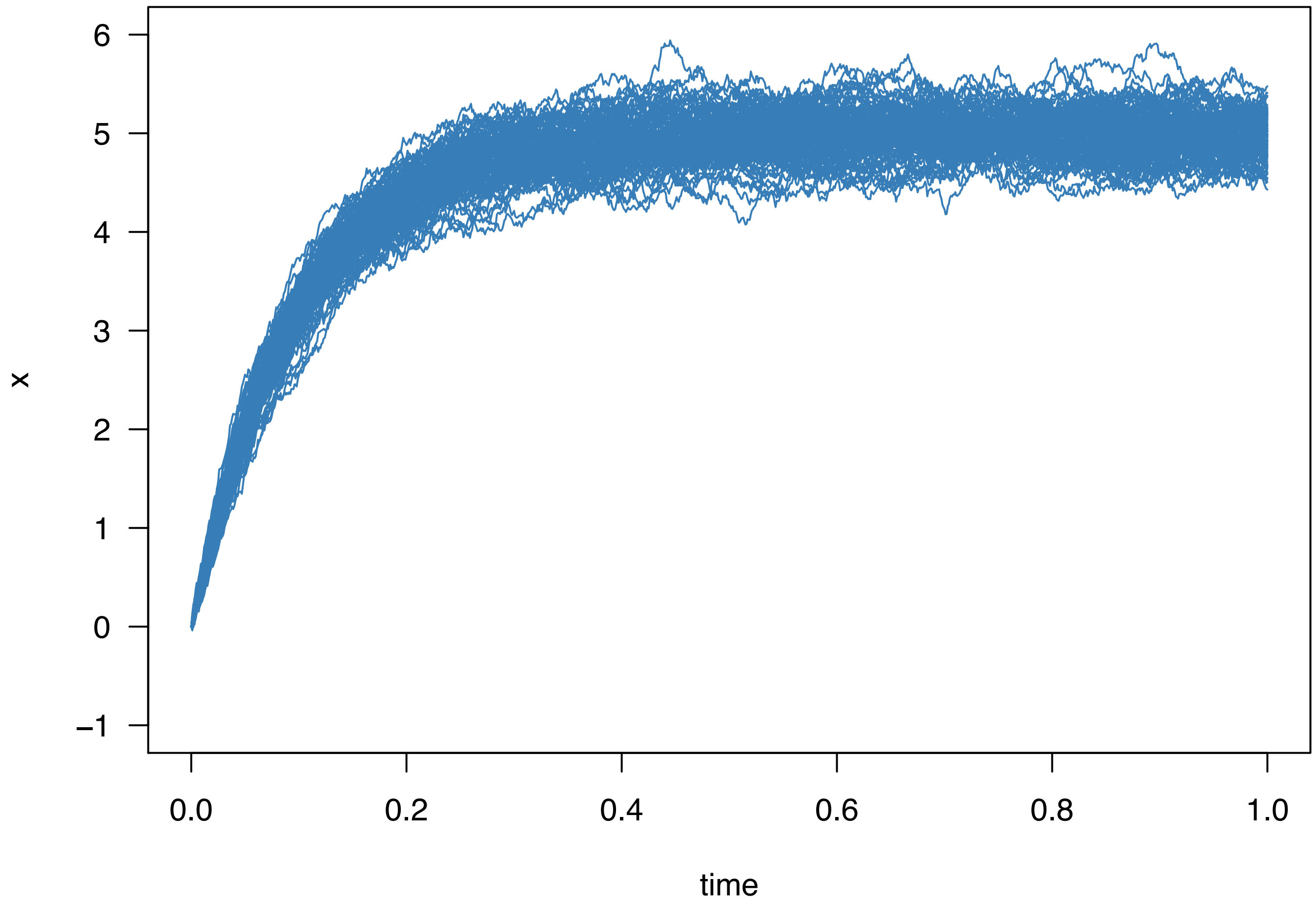
θ — optimal value

α — strength of selection

Exotic Diffusion Models

Ornstein-Uhlenbeck (OU) model

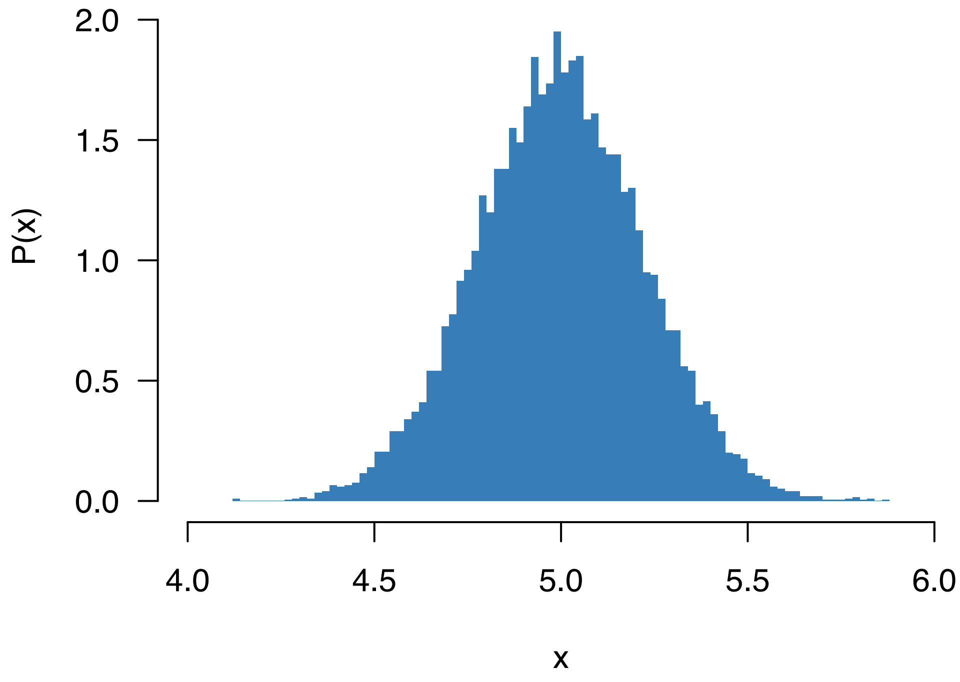
Many sample paths under OU



Exotic Diffusion Models

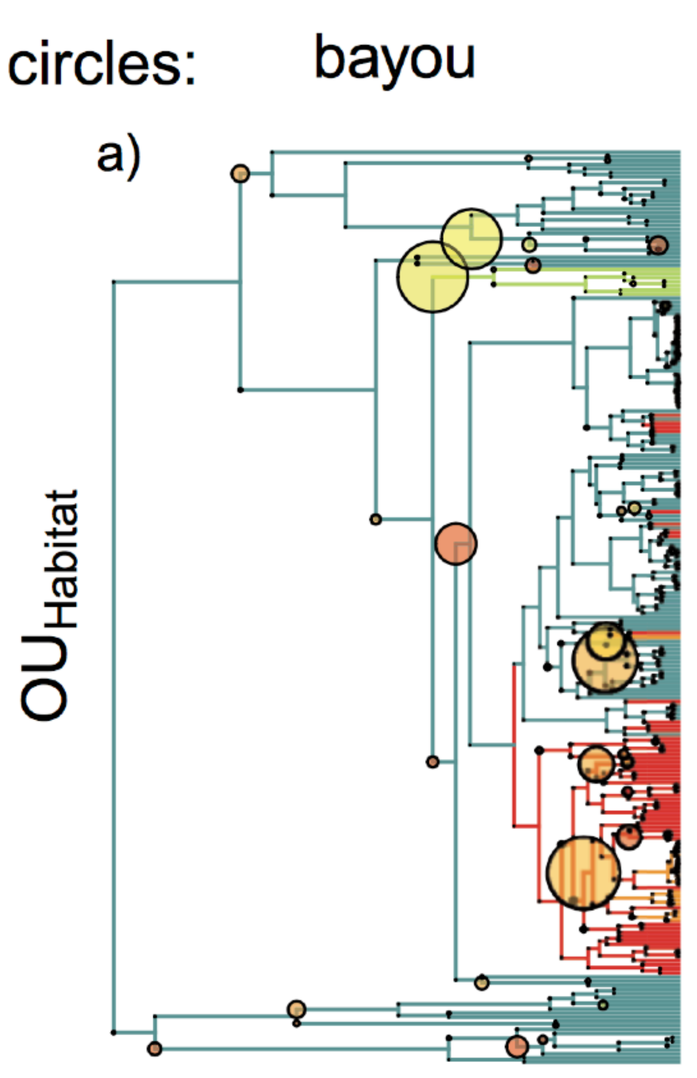
Ornstein-Uhlenbeck (OU) model

The transition probability under the OU process is a known normal probability density (with complicated parameters!)



Exotic Diffusion Models

Ornstein-Uhlenbeck (OU) model



Uyeda and Harmon 2014

Exotic Diffusion Models

Lévy process models

The Lévy processes are a family of models that allow for both continuous diffusion (as with the Brownian motion model) and sudden changes in the state of the character.

The Jump-Normal model is a Lévy process that models jumps using a Poisson process. At each jump event, the character changes by a normal random variable.

