
Lecture 2.2

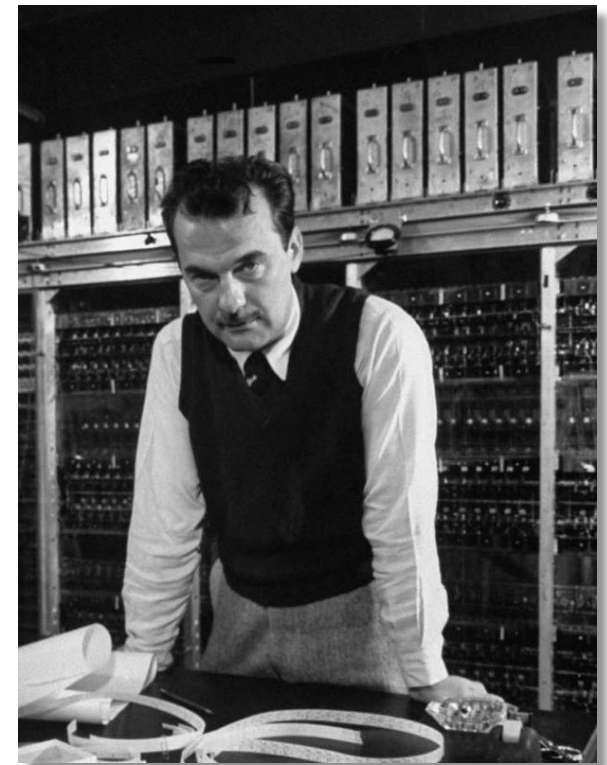
MCMC Sampling

Posterior Distribution

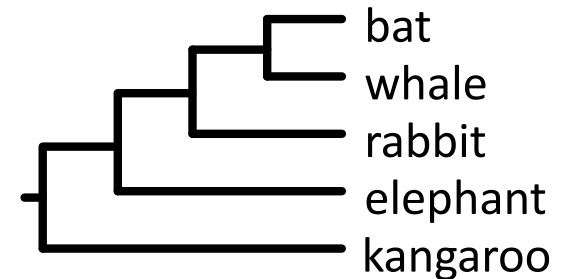
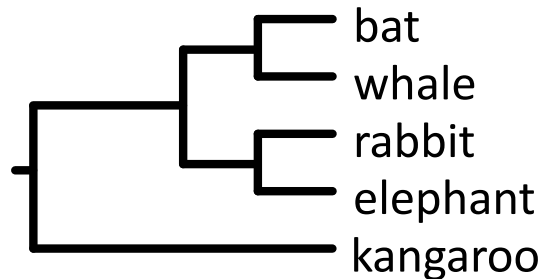
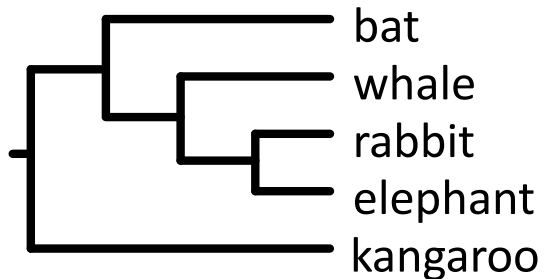
Estimating the posterior

- Impossible to obtain the posterior directly
- Instead, the posterior can be estimated using **Markov chain Monte Carlo simulation**
- This is usually done using the **Metropolis-Hastings algorithm**

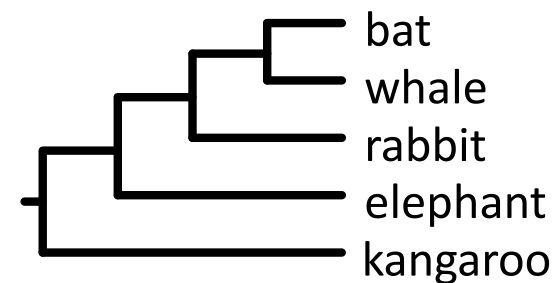
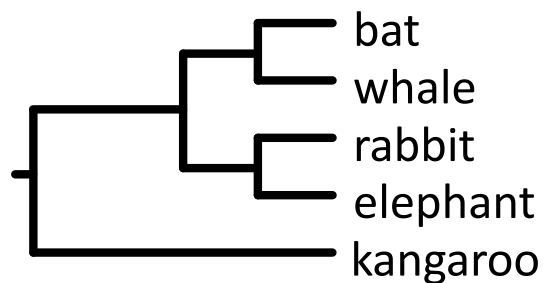
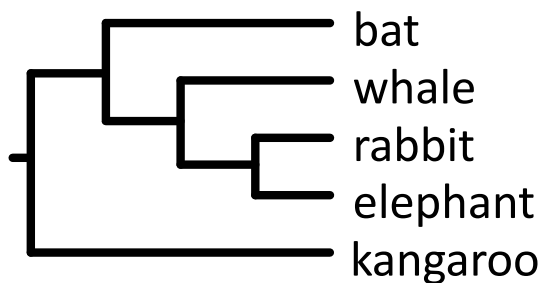
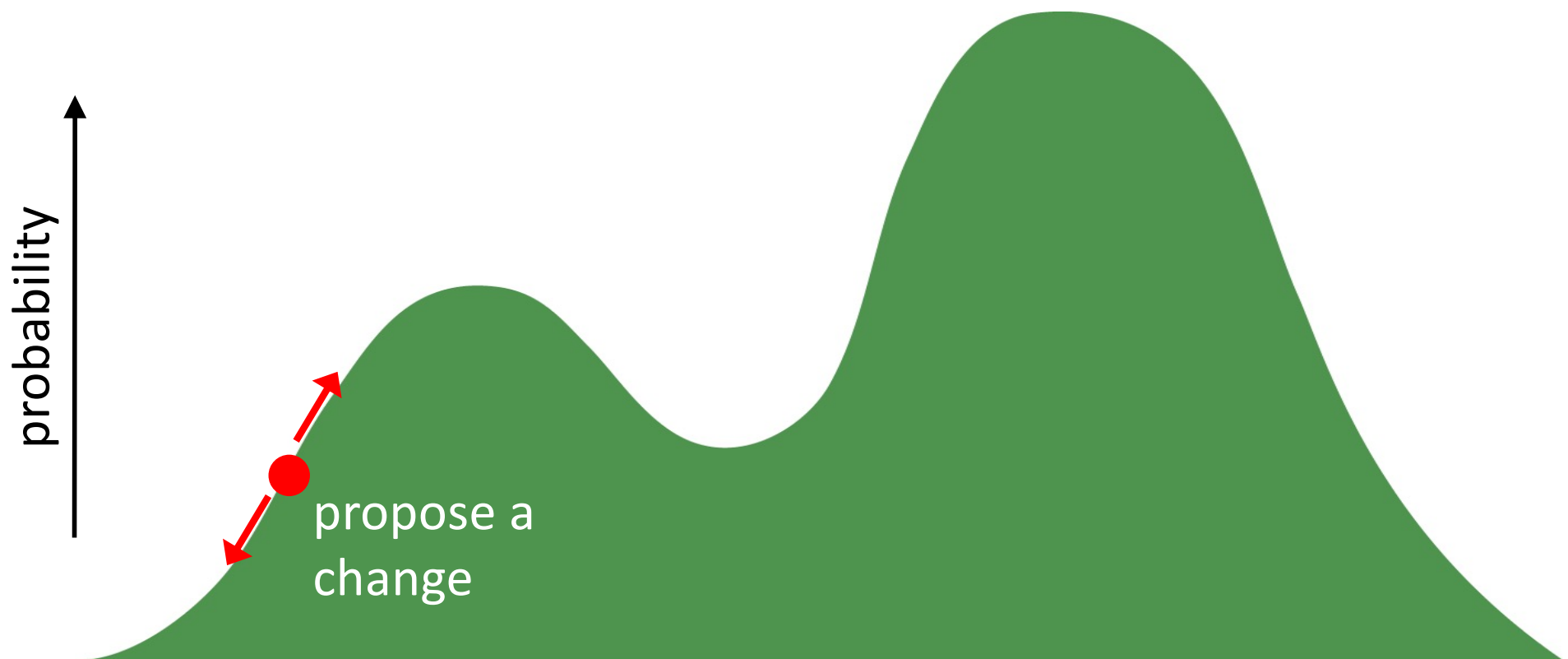
Nicholas Metropolis
Los Alamos, 1953



