

A Brief Introduction to Bayesian Inference of Phylogeny

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Outline

I. Introduction to Bayesian inference

What is Bayesian inference?

- Deriving Bayes theorem
- Two non-phylogenetic examples
- Bayesian inference of phylogeny

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What's the deal with priors?

Learning to embrace your inner Bayesian

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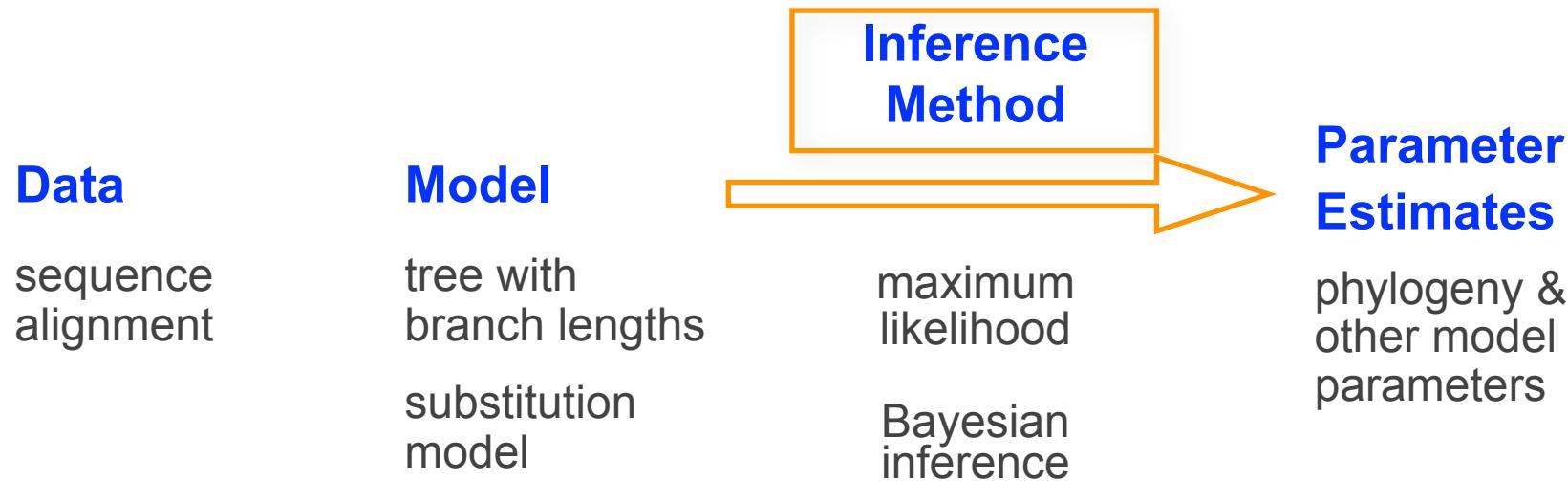
III. Numerical algorithms for Bayesian inference

Markov-chain Monte Carlo (MCMC)

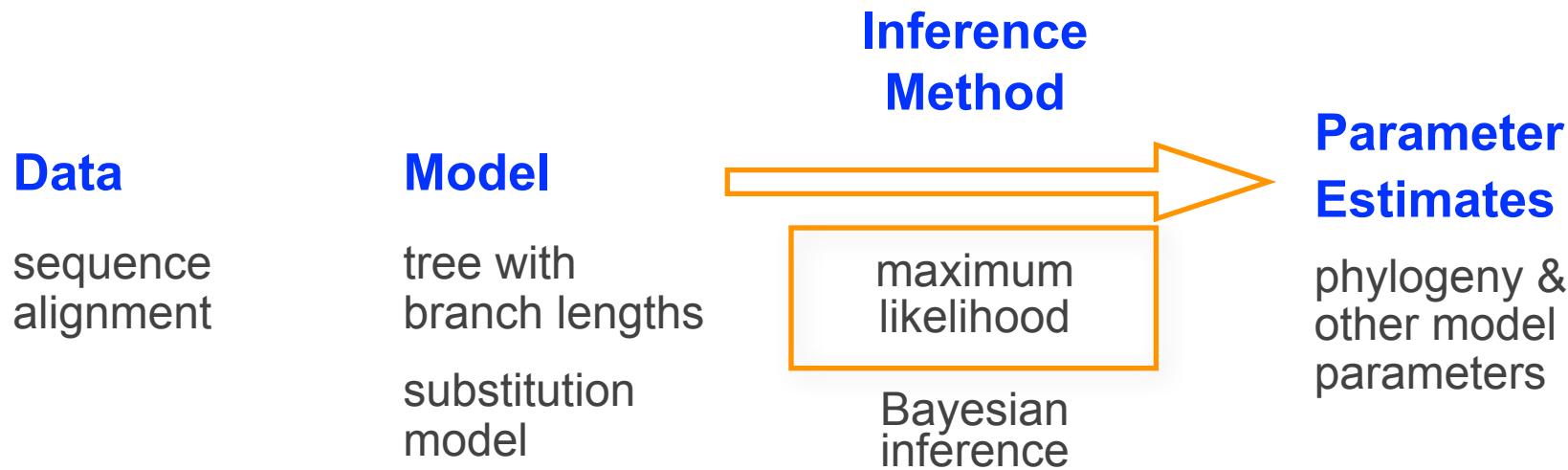
- Metropolis-Hastings algorithm
- Metropolis-Coupled algorithm

Summarizing posterior samples

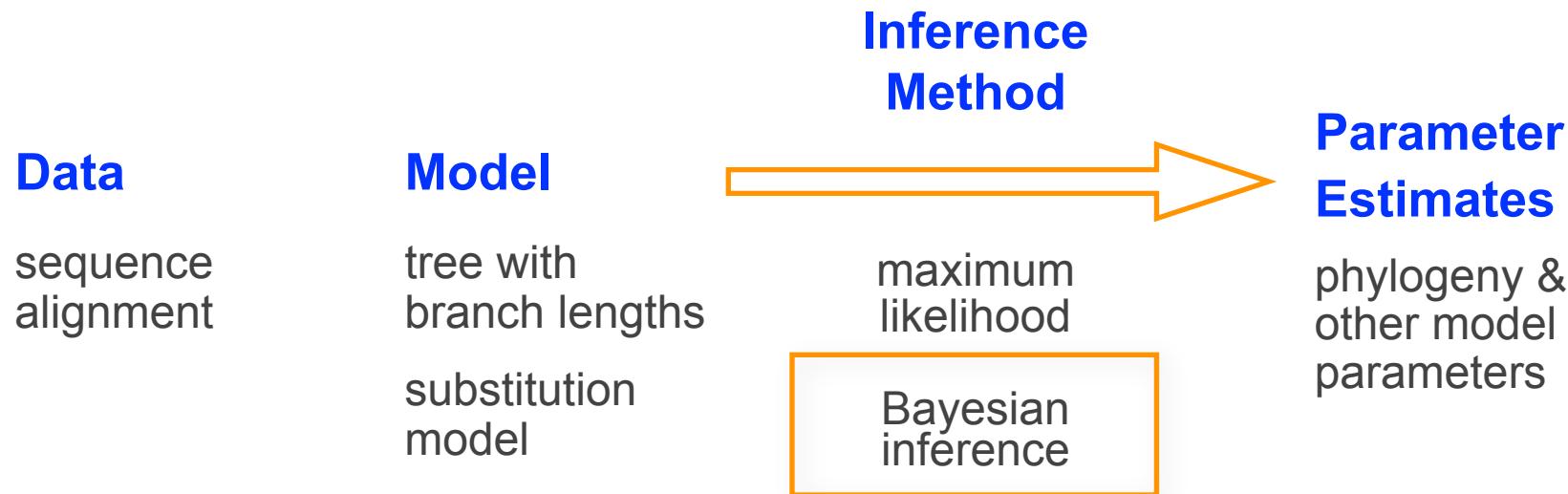
Statistical Estimation of Phylogeny: An Outline



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Bayesian Inference

Joint and Conditional Probabilities

The *joint probability* of A and B is the probability that events A and B occur together.

$$\Pr(A, B)$$

Bayesian Inference

Joint and Conditional Probabilities

The *joint probability* of A and B is the probability that events A and B occur together.

It is equal to the *marginal probability* of A times the *conditional probability* of B given A .

$$\Pr(A, B) = \Pr(A) \times \Pr(B | A)$$

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Bayesian Inference

Bayes' Theorem

$$\Pr(A \mid B) = \frac{\Pr(A) \times \Pr(B \mid A)}{\Pr(B)}$$

Bayesian Inference

Bayes' Theorem

$$\boxed{\Pr(A \mid B)} = \frac{\Pr(A) \times \Pr(B \mid A)}{\Pr(B)}$$

posterior probability

Bayesian Inference

Bayes' Theorem

$$\Pr(A | B) = \frac{\Pr(A) \times \Pr(B | A)}{\Pr(B)}$$

prior probability

posterior probability

The diagram illustrates the components of Bayes' Theorem. The formula is $\Pr(A | B) = \frac{\Pr(A) \times \Pr(B | A)}{\Pr(B)}$. An orange arrow points from the label "prior probability" to the term $\Pr(A)$. Another orange arrow points from the same label to the term $\Pr(B | A)$. A third orange arrow points from the label "posterior probability" to the term $\Pr(B)$.