σ^2 — rate of evolution

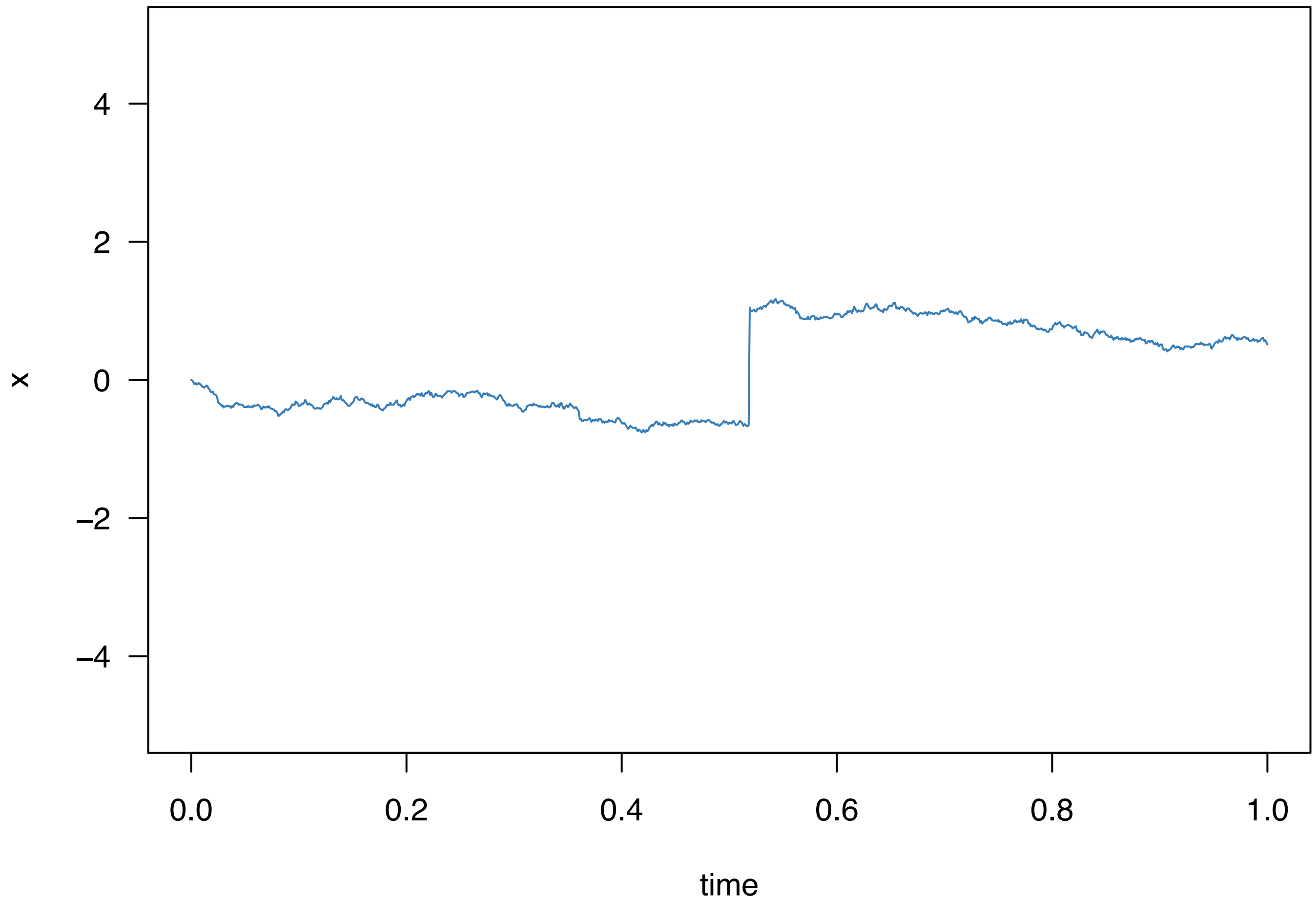
λ — rate of jumps

δ — size of jumps

Exotic Diffusion Models

Jump-Normal (JN) model

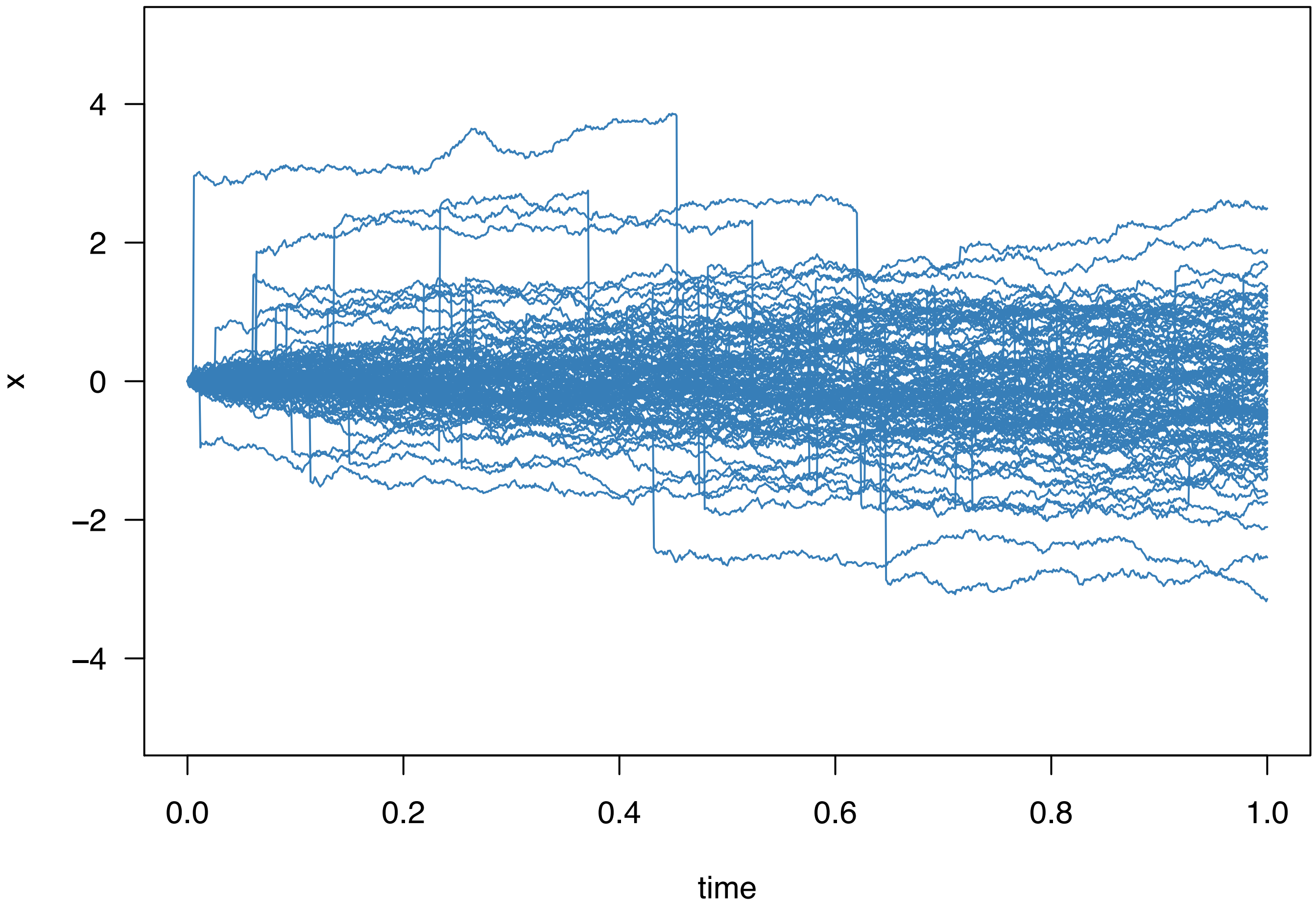