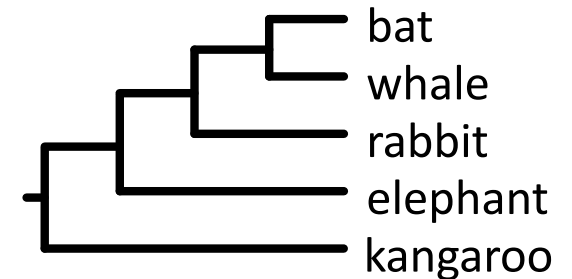
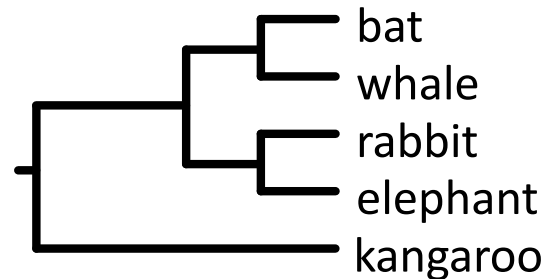
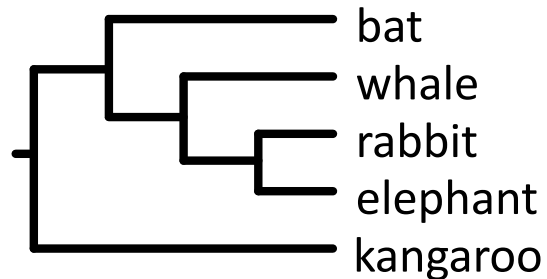
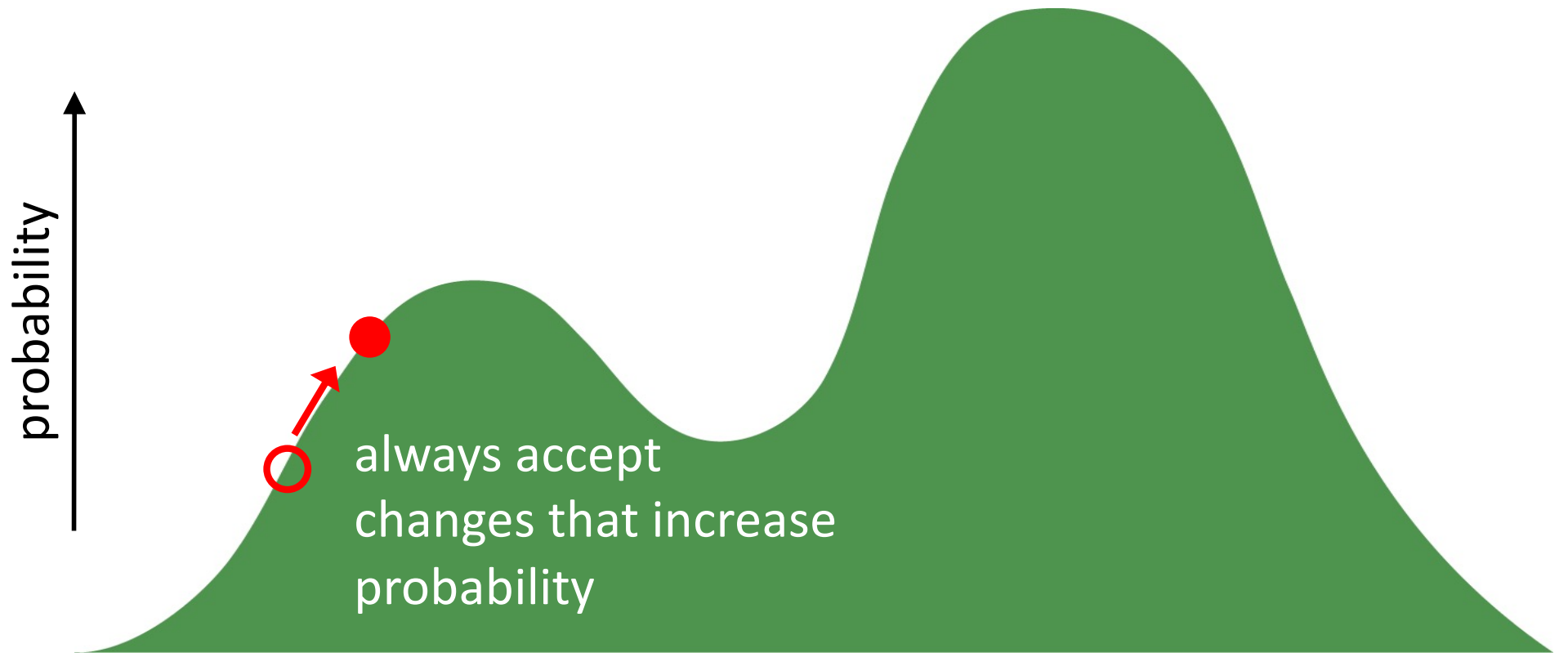
MCMC simulation



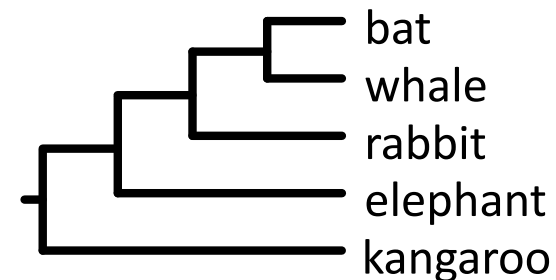
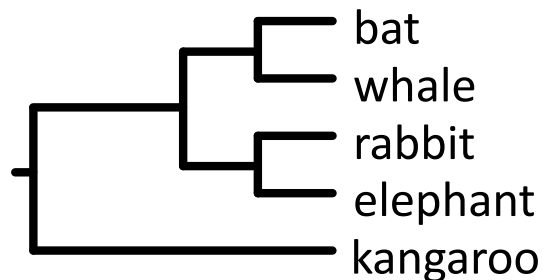
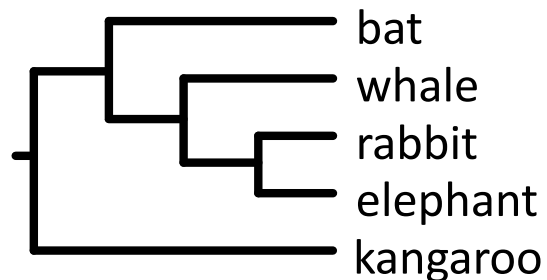
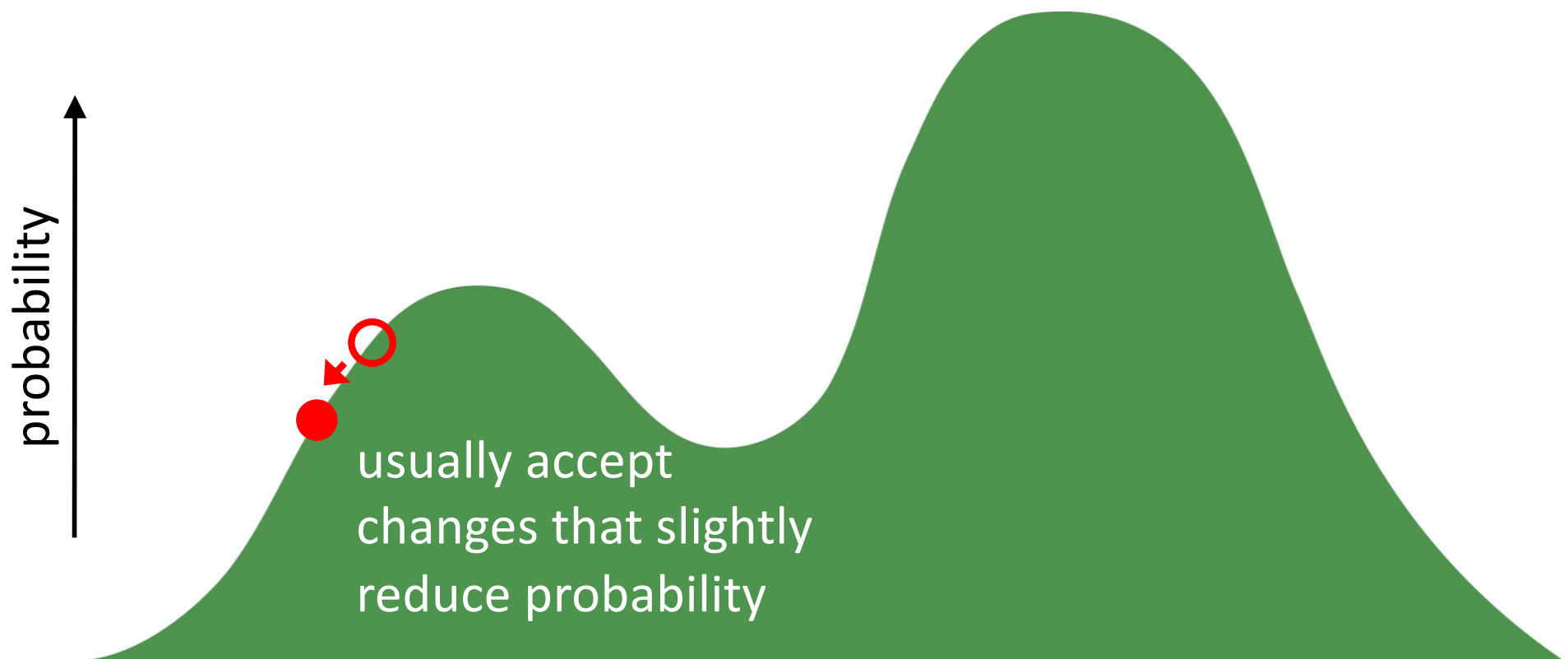
MCMC simulation