Bayesian Inference

Bayes' Theorem

$$\Pr(A | B) = \frac{\Pr(A) \times \Pr(B | A)}{\Pr(B)}$$

prior probability

likelihood function

posterior probability

The diagram illustrates the components of Bayes' Theorem. At the top, 'prior probability' and 'likelihood function' are shown as inputs pointing towards the formula. The output of the formula, 'posterior probability', is shown at the bottom. All components are enclosed in orange boxes.

Bayesian Inference

Bayes' Theorem

$$\Pr(A | B) = \frac{\Pr(A) \times \Pr(B | A)}{\Pr(B)}$$

Diagram illustrating Bayes' Theorem:

- prior probability**: $\Pr(A)$
- likelihood function**: $\Pr(B | A)$
- posterior probability**: $\Pr(A | B)$
- marginal likelihood**: $\Pr(B)$

The diagram shows the components of Bayes' Theorem: prior probability, likelihood function, posterior probability, and marginal likelihood. The posterior probability is shown as a fraction where the numerator is the product of the prior probability and the likelihood function, and the denominator is the marginal likelihood.

Bayesian Inference

Bayes' Theorem

$$\Pr(A | B) = \frac{\Pr(A) \times \Pr(B | A)}{\Pr(B)}$$

Diagram illustrating Bayes' Theorem:

- prior probability: $\Pr(A)$
- likelihood function: $\Pr(B | A)$
- posterior probability: $\Pr(A | B)$
- marginal likelihood: $\Pr(B)$

```
graph LR; A[posterior probability] --- PrA["Pr(A)"]; A --- PrBA["Pr(B | A)"]; A --- PrB["Pr(B)"]; PrA --- PrA_label[prior probability]; PrBA --- PrBA_label[likelihood function]; PrB --- PrB_label[marginal likelihood]
```

$$\Pr(B) = \sum_A \Pr(A) \Pr(B | A)$$

Bayesian Inference

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Diagram illustrating Bayes' Theorem:

