

A very small intro to CTMC in phylogenetics

Rosana Zenil-Ferguson, Will Freyman, and Jordan Koch

University of Minnesota

Botany 2018

In a Bayesian framework

We are always interested in knowing the **posterior distribution**

$$P(\theta|D) \propto P(D|\theta) P(\theta)$$

Example

$X(t)$ = Evolution of flower color at time changes according time t

Example

$X(t)$ = Evolution of flower color at time changes according time t

M is our Model (a.k.a.the hypothesis)

Red flowers evolve into purple and viceversa

$$\theta = (q_{BR}, q_{RB})$$

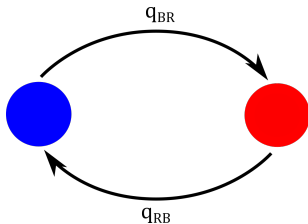
Example

$X(t)$ = Evolution of flower color at time changes according time t

M is our Model (a.k.a.the hypothesis)

Red flowers evolve into purple and viceversa

$$\theta = (q_{BR}, q_{RB})$$



The assumptions of our model in Bayesian framework

- ▶ In Bayesian framework: q_{BR} , and q_{RB} are **unknown and random variables** (they have a probability)

The assumptions of our model in Bayesian framework

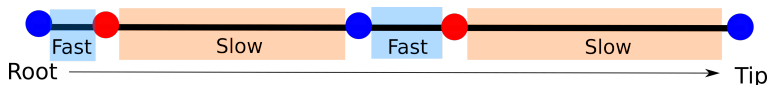
- ▶ In Bayesian framework: q_{BR} , and q_{RB} are **unknown and random variables** (they have a probability)
- ▶ q_{BR} and q_{RB} are **instantaneous rates**.


The assumptions of our model in Bayesian framework


- ▶ In Bayesian framework: q_{BR} , and q_{RB} are **unknown and random variables** (they have a probability)
- ▶ q_{BR} and q_{RB} are **instantaneous rates**.

The assumptions of our model in Bayesian framework

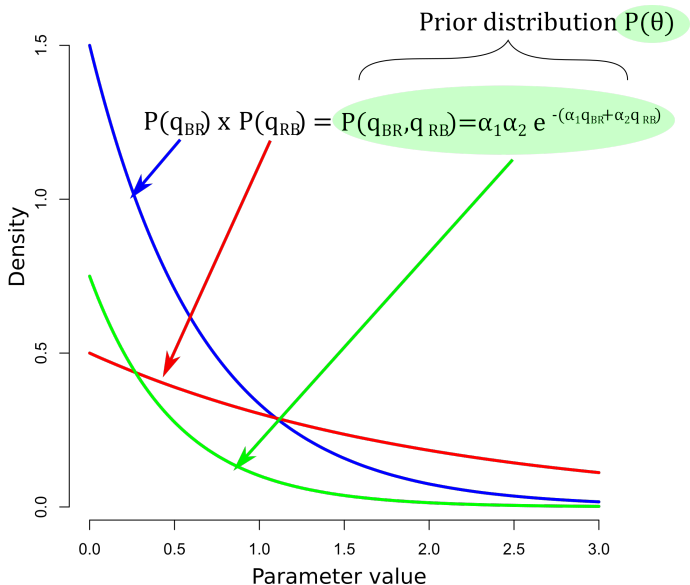
- ▶ In Bayesian framework: q_{BR} , and q_{RB} are **unknown and random variables** (they have a probability)
- ▶ q_{BR} and q_{RB} are **instantaneous rates**.



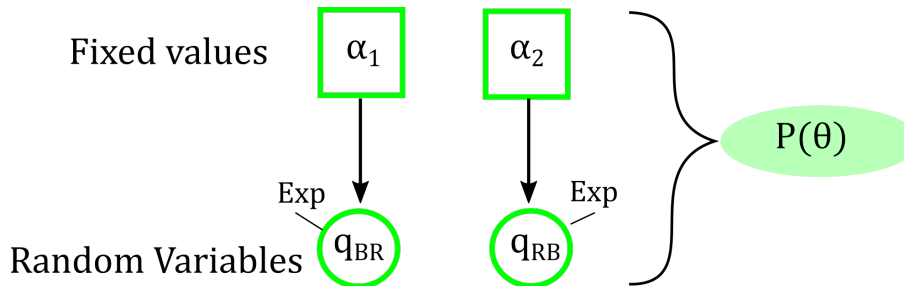
 Sojourn times from B to BR $\sim \text{Exp}(q_{BR})$,

 Sojourn times from R to B $\sim \text{Exp}(q_{RB})$,

The prior distribution: $P(\theta)$



How are these assumptions represented graphically?



D is our data

We go into our favorite herbarium, field site, or green house and we collect color of multiple species

How do we integrate our model θ and our data D ?