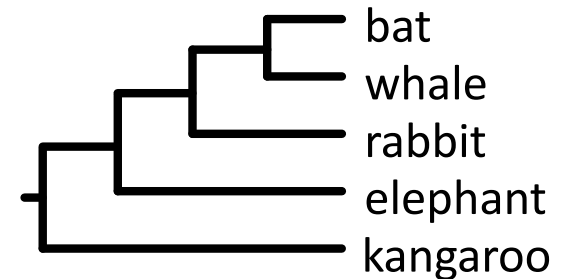
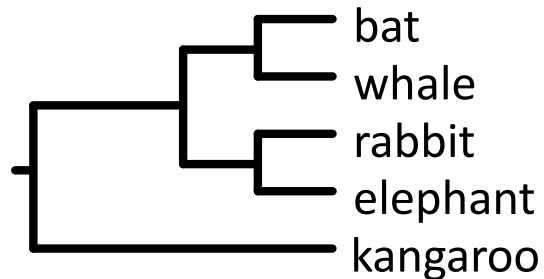
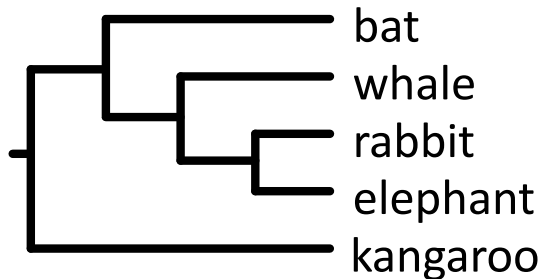
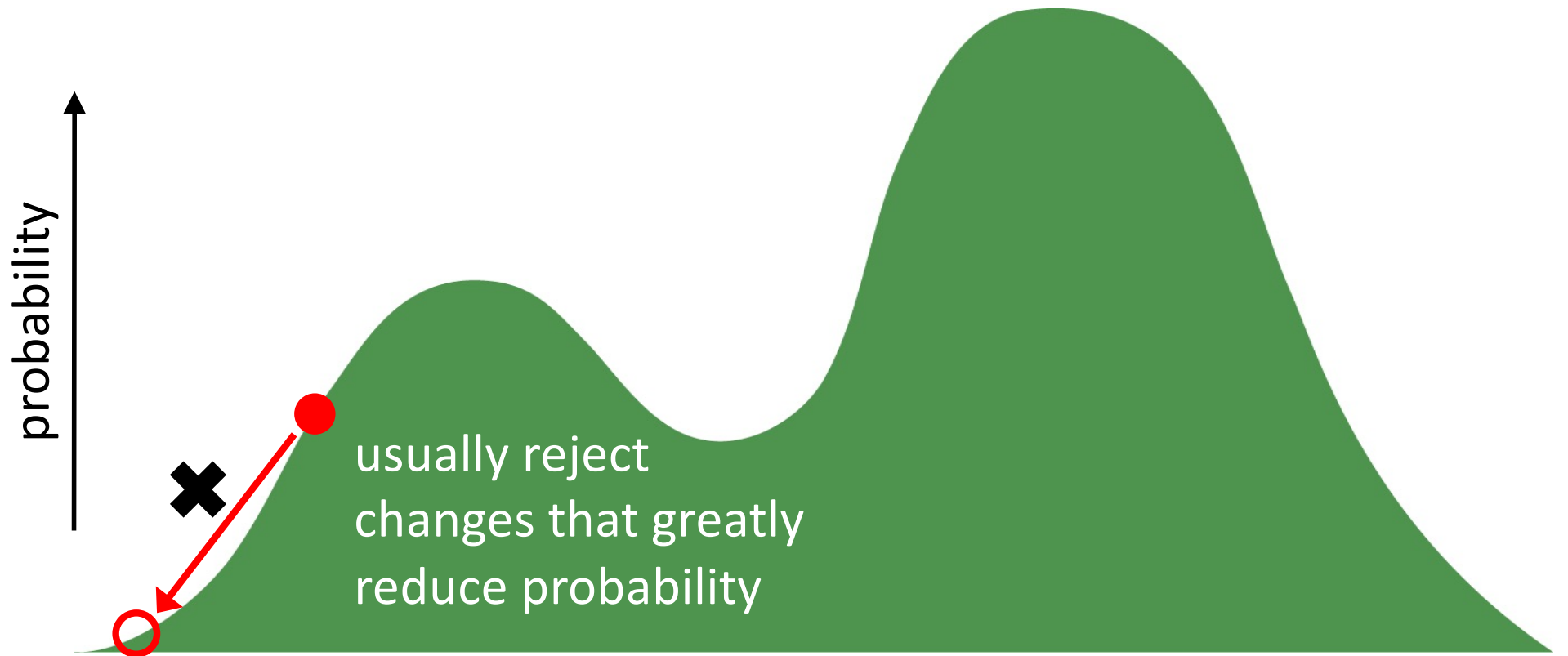
MCMC simulation



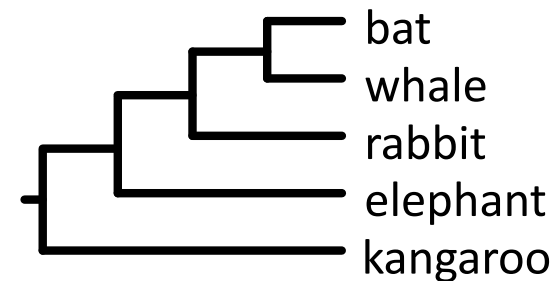
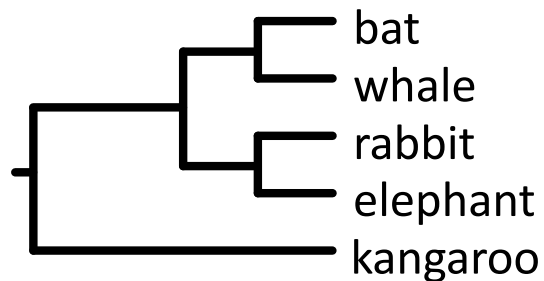
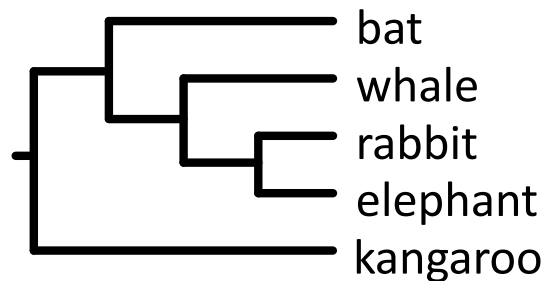
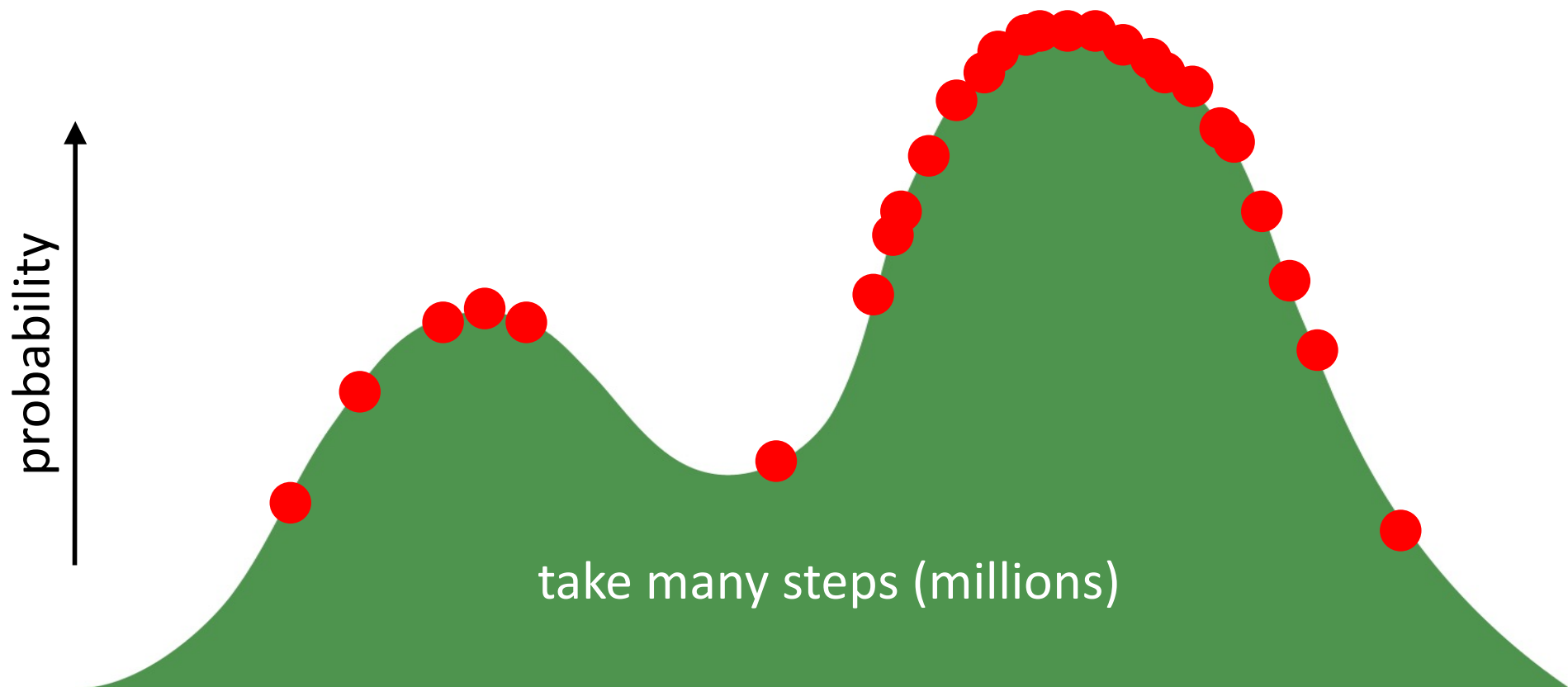
MCMC simulation