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```
graph LR; A["prior probability  
Pr(A)"] --> B["likelihood function  
Pr(B | A)"]; A --> C["posterior probability  
Pr(A | B)"]; B --> C; D["marginal likelihood  
Pr(B)"] --> C;
```

$$\begin{aligned}\Pr(B) &= \sum_A \Pr(A)\Pr(B | A) \\ &= \int \Pr(A)\Pr(B | A)dA\end{aligned}$$

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Example: The biased-die problem

There is the possibility that a die is either fair, or is biased in a specific way:

Bayesian Inference

Example: The biased-die problem

There is the possibility that a die is either fair, or is biased in a specific way:

Observation	Fair	Biased
	$\frac{1}{6}$	$\frac{1}{21}$
	$\frac{1}{6}$	$\frac{2}{21}$
	$\frac{1}{6}$	$\frac{3}{21}$
	$\frac{1}{6}$	$\frac{4}{21}$
	$\frac{1}{6}$	$\frac{5}{21}$
	$\frac{1}{6}$	$\frac{6}{21}$

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We generate some observations from a randomly selected die:

- 2 rolls with 4 and 6 pips

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Probability of the observations:

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We generate some observations from a randomly selected die:

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Probability of the observations: $\Pr(\boxed{\bullet\bullet}, \boxed{\bullet\bullet} \mid \text{Fair}) =$

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	$\frac{1}{6}$	$\frac{6}{21}$

We generate some observations from a randomly selected die:

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Probability of the observations: $\Pr(\text{[die showing 4 dots]}, \text{[die showing 6 dots]} \mid \text{Fair}) = \boxed{\frac{1}{6}}$

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We generate some observations from a randomly selected die:

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Probability of the observations: $\Pr(\text{die showing 4}, \text{die showing 6} | \text{Fair}) = \frac{1}{6} \times \frac{1}{6}$

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We generate some observations from a randomly selected die:

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Probability of the observations: $\Pr(\text{die showing 4}, \text{die showing 6} | \text{Fair}) = \frac{1}{6} \times \frac{1}{6} = \frac{1}{36} \approx 0.028$

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We generate some observations from a randomly selected die:

- 2 rolls with 4 and 6 pips

Probability of the observations: $\Pr(\text{[4, 6]} \mid \text{Fair}) = \frac{1}{6} \times \frac{1}{6} = \frac{1}{36} \approx 0.028$

$\Pr(\text{[4, 6]} \mid \text{Biased}) = \frac{4}{21} \times \frac{6}{21} = \frac{24}{441} \approx 0.054$

Bayesian Inference

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$$\Pr(\boxed{\bullet\bullet}, \boxed{\bullet\bullet\bullet} | \text{Biased}) = \frac{4}{21} \times \frac{6}{21} = \frac{24}{441} \approx 0.054$$