A single sample path under JN



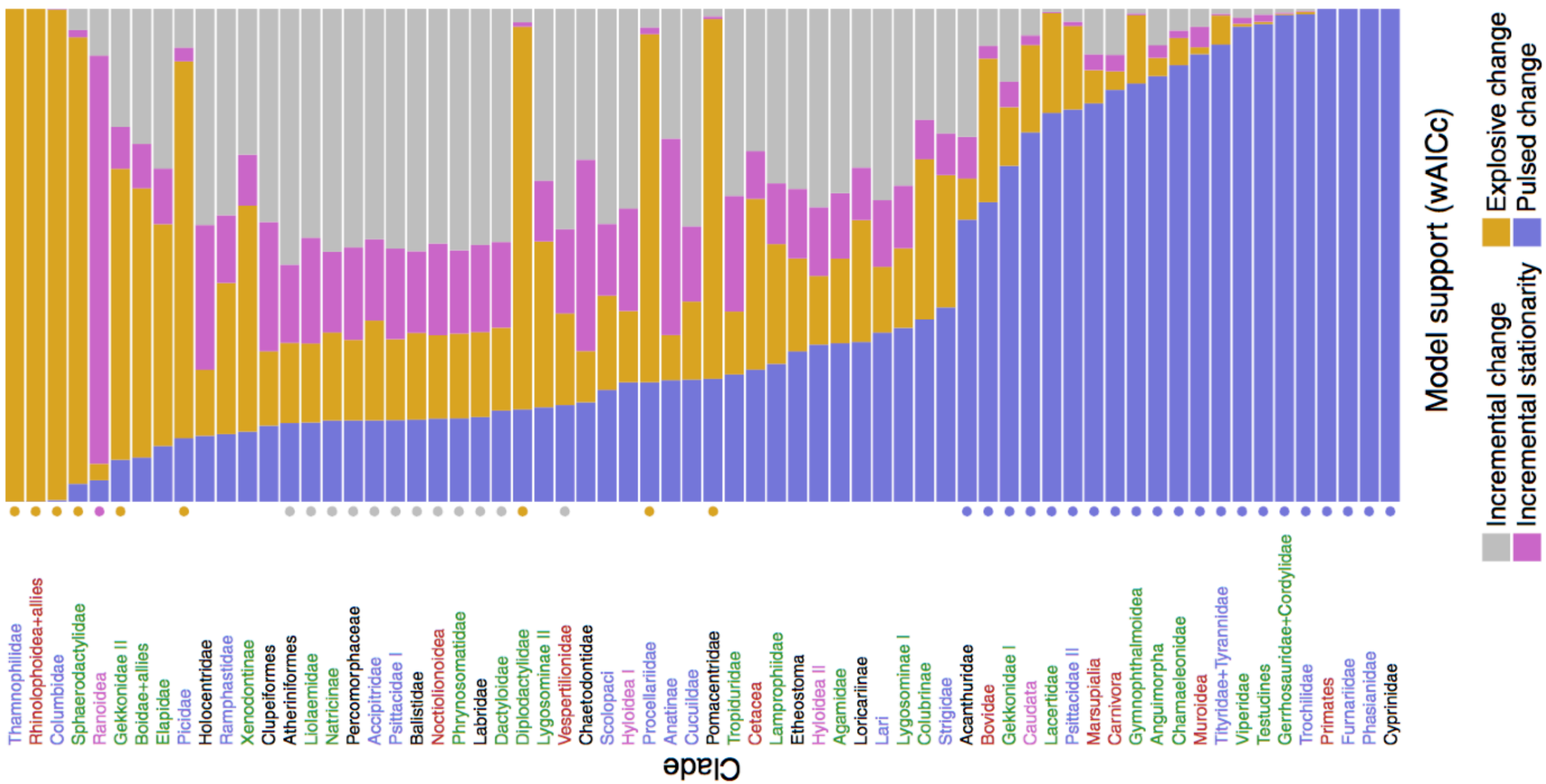
Exotic Diffusion Models

Jump-Normal (JN) model

Many sample paths under JN



Exotic Diffusion Models



Landis and Schraiber 2017