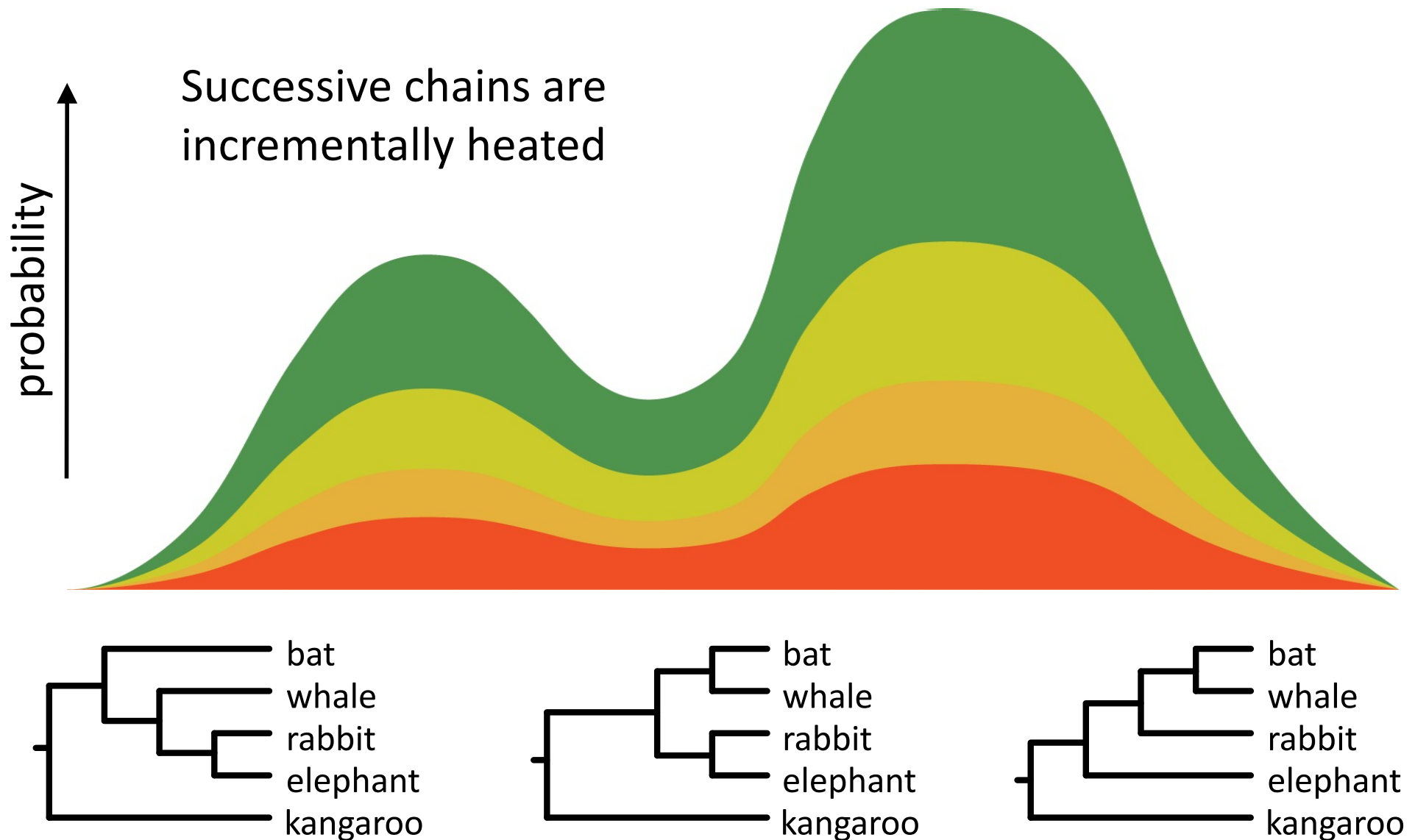
MCMC simulation



MCMC simulation



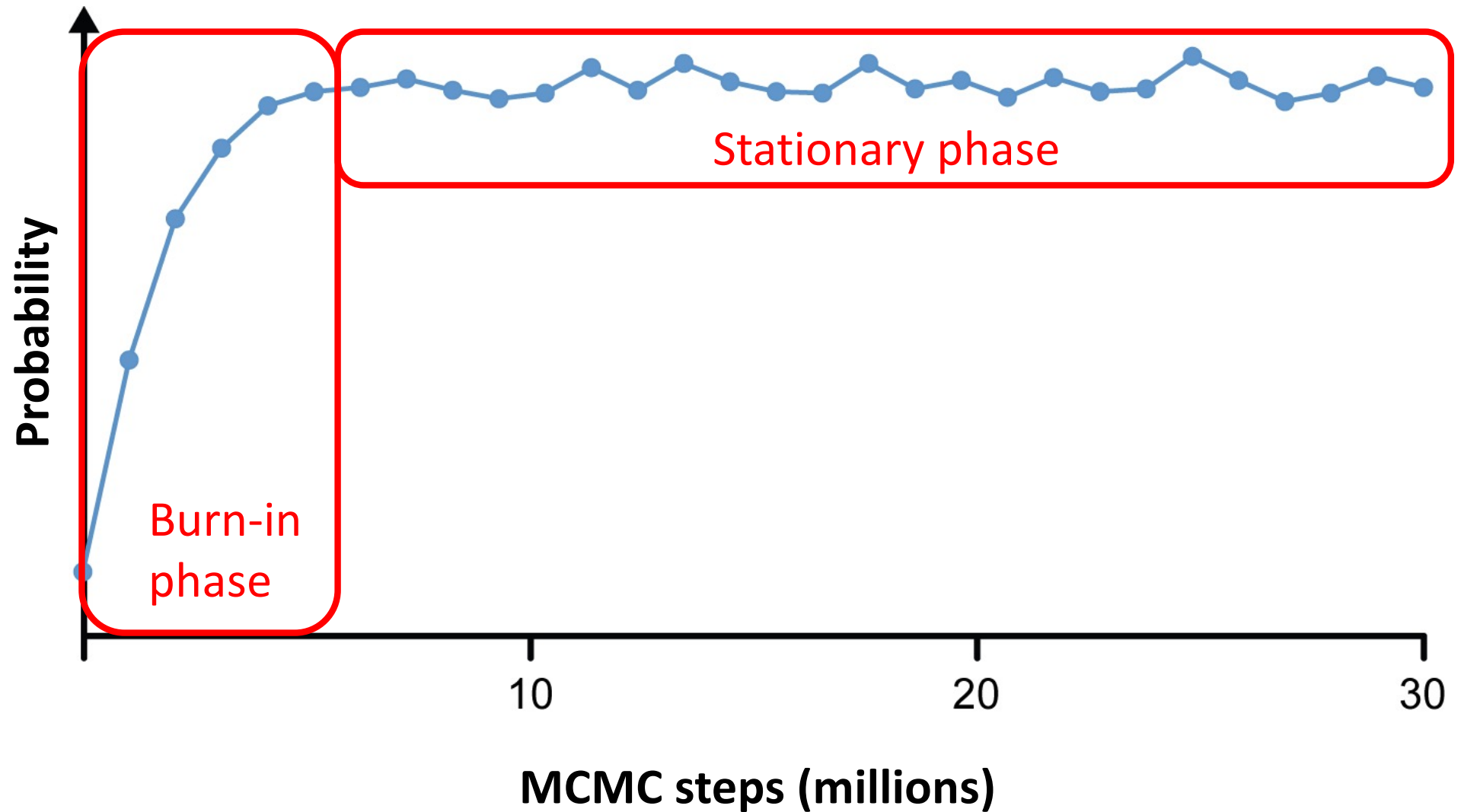
Metropolis-coupled MCMC



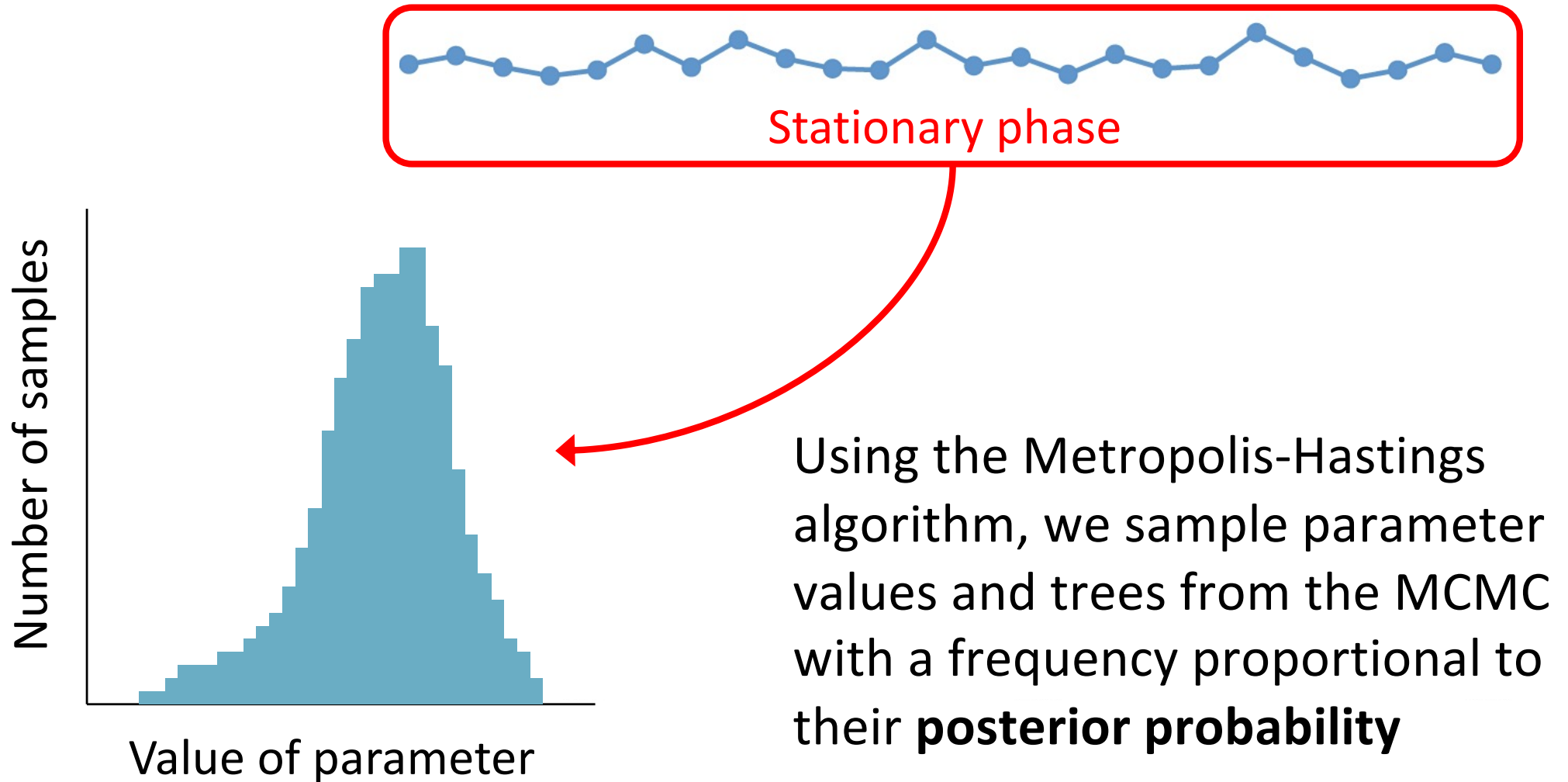
Samples from the MCMC

- Output from a Bayesian phylogenetic analysis:
 - A list of the **parameter values** visited by the Markov chain
(.p file in *MrBayes*, .log file in *BEAST*)
 - A list of the **trees** visited by the Markov chain
(.t file in *MrBayes*, .trees file in *BEAST*)