So, the observations are ~ 2 times more likely under the biased hypothesis

Bayesian Inference

Example: The biased-die problem

What is the posterior probability of the alternative hypotheses?

$$\overbrace{\Pr(\text{Biased} \mid \begin{array}{|c|c|}\hline \bullet & \bullet \\ \hline \bullet & \bullet \\ \hline \end{array}, \begin{array}{|c|c|}\hline \bullet & \bullet \\ \hline \bullet & \bullet \\ \hline \end{array})}^{\text{posterior probability}} = \frac{\Pr(\begin{array}{|c|c|}\hline \bullet & \bullet \\ \hline \bullet & \bullet \\ \hline \end{array}, \begin{array}{|c|c|}\hline \bullet & \bullet \\ \hline \bullet & \bullet \\ \hline \end{array} \mid \text{Biased}) \times \Pr(\text{Biased})}{\Pr(\begin{array}{|c|c|}\hline \bullet & \bullet \\ \hline \bullet & \bullet \\ \hline \end{array}, \begin{array}{|c|c|}\hline \bullet & \bullet \\ \hline \bullet & \bullet \\ \hline \end{array})}$$

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prior probabilities:

$$\Pr(\text{Fair}) = 0.9$$
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likelihoods: $\Pr(\begin{array}{|c|c|}\hline \bullet & \bullet \\ \hline \bullet & \bullet \\ \hline \end{array}, \begin{array}{|c|c|}\hline \bullet & \bullet \\ \hline \bullet & \bullet \\ \hline \end{array} \mid \text{Fair}) = \frac{1}{36}$

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likelihoods: $\Pr(\begin{array}{|c|c|}\hline \bullet & \bullet \\ \hline \bullet & \bullet \\ \hline \end{array}, \begin{array}{|c|c|}\hline \bullet & \bullet \\ \hline \bullet & \bullet \\ \hline \end{array} \mid \text{Fair}) = \frac{1}{36}$

$$\Pr(\begin{array}{|c|c|}\hline \bullet & \bullet \\ \hline \bullet & \bullet \\ \hline \end{array}, \begin{array}{|c|c|}\hline \bullet & \bullet \\ \hline \bullet & \bullet \\ \hline \end{array} \mid \text{Biased}) = \frac{24}{441}$$

posterior probability: $\Pr(\text{Biased} \mid \begin{array}{|c|c|}\hline \bullet & \bullet \\ \hline \bullet & \bullet \\ \hline \end{array}, \begin{array}{|c|c|}\hline \bullet & \bullet \\ \hline \bullet & \bullet \\ \hline \end{array}) = \frac{\frac{24}{441} \times \frac{1}{10}}{\frac{24}{441} \times \frac{1}{10} + \frac{1}{36} \times \frac{9}{10}} \approx 0.18$

Bayesian Inference

Example: The biased-die problem

What is the posterior probability of the alternative hypotheses?

$$\Pr(\text{Biased} \mid \begin{array}{|c|c|}\hline \bullet & \bullet \\ \hline \bullet & \bullet \\ \hline \end{array}, \begin{array}{|c|c|}\hline \bullet & \bullet \\ \hline \bullet & \bullet \\ \hline \end{array}) = \frac{\underbrace{\Pr(\begin{array}{|c|c|}\hline \bullet & \bullet \\ \hline \bullet & \bullet \\ \hline \end{array}, \begin{array}{|c|c|}\hline \bullet & \bullet \\ \hline \bullet & \bullet \\ \hline \end{array} \mid \text{Biased}) \times \Pr(\text{Biased})}_{\text{likelihood}}}{\underbrace{\Pr(\begin{array}{|c|c|}\hline \bullet & \bullet \\ \hline \bullet & \bullet \\ \hline \end{array}, \begin{array}{|c|c|}\hline \bullet & \bullet \\ \hline \bullet & \bullet \\ \hline \end{array} \mid \text{Biased}) \times \Pr(\text{Biased}) + \Pr(\begin{array}{|c|c|}\hline \bullet & \bullet \\ \hline \bullet & \bullet \\ \hline \end{array}, \begin{array}{|c|c|}\hline \bullet & \bullet \\ \hline \bullet & \bullet \\ \hline \end{array} \mid \text{Fair}) \times \Pr(\text{Fair})}_{\text{marginal likelihood}}}$$

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So, our posterior belief in the biased hypothesis is $\Pr = 0.18$, which is an updated version of our prior belief in the biased hypothesis is $\Pr = 0.10$

Bayesian Inference

Generic statistical paradigm

pose a substantive question

develop a stochastic model
with parameters that, if known,
would answer the question

collect observations that
are informative about model
parameters

find the best estimate of
model parameters (by some
means) conditioned on (*i.e.*,
given) the data at hand

Coin tossing

Is this a fair coin? Or, what is the probability
of observing heads in a single toss?

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toss the coin n times and record the
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Binomial probability distribution with
parameter θ (probability of observing
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toss the coin n times and record the
number of heads, x .

find the best estimate of the θ parameter
using Bayesian inference

Bayesian Inference

Example: Coin tossing

$$\Pr(\theta | x) = \frac{\Pr(x | \theta) \Pr(\theta)}{\Pr(x)}$$

Diagram illustrating the Bayesian formula:

- The term $\Pr(\theta | x)$ is labeled "posterior probability".
- The term $\Pr(x | \theta) \Pr(\theta)$ is labeled "likelihood function" above and "prior probability" to its right.
- The term $\Pr(x)$ is labeled "marginal likelihood" below it.

Bayesian Inference

Example: Coin tossing

$$\Pr(\theta | x) = \frac{\Pr(x | \theta)\Pr(\theta)}{\int \Pr(x | \theta)\Pr(\theta)d\theta}$$

likelihood function

prior probability

posterior probability

marginal likelihood

The diagram illustrates the Bayesian inference formula. The formula is $\Pr(\theta | x) = \frac{\Pr(x | \theta)\Pr(\theta)}{\int \Pr(x | \theta)\Pr(\theta)d\theta}$. Four orange arrows point from labels to specific parts of the formula: 'likelihood function' points to $\Pr(x | \theta)$, 'prior probability' points to $\Pr(\theta)$, 'posterior probability' points to the entire fraction, and 'marginal likelihood' points to the denominator $\int \Pr(x | \theta)\Pr(\theta)d\theta$.

Bayesian Inference

Example: Coin tossing

$$\Pr(\theta | x) = \frac{\Pr(x | \theta)\Pr(\theta)}{\int \Pr(x | \theta)\Pr(\theta)d\theta}$$

likelihood function

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marginal likelihood