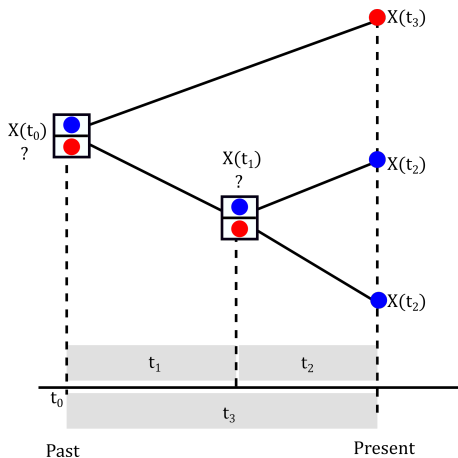
Calculating the likelihood $P(D|\theta)$

- ▶ We assume a phylogenetic tree Ψ (for this example is fixed)

Calculating the likelihood $P(D|\theta)$

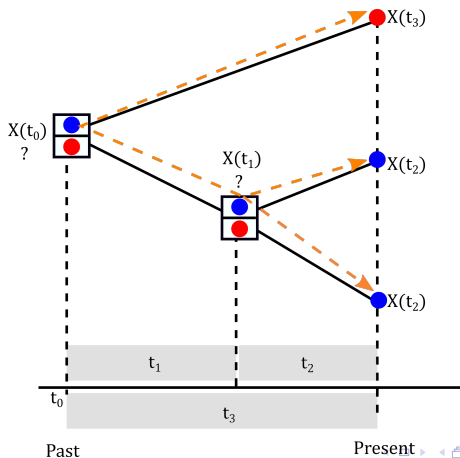
- ▶ We assume a phylogenetic tree Ψ (for this example is fixed)
- ▶ **Data:** a sample of red and purple flowers on the tips of our phylogeny tree

Likelihood function: The probability of the sample given our hypothesis θ



The probability of a single possible story in phylogenetics

$$P(X(t_2) = B|X(t_1) = B)P(X(t_2) = B|X(t_1) = B) \times \\ \times P(X(t_1) = B|X(t_0) = B)P(X(t_3) = R|X(t_0) = B)P(X(t_0) = B)$$



Calculating the likelihood is computationally challenging

- ▶ Felsenstein (1981)= Pruning algorithm, reduces the complexity in the calculation.

Calculating the likelihood is computationally challenging

- ▶ Felsenstein (1981)= Pruning algorithm, reduces the complexity in the calculation.
- ▶ Reminder: Optimizations to find maximum likelihood estimates and confident intervals require challenging numerical algorithms

How do the rates connect with the probabilities?

Q-matrix= The infinitesimal probability matrix is the derivative of the probability

$$\frac{dP(t)}{dt} = Q$$

$$Q = \begin{matrix} & \bullet & \bullet \\ \bullet & \begin{pmatrix} -q_{BR} & q_{BR} \\ q_{RB} & -q_{RB} \end{pmatrix} & \\ \bullet & & \end{matrix} \quad P(t) = e^{Qt}$$

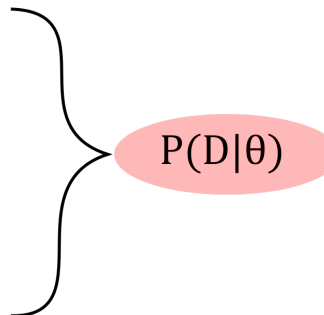
Likelihood in graphical form $P(D|\theta)$

Fixed value

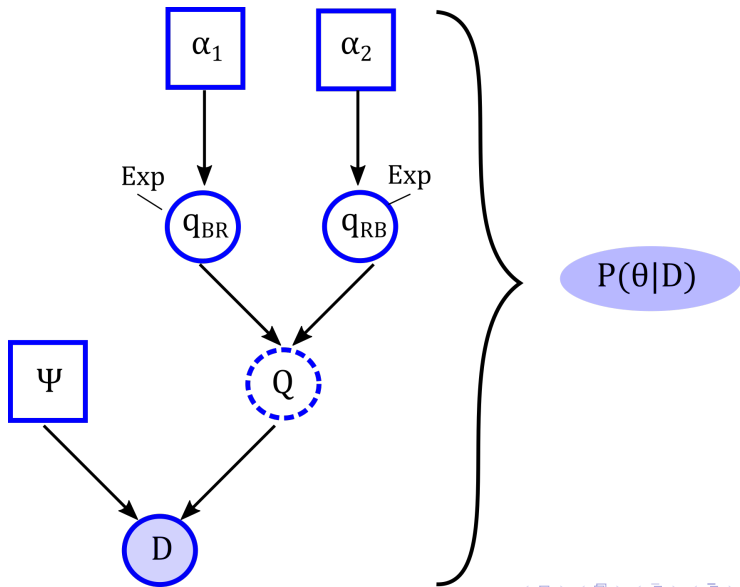
Function calculated from r.v.



Evaluate in observed data.



The posterior distribution: the model conditional to the observed data



- ▶ **Explicit notation:** In RevBayes we have notation for fixed variables, random variables, observed data, deterministic function,...

Graphical model benefits

- ▶ **Explicit notation:** In RevBayes we have notation for fixed variables, random variables, observed data, deterministic function,...
- ▶ **Modularity:** Once I have built a model I can connect other as a module (building blocks!)