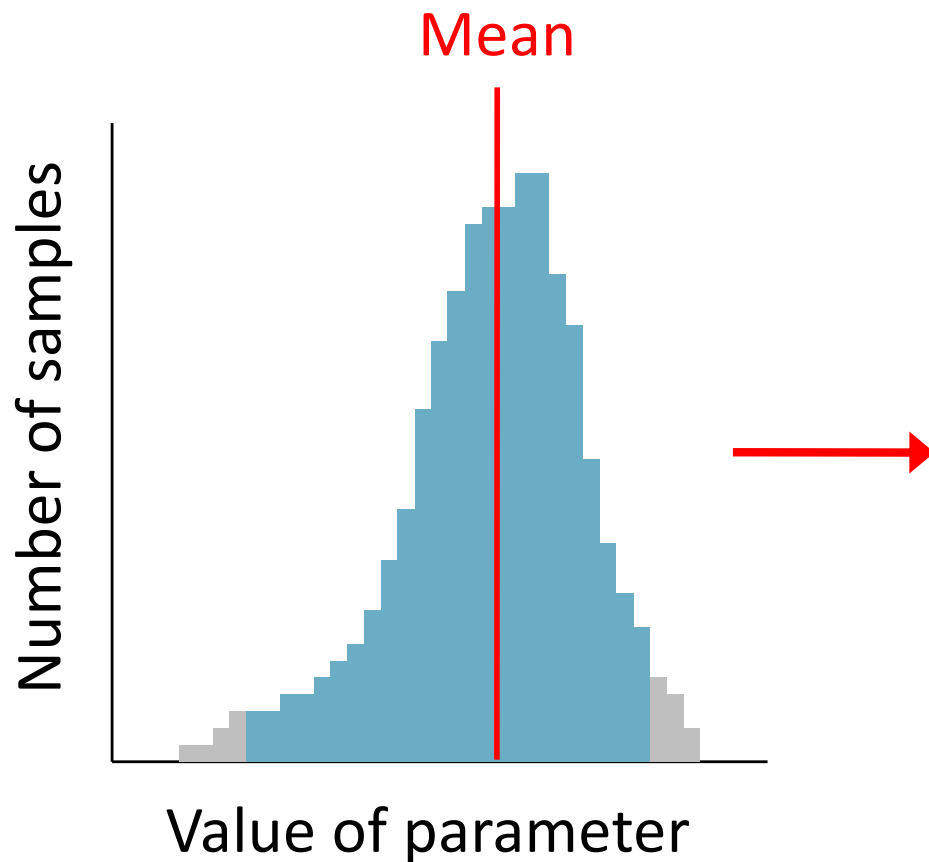
Samples from the MCMC



Samples from the MCMC



Samples from the MCMC



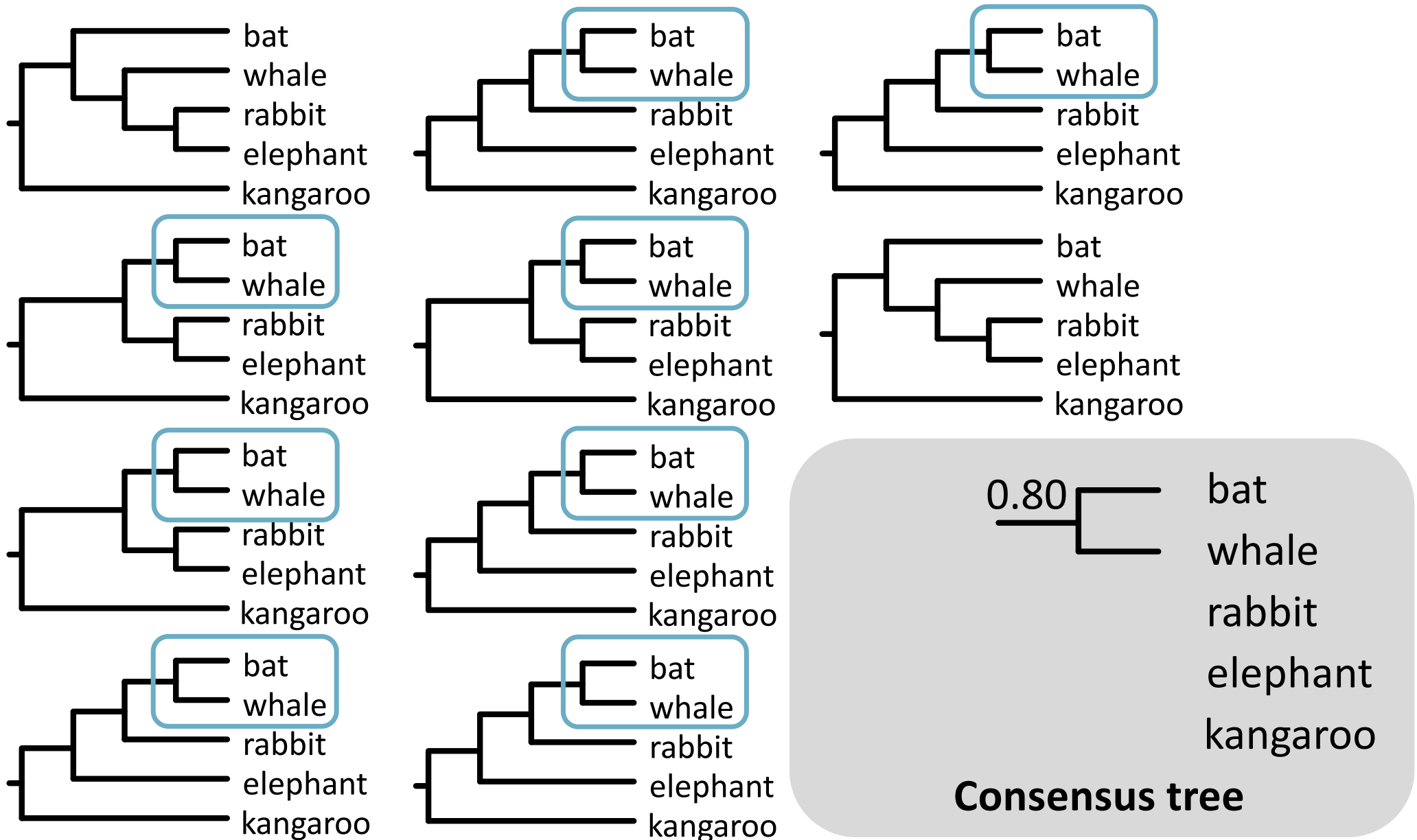
- Take the mean of the sampled values

Mean posterior estimate

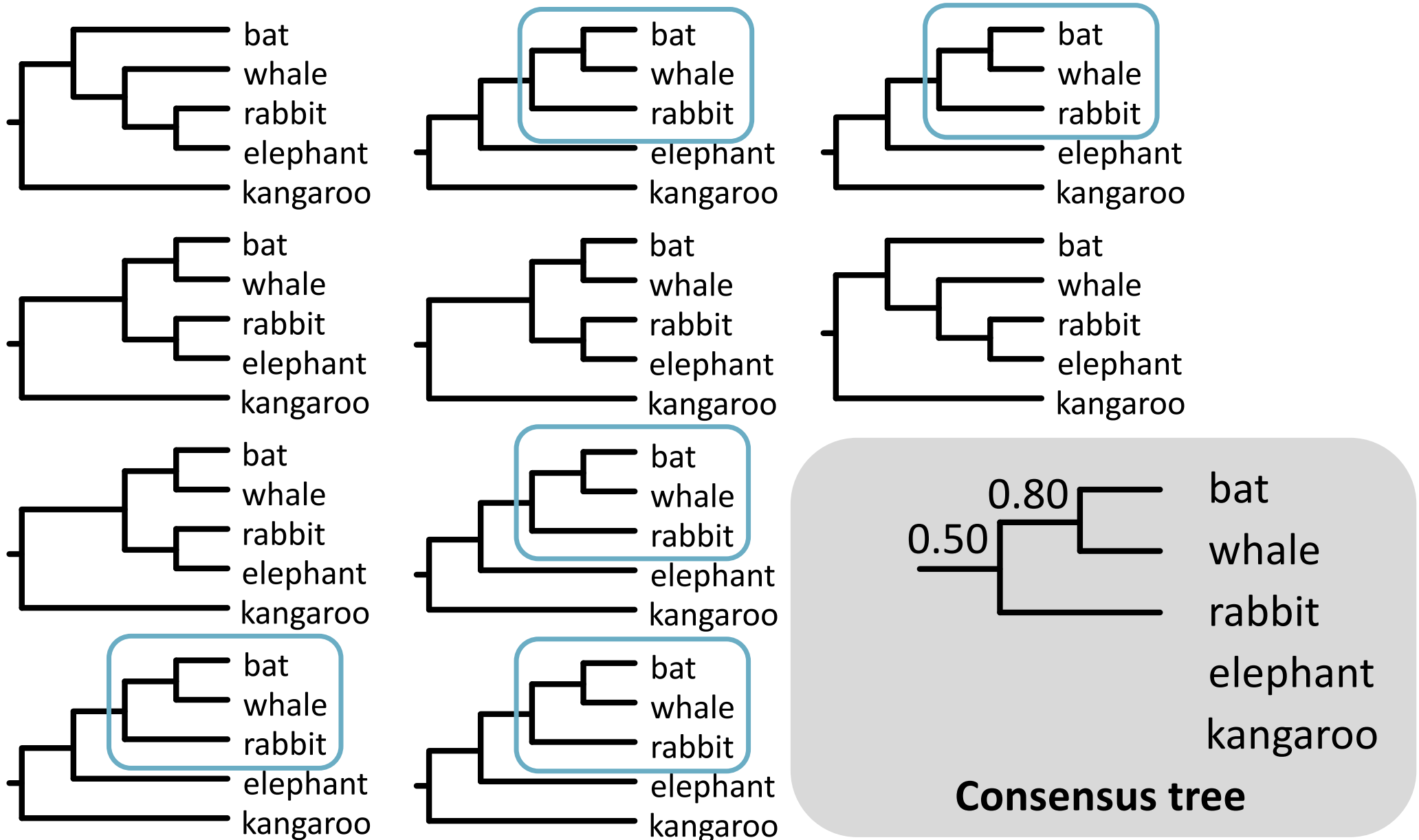
- Take the 'central' 95% of the sampled values