The diagram illustrates the Bayesian inference formula for coin tossing. The formula is $\Pr(\theta | x) = \frac{\Pr(x | \theta)\Pr(\theta)}{\int \Pr(x | \theta)\Pr(\theta)d\theta}$. Four orange arrows point to different parts of the formula: one from the left points to the term $\Pr(\theta | x)$ labeled 'posterior probability'; another from the top left points to $\Pr(x | \theta)$ labeled 'likelihood function'; a third from the top right points to $\Pr(\theta)$ labeled 'prior probability'; and a fourth from the bottom right points to the denominator $\int \Pr(x | \theta)\Pr(\theta)d\theta$ labeled 'marginal likelihood'.

Bayesian Inference

Example: Coin tossing

We will adopt the Binomial distribution as our model of coin tossing:
discrete probability distribution that has two outcomes (e.g., T/F, Y/N, H/T)

$$\Pr(x | \theta) = \binom{n}{x} \theta^x (1 - \theta)^{n-x}$$

↑
heads

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↑
possible orderings
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This is called the Binomial coefficient, and is read 'n choose x ':

$$\binom{n}{x} = \frac{n!}{x!(n-x)!}$$

Bayesian Inference

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discrete probability distribution that has two outcomes (e.g., T/F, Y/N, H/T)

$$\Pr(x | \theta) = \binom{n}{x} \theta^x (1 - \theta)^{n-x}$$

The likelihood function for the Binomial distribution:

$$L(\theta; x) \propto \Pr(x | \theta) = \binom{n}{x} \theta^x (1 - \theta)^{n-x}$$

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With some algebra, we can solve for θ to find the MLE:

$$\hat{\theta} = \frac{x}{n}$$

Bayesian Inference

Example: Coin tossing

$$\Pr(\theta | x) = \frac{\Pr(x | \theta)\Pr(\theta)}{\int \Pr(x | \theta)\Pr(\theta)d\theta}$$

likelihood function

prior probability

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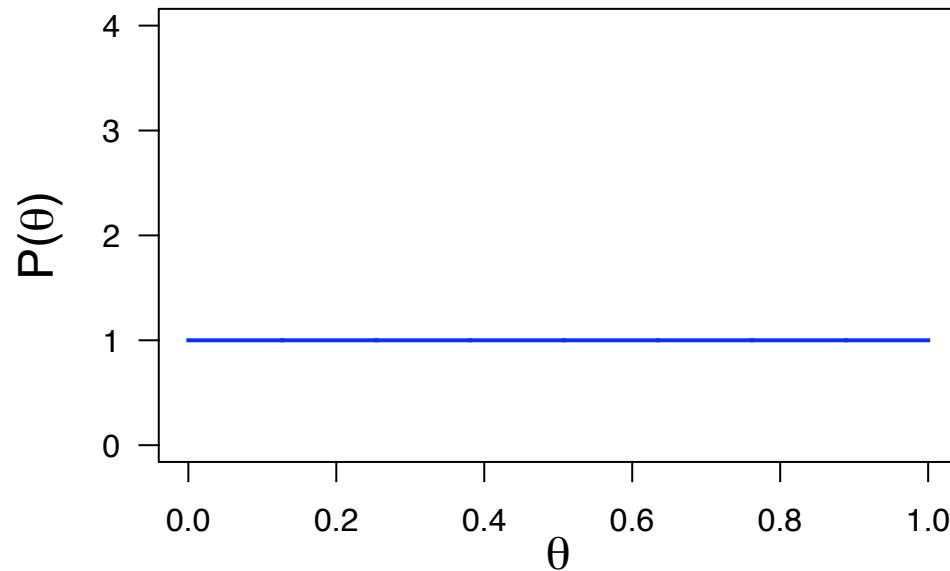
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Bayesian Inference

Example: Coin tossing

The Beta prior probability distribution:

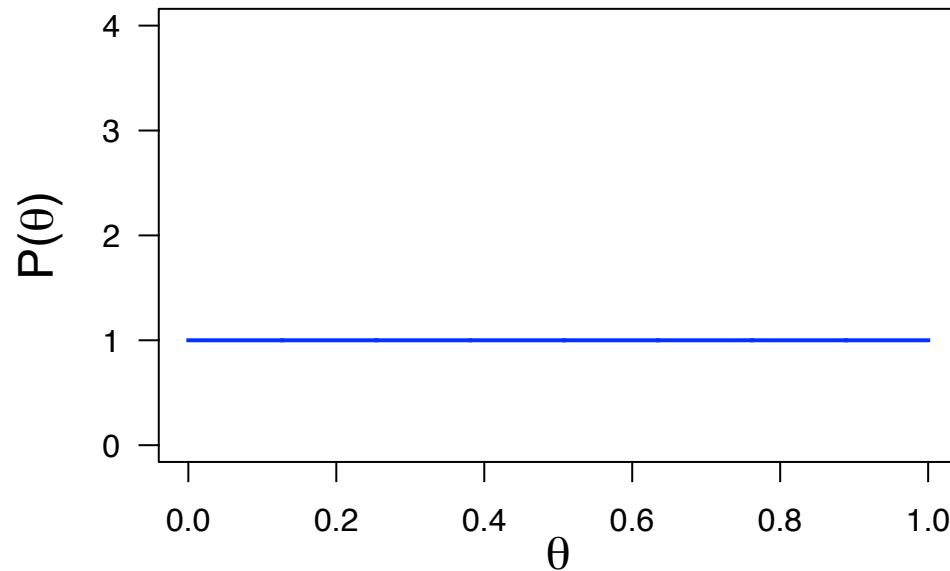


uniform prior: $\alpha = \beta = 1$

Bayesian Inference

Example: Coin tossing

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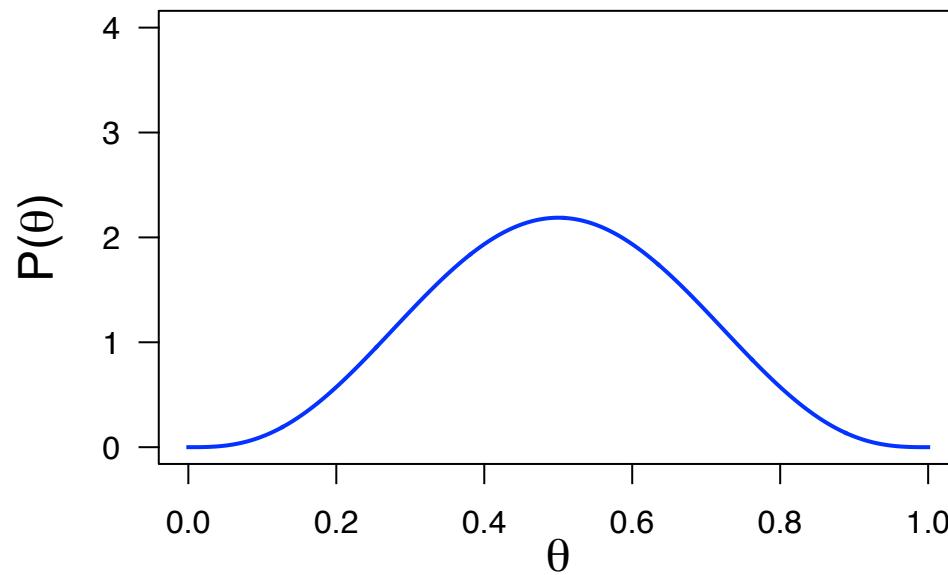
uniform prior: $\alpha = \beta = 1$

NOTE: uniform prior \neq uninformative

Bayesian Inference

Example: Coin tossing

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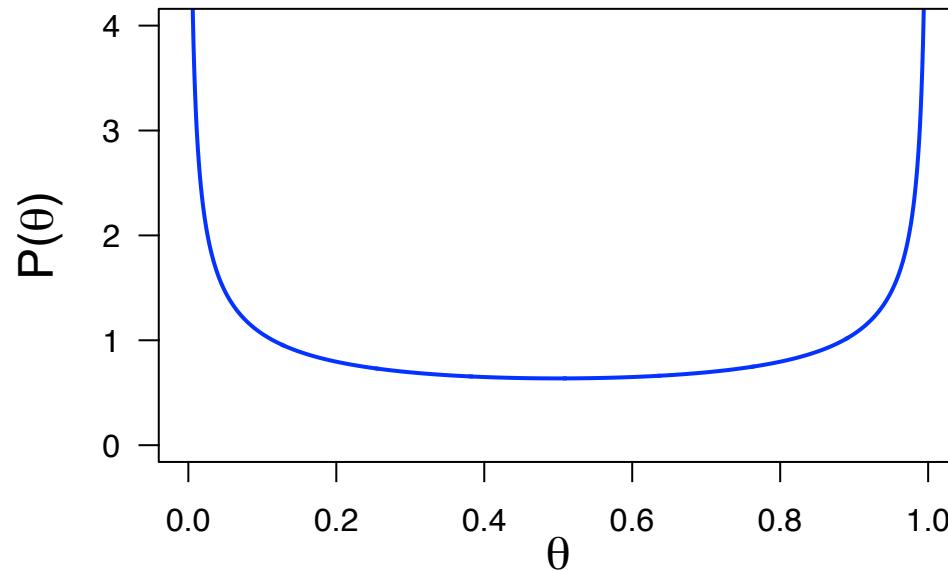


nonuniform prior: $\alpha = \beta = 4$

Bayesian Inference

Example: Coin tossing

The Beta prior probability distribution:

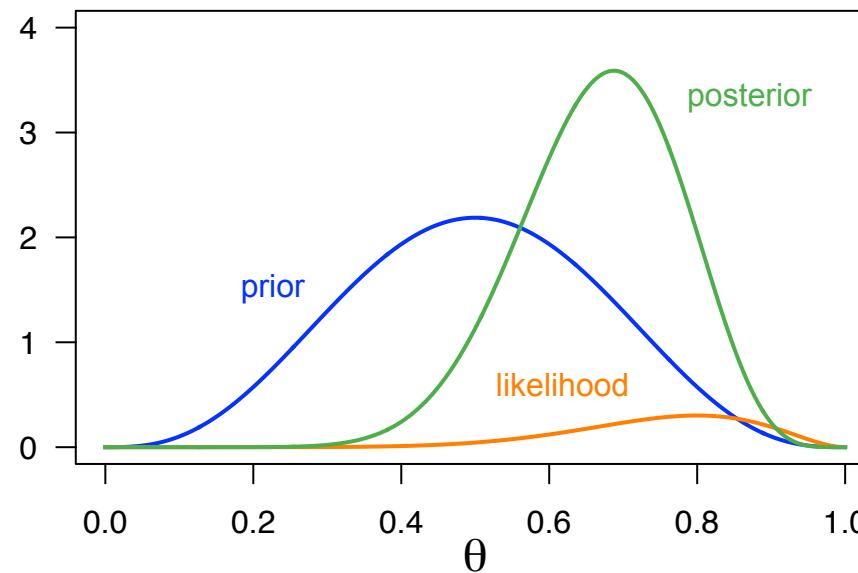


nonuniform prior: $\alpha = \beta = 0.5$

Bayesian Inference

Example: Coin tossing

The impact of the prior probability distribution on the estimated posterior probability:



$x = 8$ heads in $n = 10$ tosses

Outline