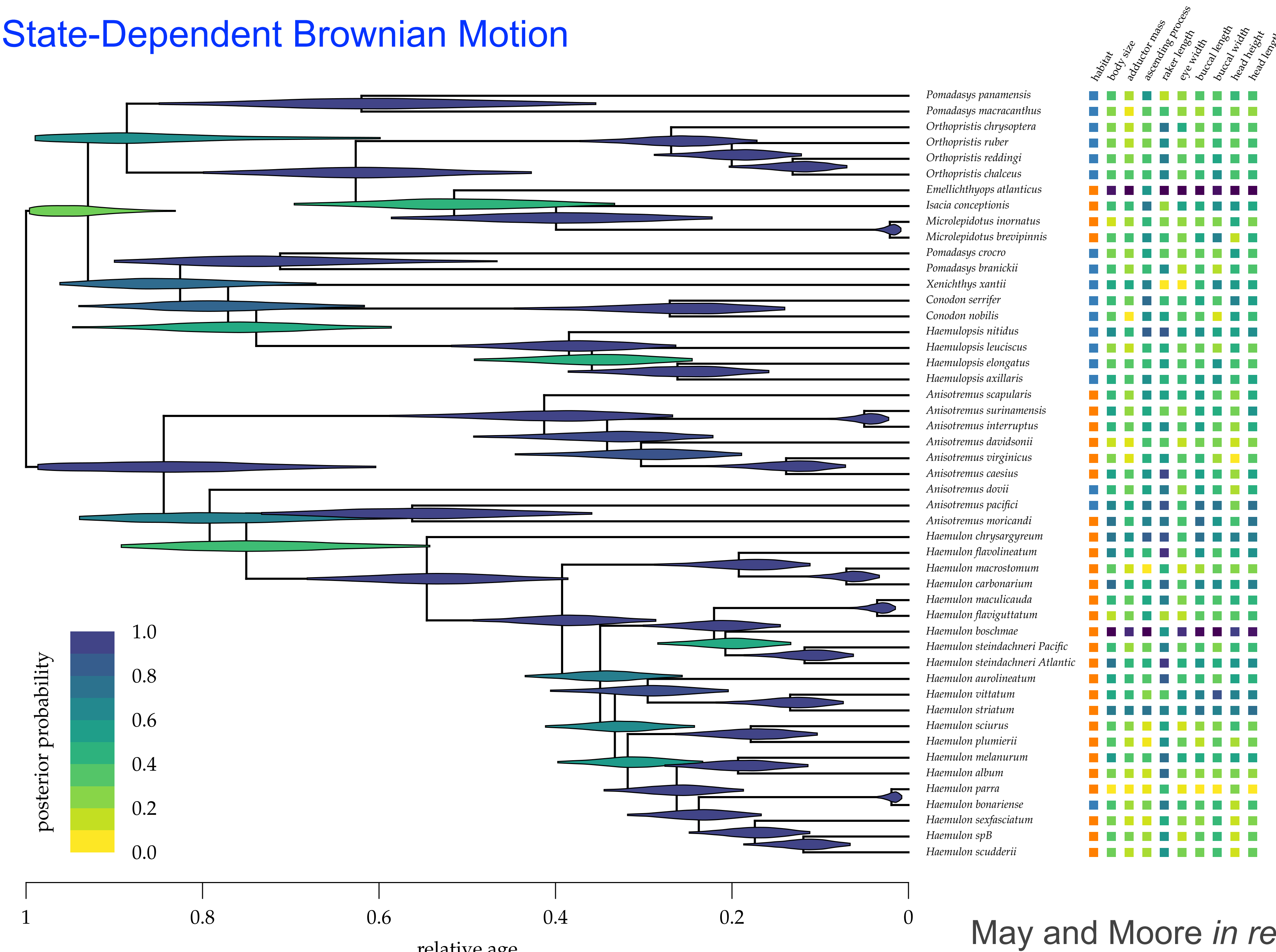
Exotic Diffusion Models

State-Dependent Brownian Motion

Sometimes we expect (or hypothesize) that rates of continuous-character evolution depend on the state of a discrete character.