95% credibility interval

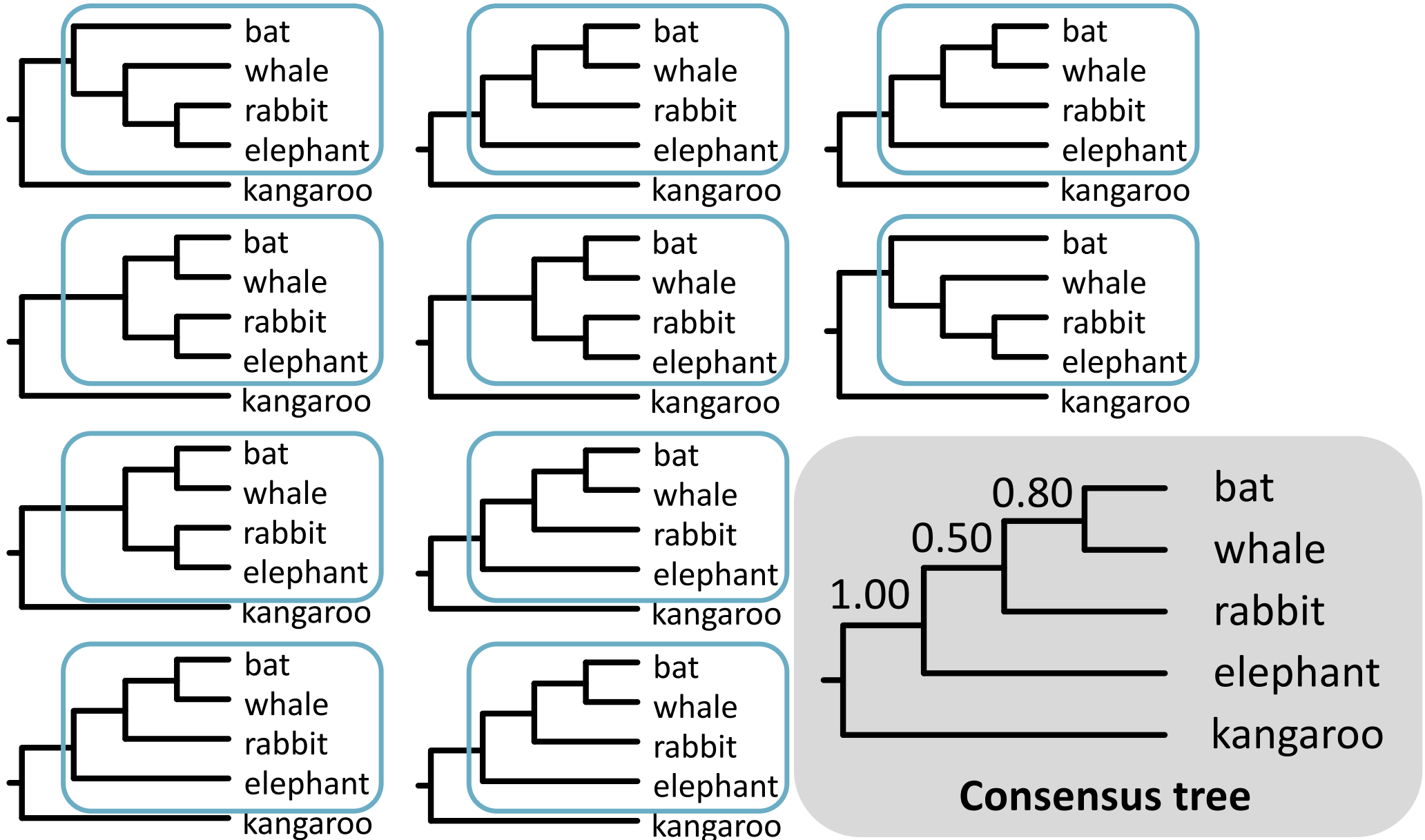
Samples from the MCMC



Samples from the MCMC



Samples from the MCMC



Samples from the MCMC

- **Majority-rule consensus tree (*MrBayes*)**
Shows all nodes with posterior probability >0.50
- **Maximum a posteriori (MAP) tree**
Sampled tree with highest posterior probability
- **Maximum clade credibility (MCC) tree (*BEAST/TreeAnnotator*)**
Sampled tree with highest sum or product of posterior node probabilities

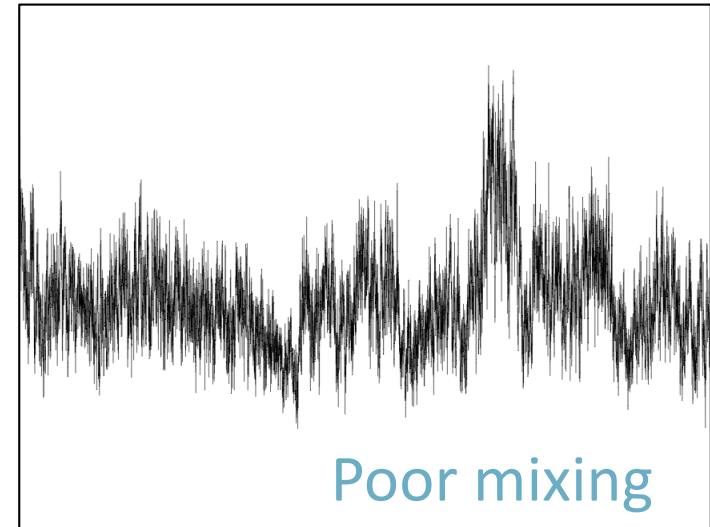
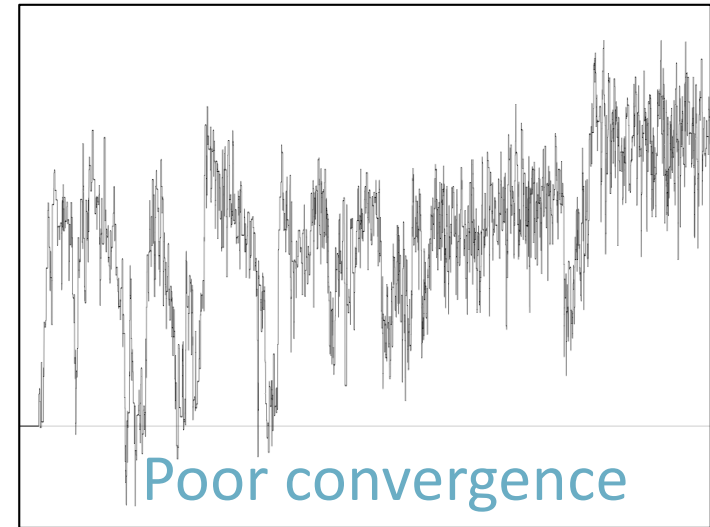
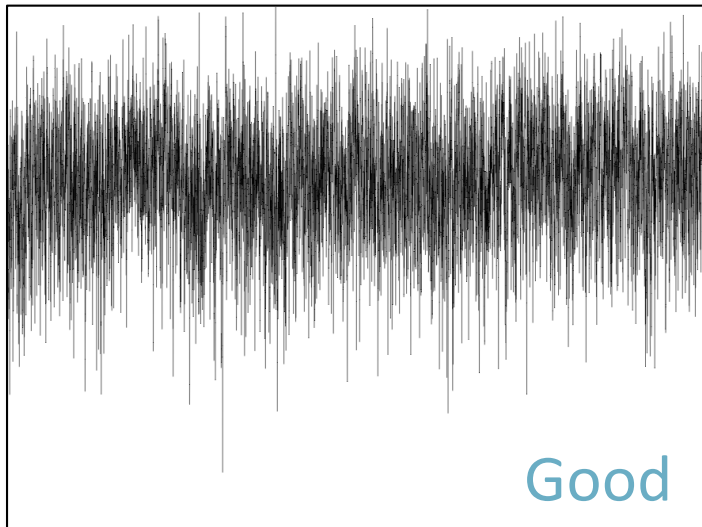
Diagnostics

1. Convergence

Are we drawing samples from the stationary distribution?

2. Sufficient sampling

Have we drawn enough samples to allow a reliable estimate of the posterior distribution?



Convergence

- Run at least 2 independent chains
- Likelihoods should be similar
- Estimates of model parameters should be similar

Sufficient sampling

- **Effective sample size (ESS)**

Have we drawn enough independent samples to produce a reliable estimate of the posterior distribution?