I. Introduction to Bayesian inference

What is Bayesian inference?

- Deriving Bayes theorem
- Two non-phylogenetic examples
- Bayesian inference of phylogeny

II. The Bayesian hard sell

What's the deal with priors?

Learning to embrace your inner Bayesian

III. Numerical algorithms for Bayesian inference

Markov-chain Monte Carlo (MCMC)

- Metropolis-Hastings algorithm
- Metropolis-Coupled algorithm

Summarizing posterior samples

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Bayesian Inference of Phylogeny (on one slide)

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I. Data

Assume an alignment, \mathbf{X} , of N sites for S species: $\mathbf{X} = (x_1, x_2, x_3, \dots, x_N)$

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II. Phylogenetic model parameters

1. Tree

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1. Tree topology $\tau = \{\tau_1, \tau_2, \dots, \tau_{(2S-5)!!}\}$

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V. Posterior Probability

$$\Pr(\tau, \nu, \theta, \pi \mid X) = \frac{\Pr(X \mid \tau, \nu, \theta, \pi) \Pr(\tau) \Pr(\nu) \Pr(\theta) \Pr(\pi)}{\Pr(X)}$$

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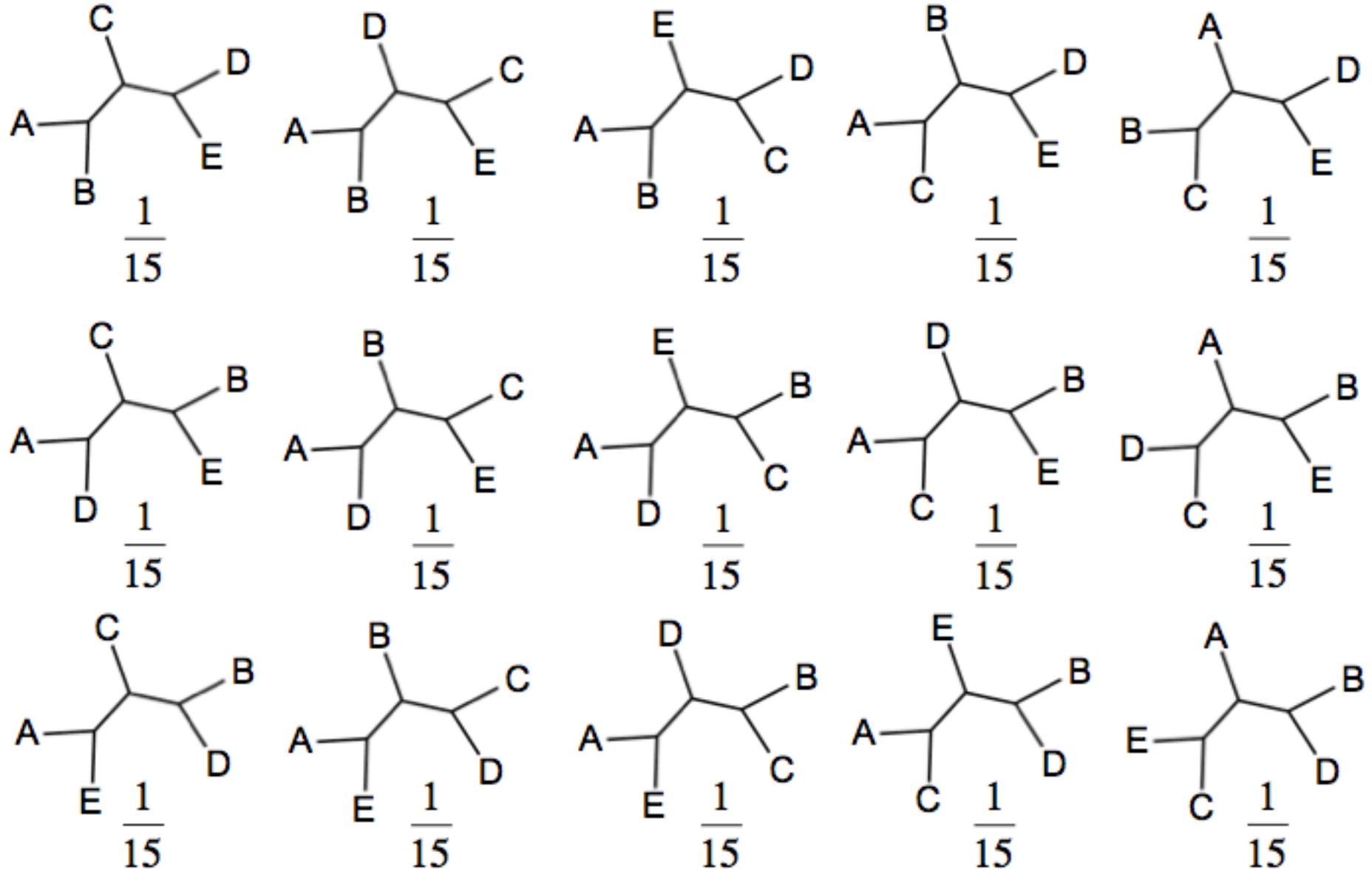
$$Q = \mu \begin{pmatrix} - & a\pi_C & b\pi_G & c\pi_T \\ a\pi_A & - & d\pi_G & e\pi_T \\ b\pi_A & d\pi_C & - & f\pi_T \\ c\pi_A & e\pi_C & f\pi_G & - \end{pmatrix}$$

V. Posterior Probability

$$\Pr(\tau, \nu, \theta, \pi \mid X) = \frac{\Pr(X \mid \tau, \nu, \theta, \pi) \Pr(\tau) \Pr(\nu) \Pr(\theta) \Pr(\pi)}{\Pr(X)}$$

Bayesian Inference of Phylogeny

Discrete-uniform prior on topologies



Bayesian Inference of Phylogeny

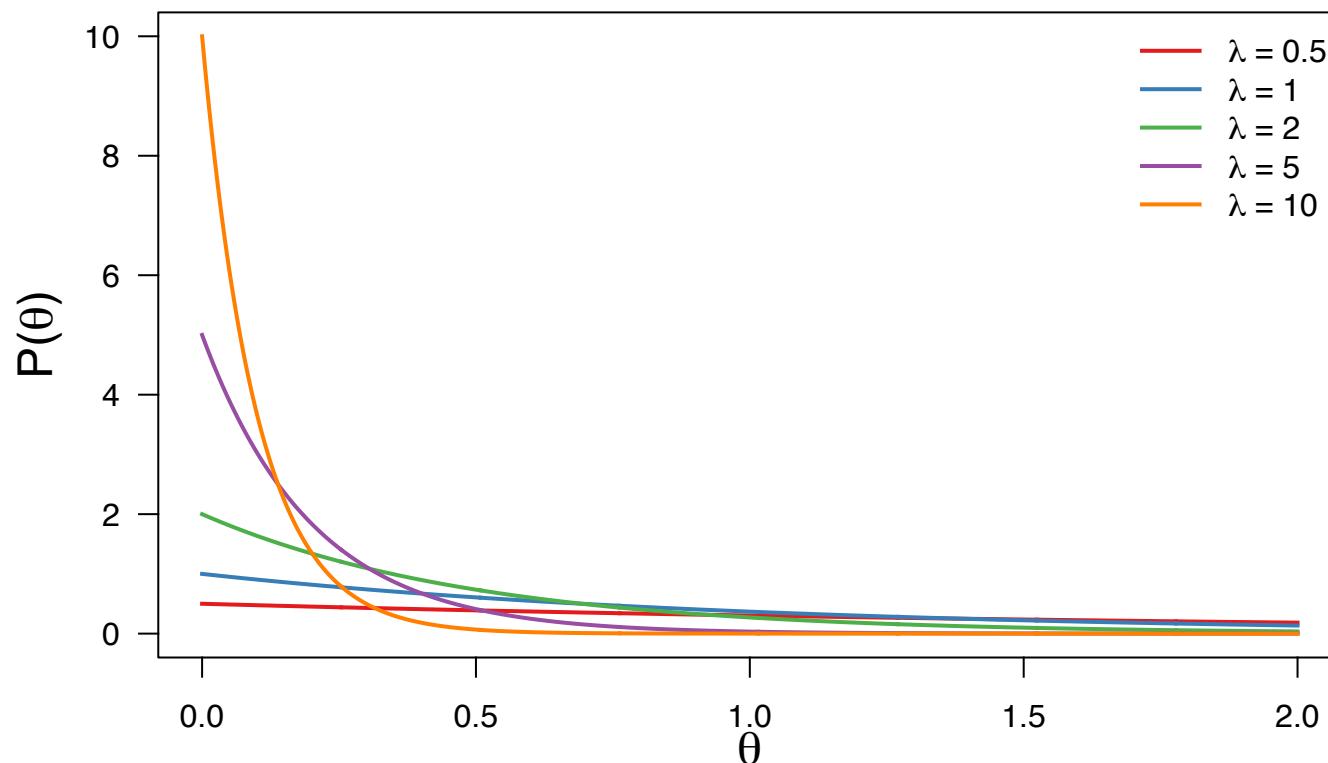
Exponential priors

Often used for branch lengths with rate parameter λ and mean $1/\lambda$

Bayesian Inference of Phylogeny

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Bayesian Inference of Phylogeny

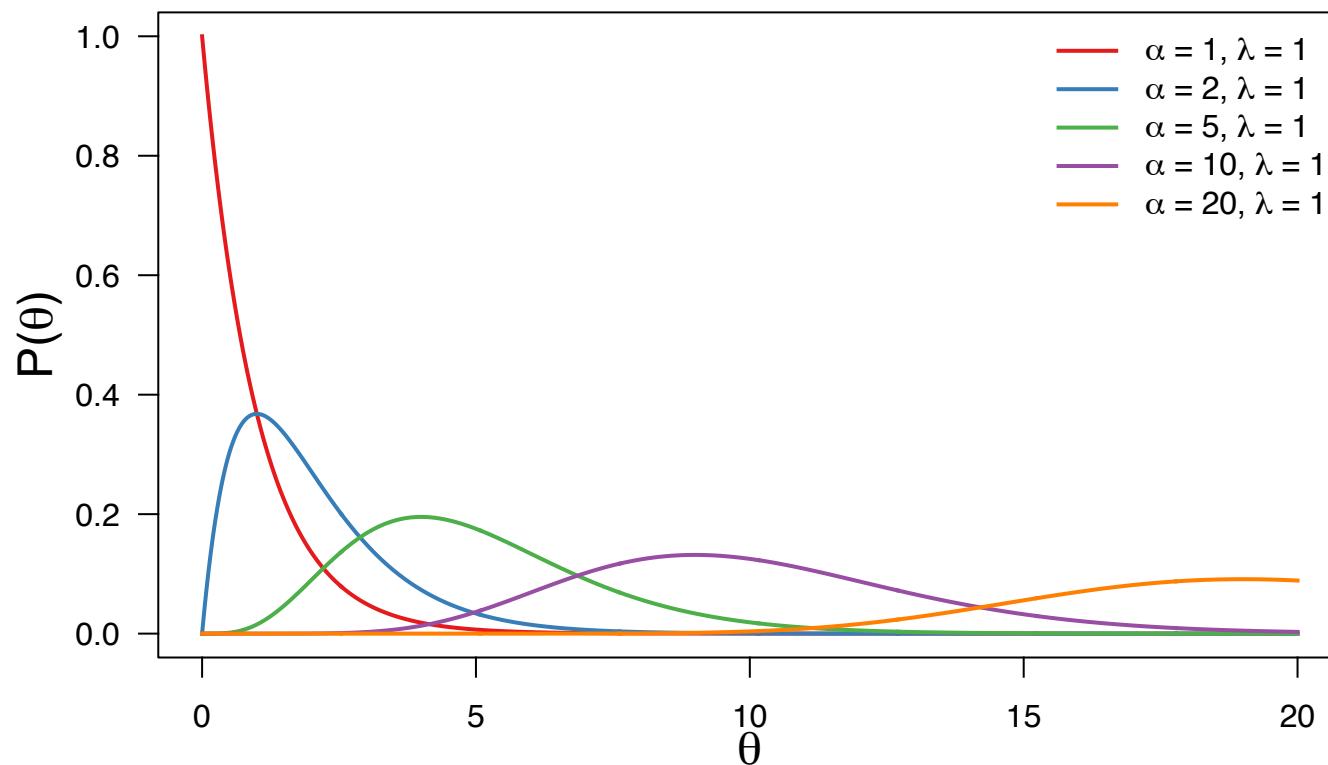
Gamma priors

A sum of α iid exponential variables

Bayesian Inference of Phylogeny

Gamma priors

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Bayesian Inference of Phylogeny

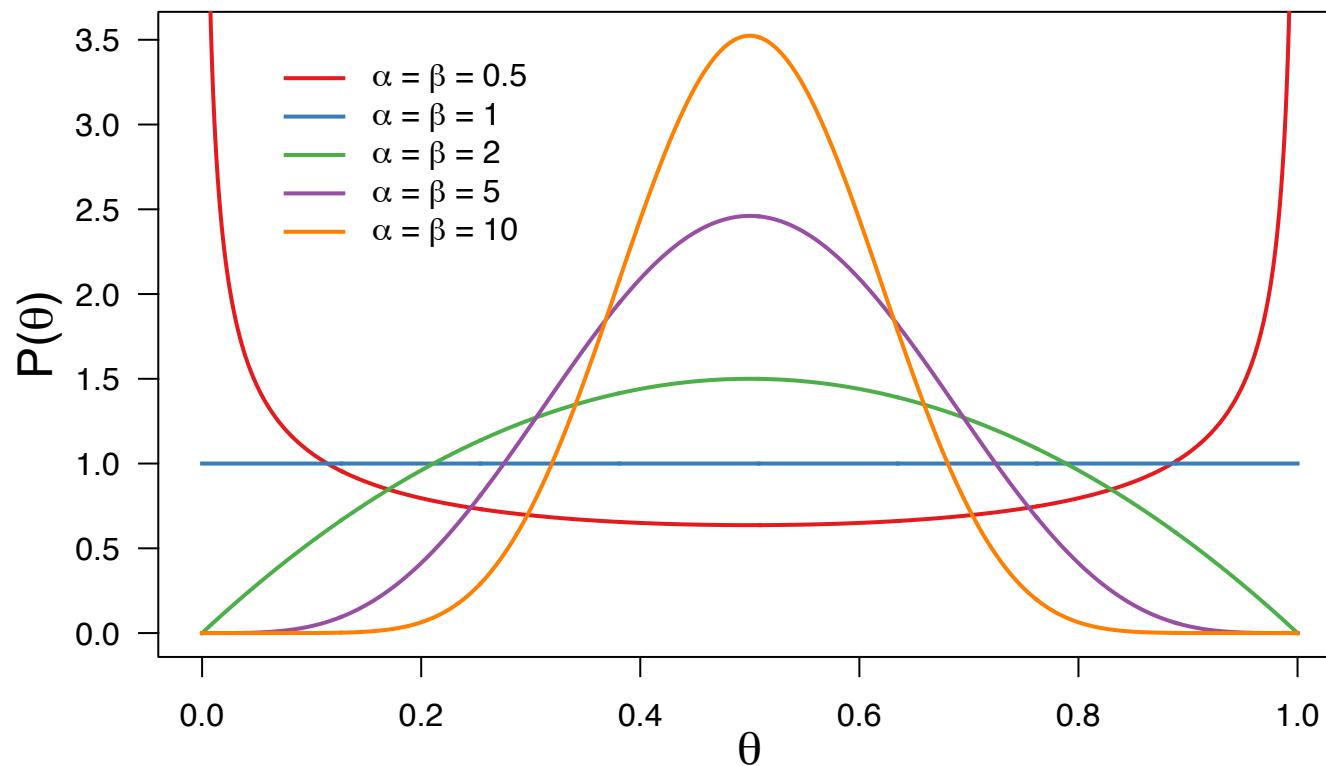
Beta prior

Often used for probabilities (like probability of heads) and fractions

Bayesian Inference of Phylogeny

Beta prior

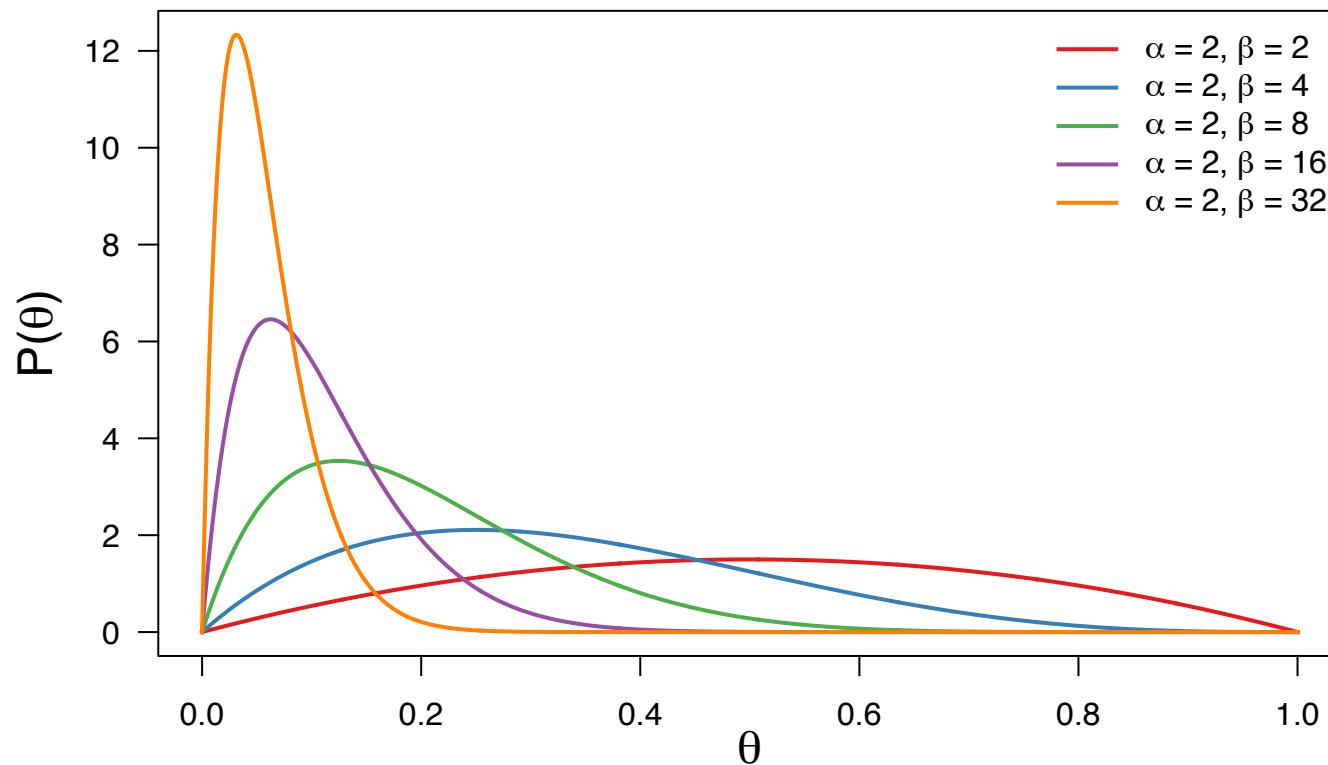
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Bayesian Inference of Phylogeny

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Often used for probabilities (like probability of heads) and fractions



Bayesian Inference of Phylogeny

Dirichlet prior

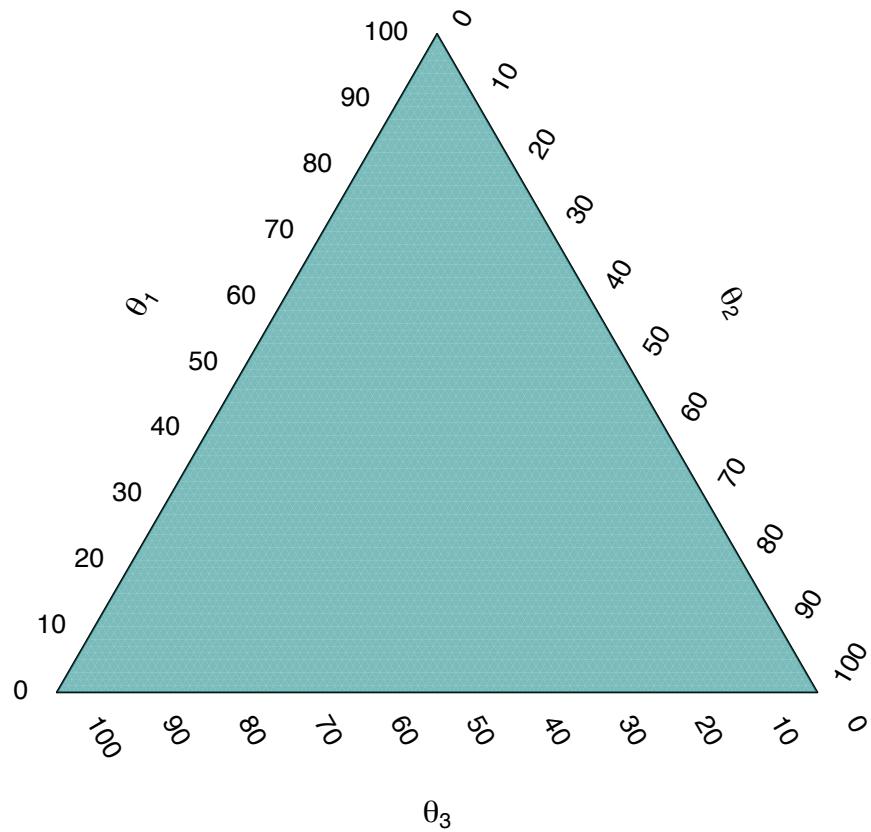
Generalization of the beta often used for proportions

Bayesian Inference of Phylogeny

Dirichlet prior

A “flat” Dirichlet distribution

$$\theta \sim \text{Dirichlet}(1, 1, 1)$$

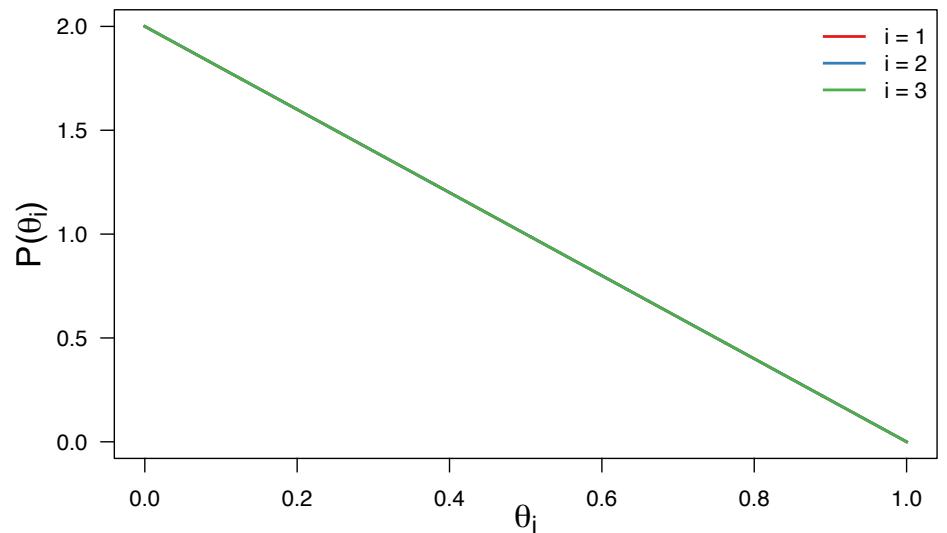
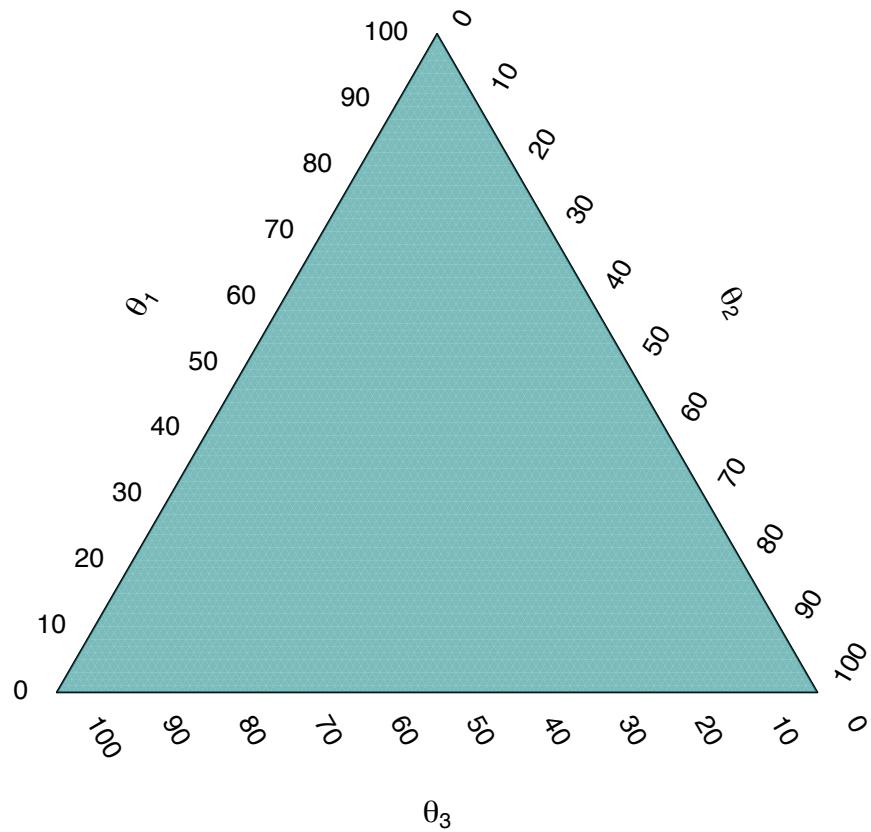