Exotic Diffusion Models

State-Dependent Brownian Motion



May and Moore *in review*

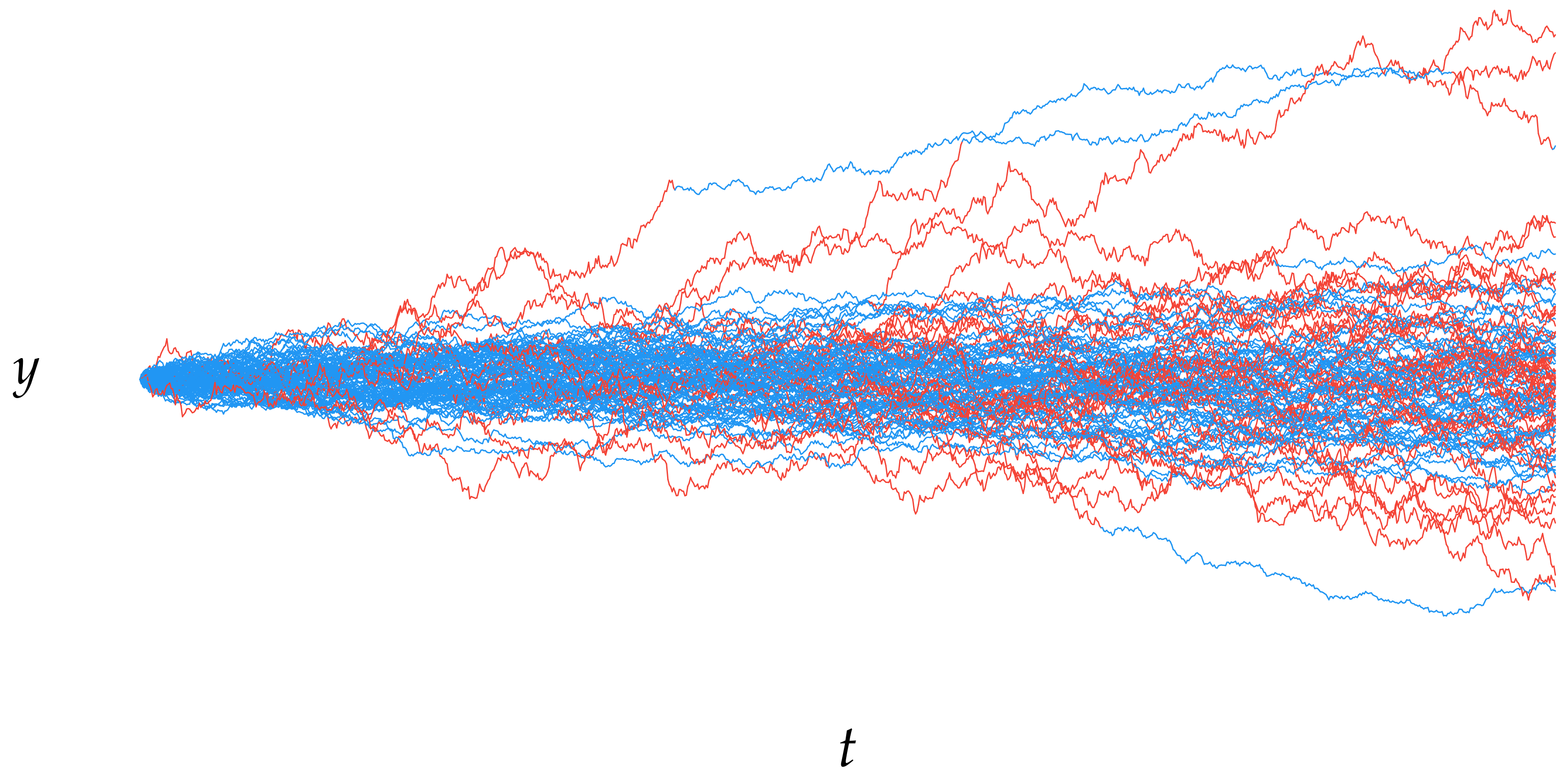
Exotic Diffusion Models

State-Dependent Brownian Motion

$X \in \{0, 1\}$	Binary discrete character
$q_{01},\ q_{10}$	Rates of change between discrete characters
$Y \in \mathbb{R}$	Continuous character
$\sigma_0^2,\ \sigma_1^2$	Rates of change for continuous character (depending on the state of the discrete character) under Brownian motion