- ESS is preferably **>200** for each parameter
- ESS can be increased by:
 - Increasing the length of the MCMC
(and decreasing the frequency of sampling)
 - Modifying the MCMC proposals

Advantages and Problems

Advantages

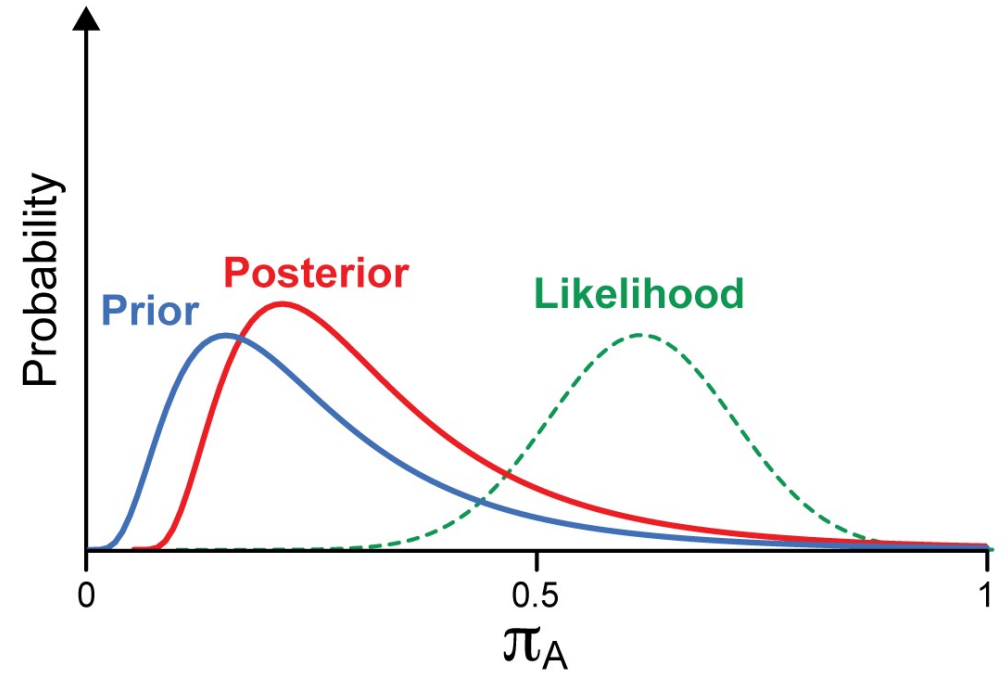
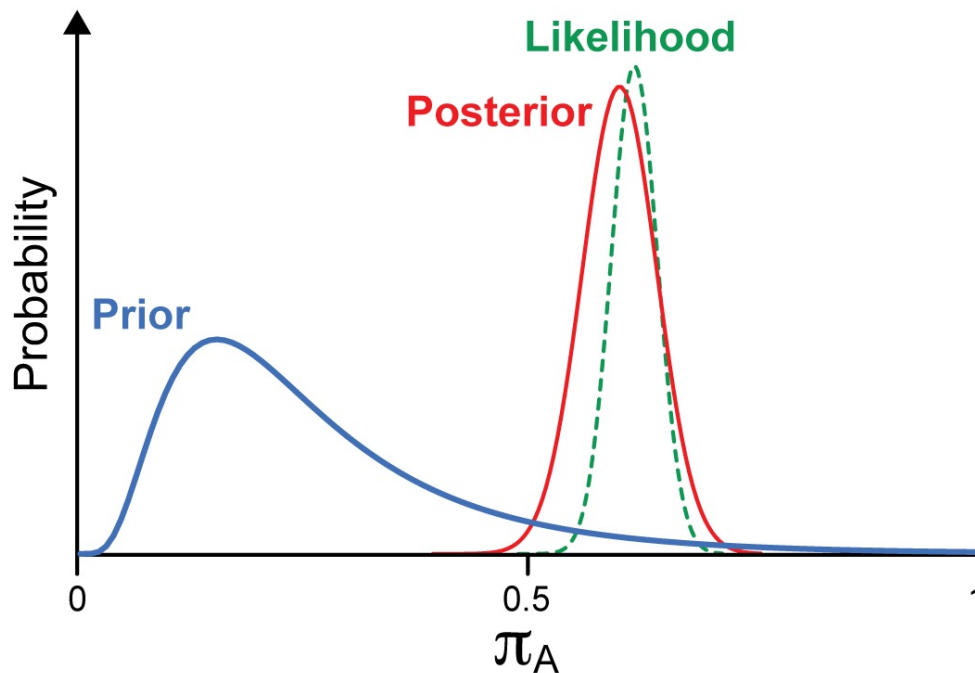
- Able to **implement complex (highly parameterised) models**
- **Estimating node support** is straightforward
- **Posterior probabilities** have an intuitive interpretation
- Can incorporate **independent information** (in the prior)

Nuisance parameters

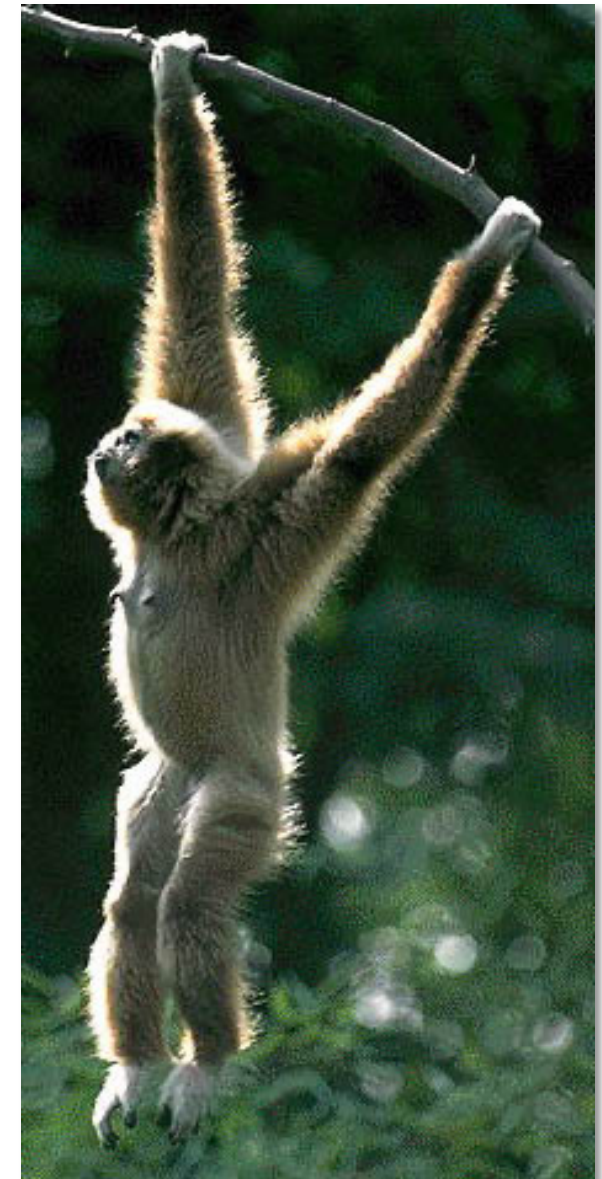
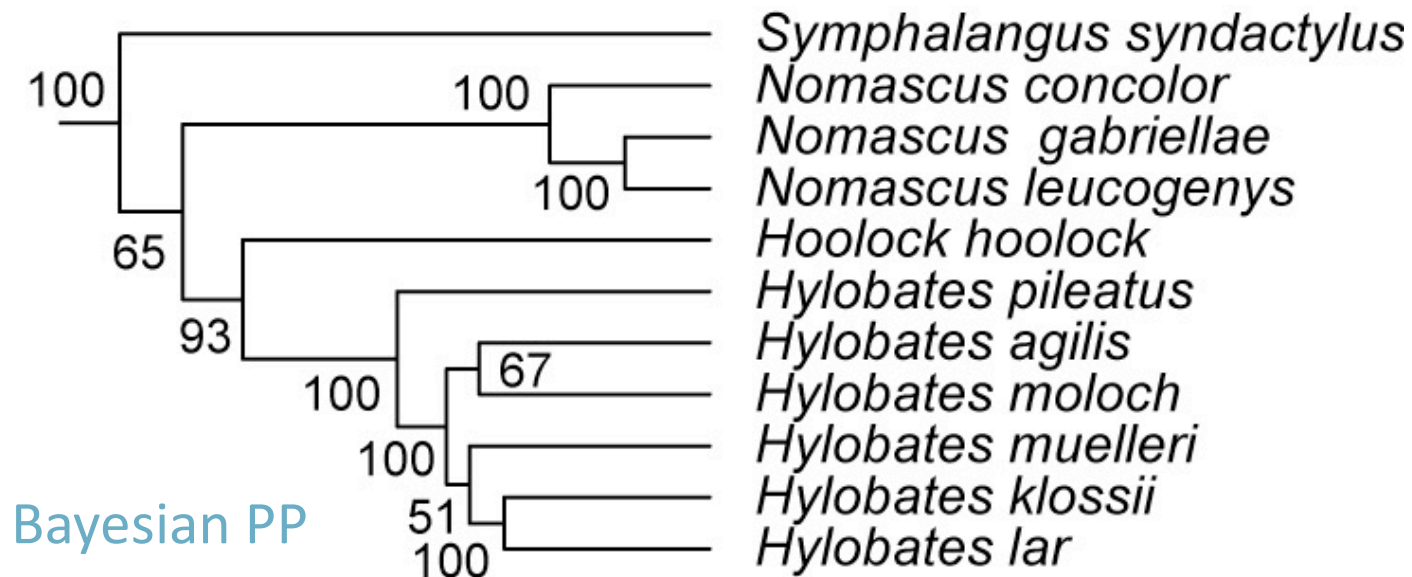
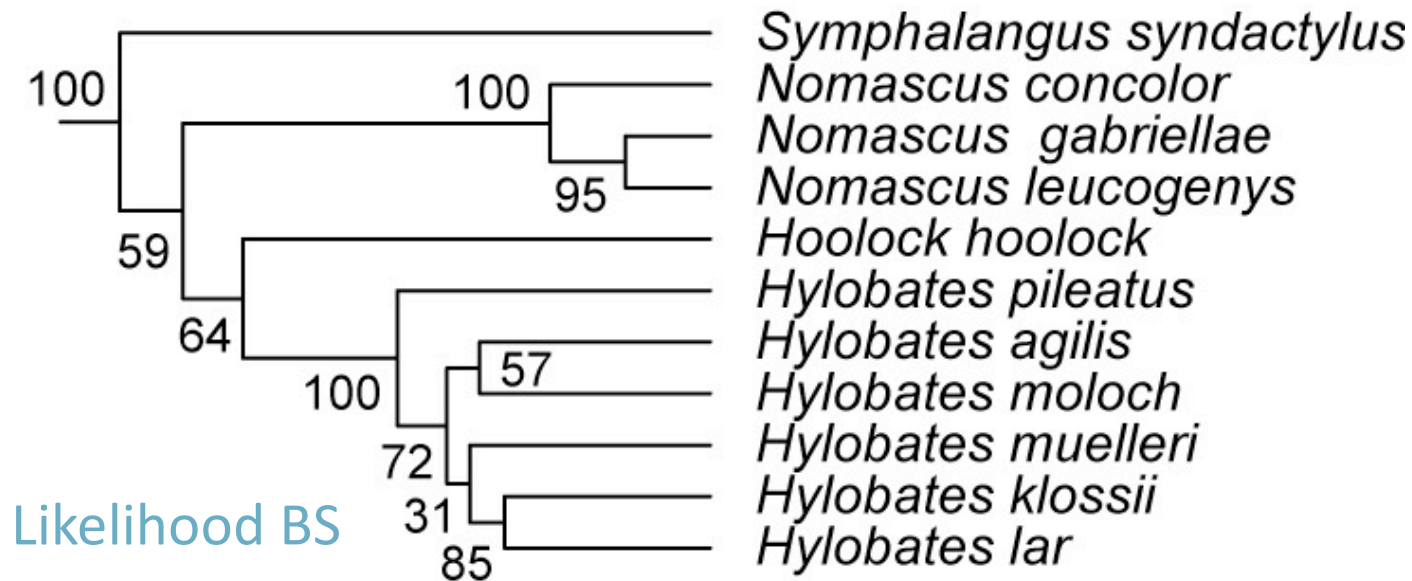
- Integrate over 'nuisance' parameters
- Marginal distribution of a parameter of interest

Influence of priors

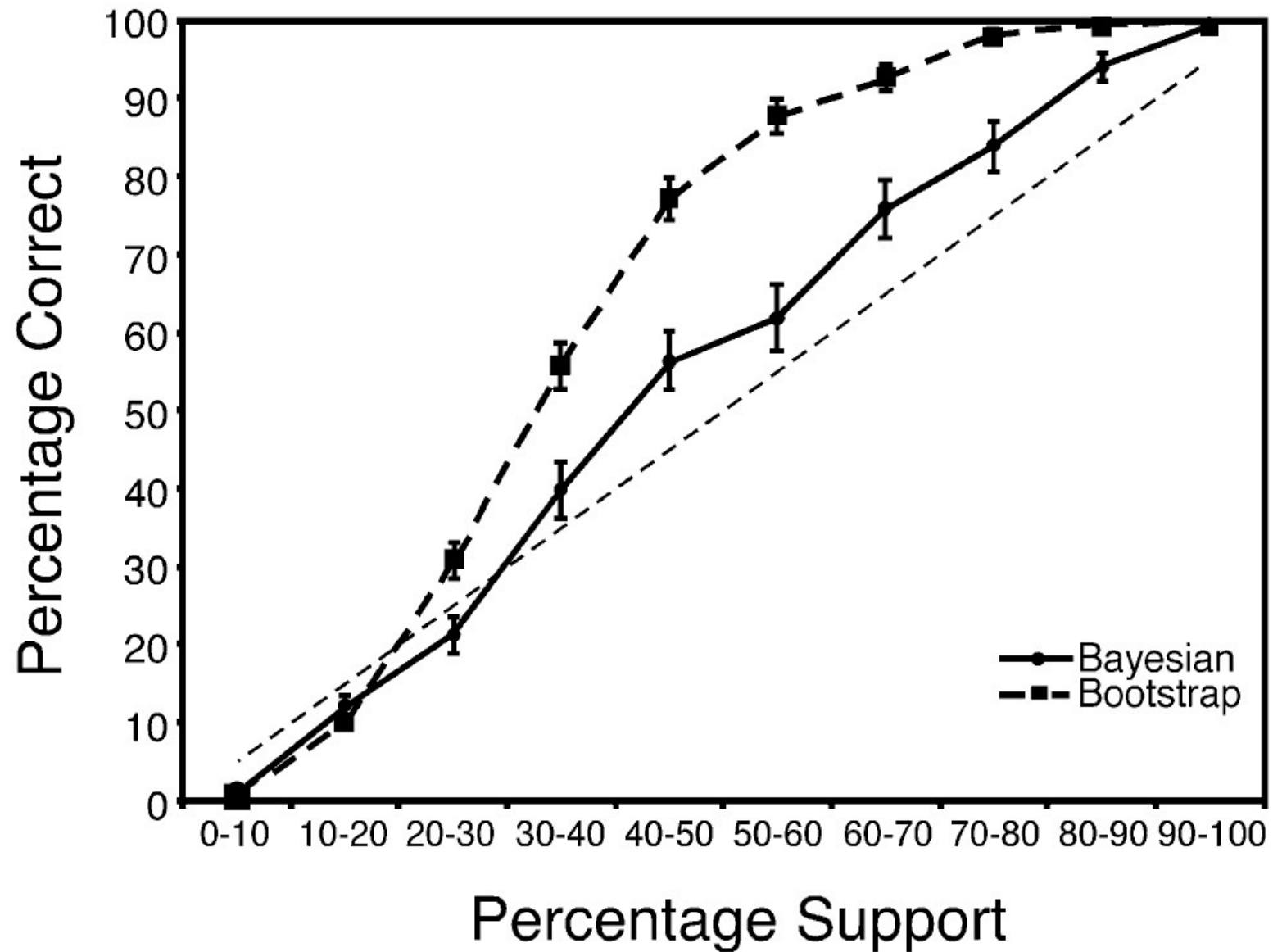
- Sensitivity of the posterior to the prior
- This problem can occur if the data are uninformative, the prior is strong, or both



Node support



Node support



Software for Bayesian Phylogenetics

BEAST 1



- **B**ayesian **E**volutionary **A**nalysis by **S**ampling **T**rees
- Analyse population- or species-level data
- Simultaneous estimation of tree and node times
- Range of clock models
- Range of tree priors and demographic models



Beast2

Bayesian evolutionary analysis by sampling trees

- Re-write of *BEAST* to increase modularity
- Users can extend *BEAST* by adding packages
- Additional tree priors not available in *BEAST* 1
- Capacity to perform simulations

**For a comparison of *BEAST* 1 and 2:
www.beast2.org/beast-features**



MrBayes

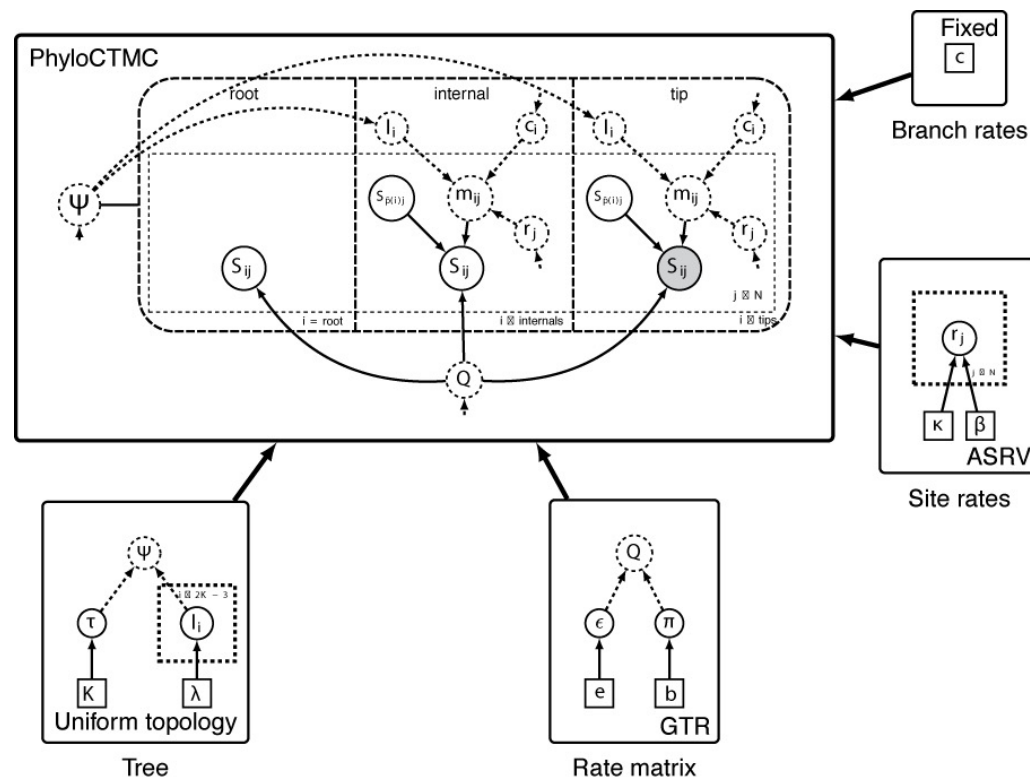
- Primarily designed for species-level data
- Simultaneous estimation of tree and node times
- Range of clock models
- Range of tree priors
- Multiple chains and MCMC diagnostics



RevBayes

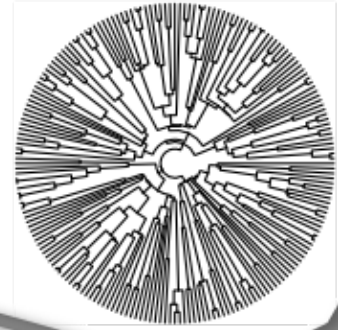


- Uses its own R-like language, Rev
- Interactive construction of graphical model
- Flexible and can be used for simulation and inference



EXABAYES

XXDRESIT



- Analyses of large data sets on computing clusters
- Available priors similar to those in older versions of *MrBayes*
- Limited options, no molecular dating
- Likelihood component adapted from *RAxML*

Useful references