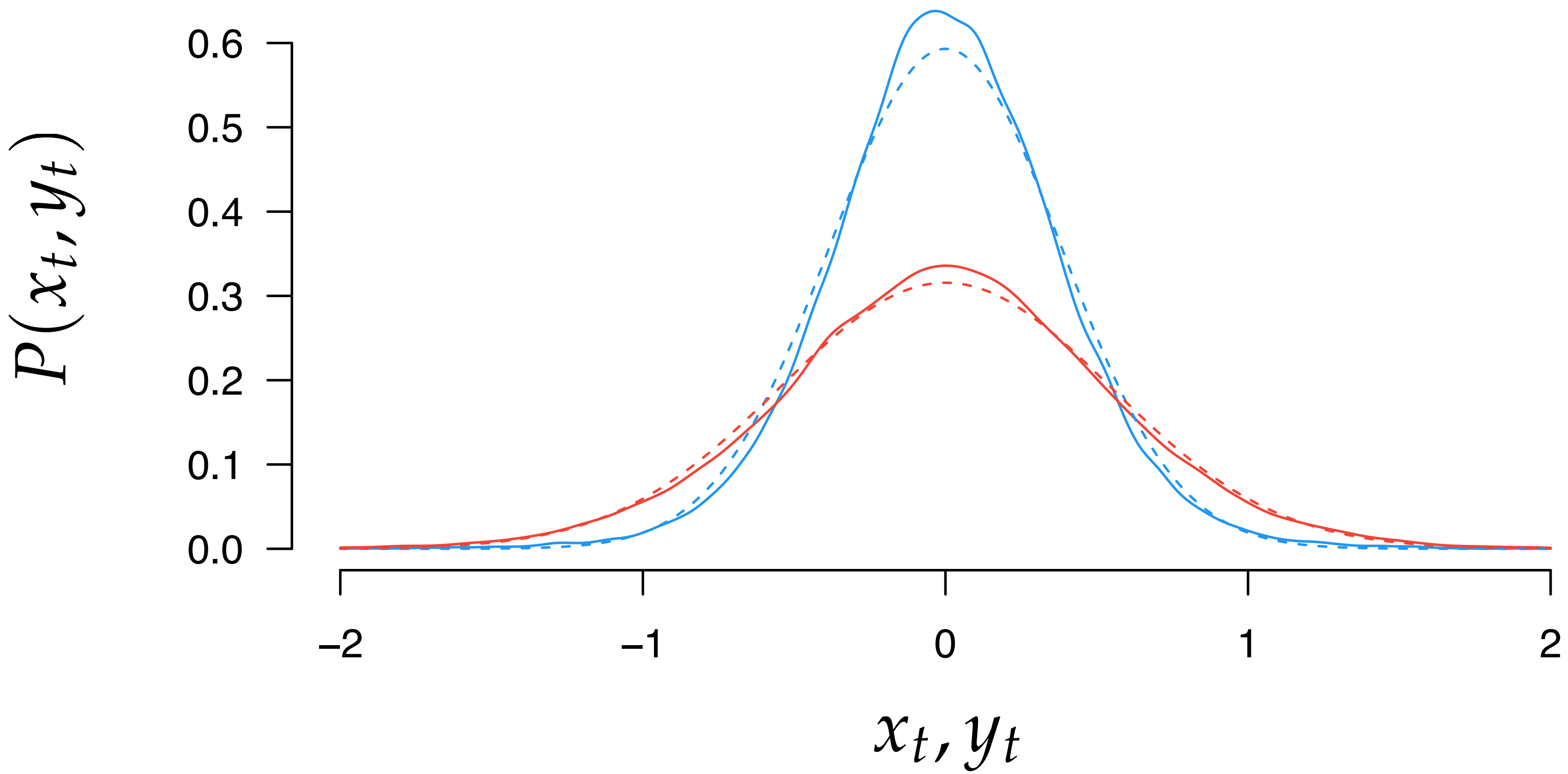
Exotic Diffusion Models

State-Dependent Brownian Motion



Exotic Diffusion Models

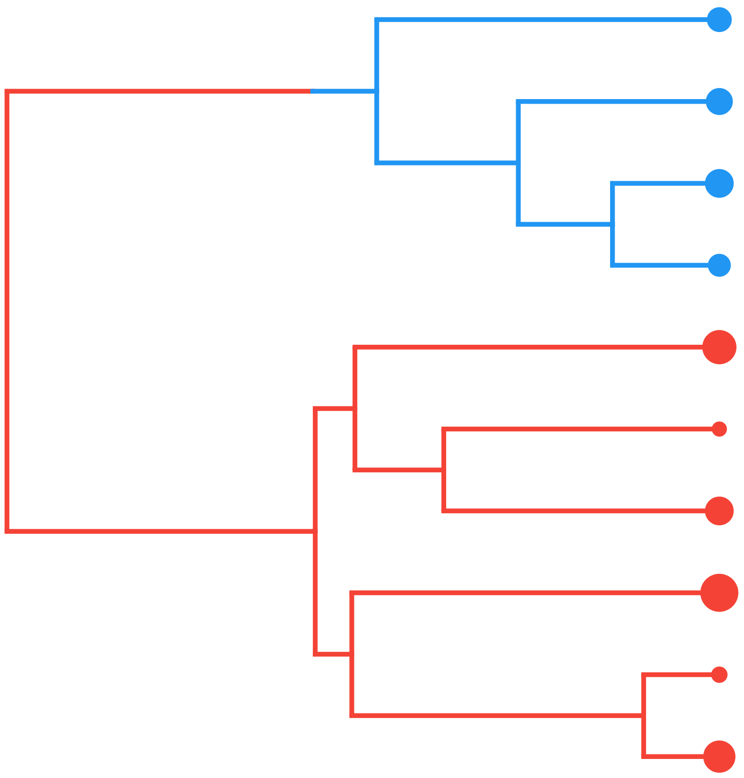
State-Dependent Brownian Motion



Exotic Diffusion Models

State-Dependent Brownian Motion

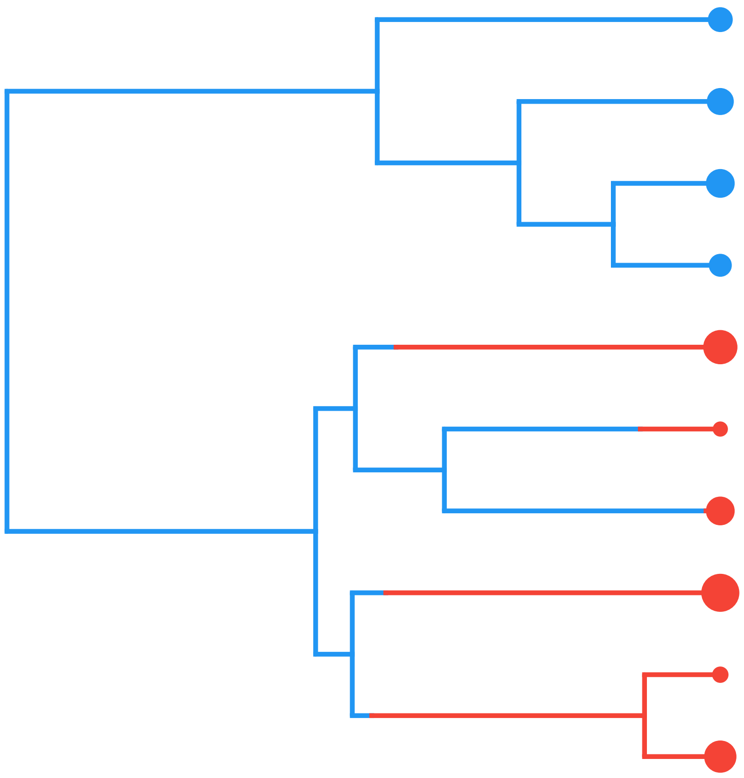
We can calculate the likelihood conditional on the complete history of the discrete character.



Exotic Diffusion Models

State-Dependent Brownian Motion

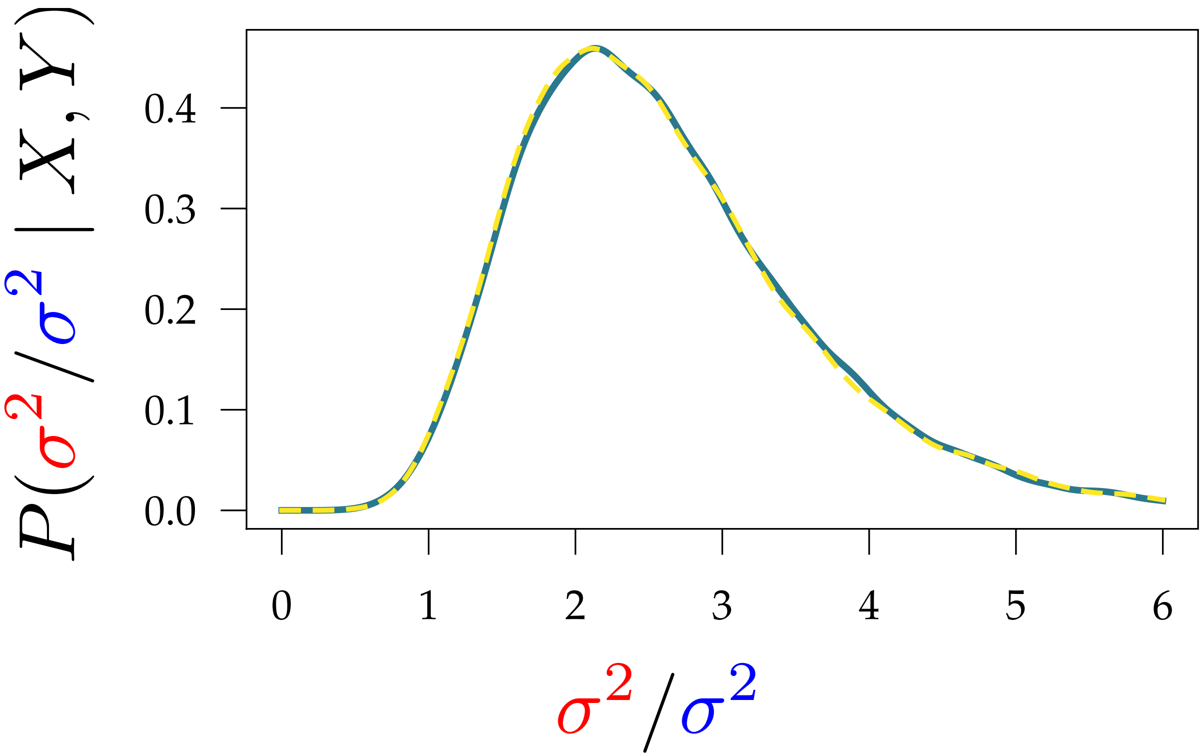
We integrate over all possible histories of the discrete character using a Bayesian technique called data augmentation.



Exotic Diffusion Models

State-Dependent Brownian Motion

We estimate the posterior distribution of the state-specific rate parameters.



May and Moore *in review*

Outline

I. Calculating likelihoods for continuous traits

A generic framework for calculating probabilities

II. A simple model of continuous-character evolution

Brownian motion model

Multivariate Brownian motion model

III. Exotic models of continuous-character evolution

Ornstein-Uhlenbeck model

Lévy models

State-dependent models