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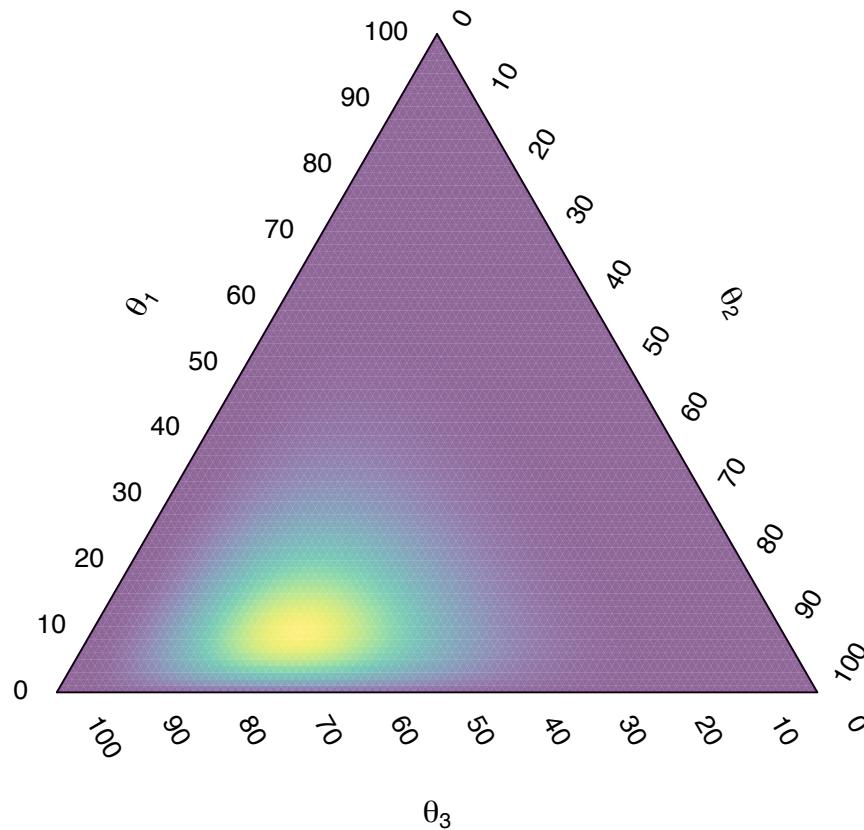


Bayesian Inference of Phylogeny

Dirichlet prior

An asymmetric Dirichlet distribution

$$\theta \sim \text{Dirichlet}(2, 4, 8)$$

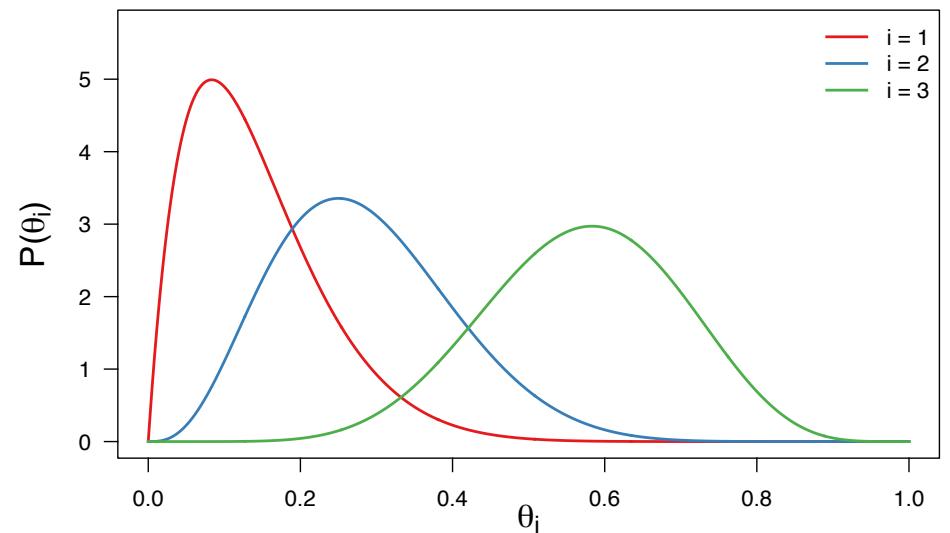
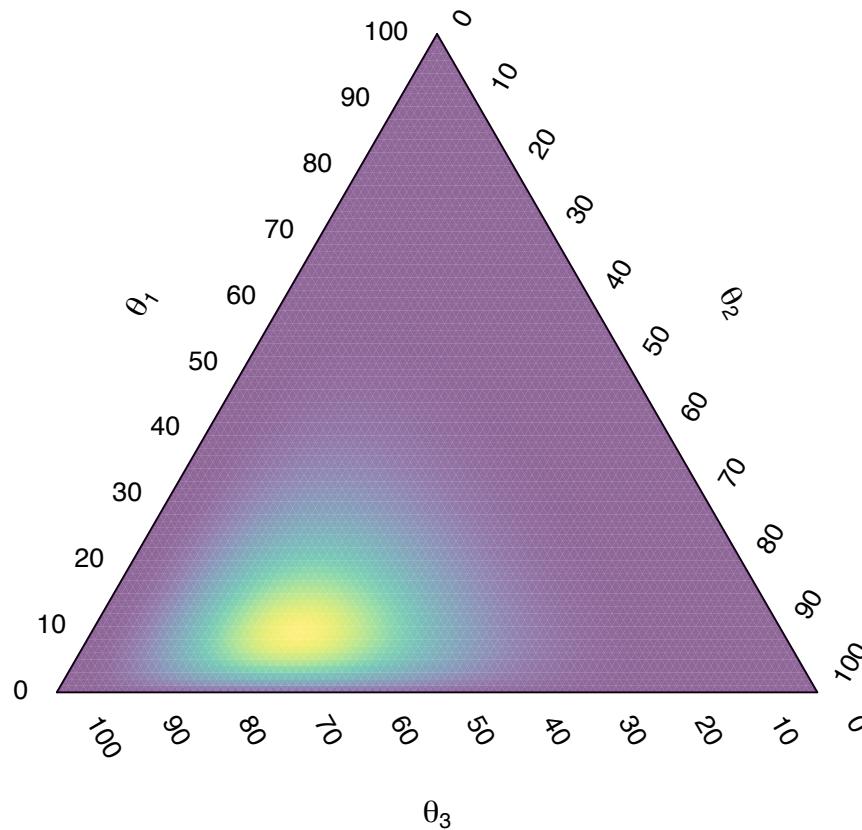


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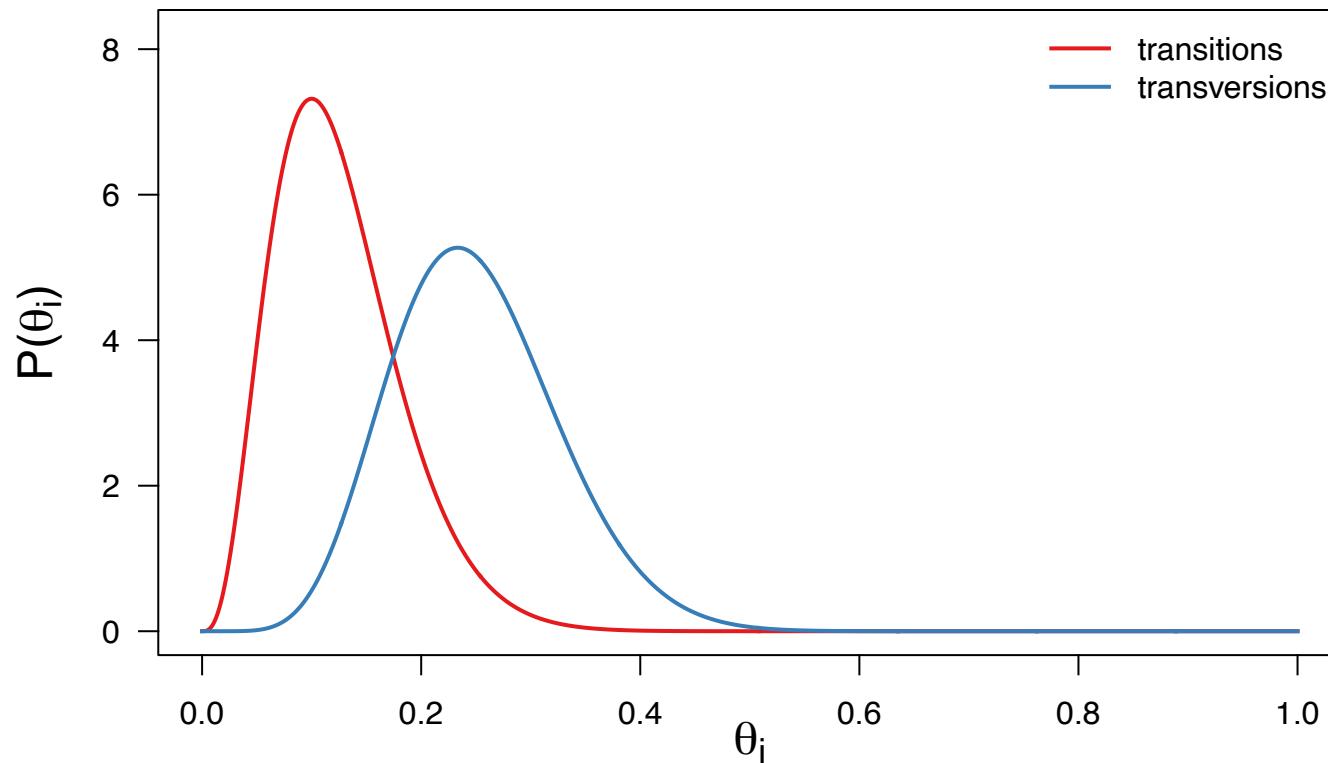


Bayesian Inference of Phylogeny

Dirichlet prior

We can express prior beliefs about transition/transversion rates

$$\theta \sim \text{Dirichlet}(4, 8, 4, 4, 8, 4)$$

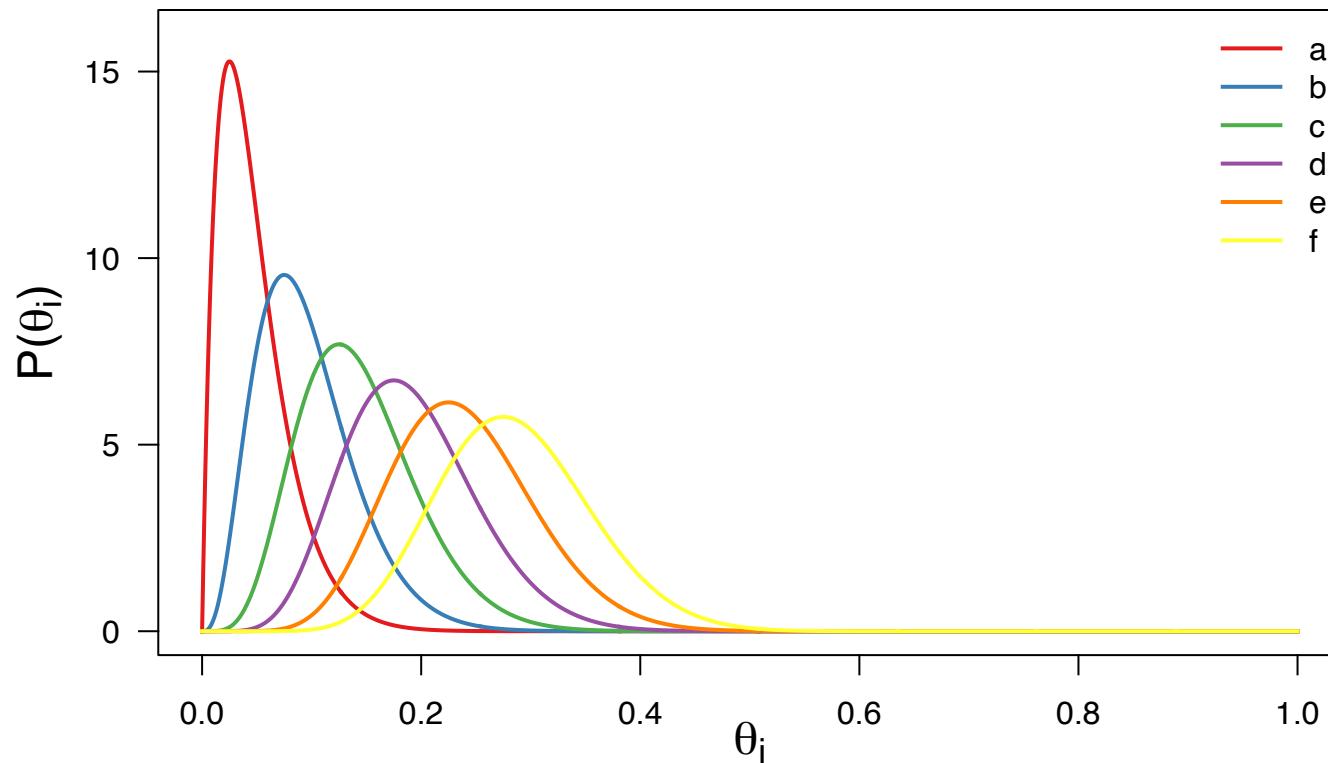


Bayesian Inference of Phylogeny

Dirichlet prior

Or any prior beliefs about exchangeability rates

$$\theta \sim \text{Dirichlet}(2, 4, 6, 8, 10, 12)$$



Bayesian Inference of Phylogeny

<https://mikeryanmay.shinyapps.io/plotprior/>



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I. Introduction to Bayesian inference

What is Bayesian inference?

- Deriving Bayes theorem
- Two non-phylogenetic examples
- Bayesian inference of phylogeny



II. The Bayesian hard sell

What's the deal with priors?

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III. Numerical algorithms for Bayesian inference

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What is there to disagree about?

Not much, actually:

- model-based statistical inference

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Lots to love about maximum-likelihood estimation

Desirable statistical properties

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Maximum-likelihood perspective on parameters:

Data are random variables, but the parameters are fixed

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Bayesian perspective on parameters:

Data are random variables, and so are the model parameters

Maximum Likelihood and Bayesian Inference

Maximum-likelihood perspective on parameters:

Data are random variables, but the parameters are fixed

Bayesian perspective on parameters:

Data are random variables, and so are the model parameters

If we treat the parameters as random variables, what do we have to specify?

Bayesian Inference

A priori...

We usually (*i.e.*, always) have prior beliefs, so why not be explicit about it?

- this is consistent with making assumptions clear (model-based inference)

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- the posterior is typically dominated by the likelihood function
- when this is not the case, the ability to detect prior sensitivity is a good thing!

Bayesian Inference

is my prior ***informative?***

is my prior ***informed?***

	no	yes
no		
yes		

Bayesian Inference

is my prior **informative?**

		no	yes
		no	
no	no		
	yes		
is my prior informed?		no	
		yes	

Bayesian Inference

is my prior **informative?**

		no	yes
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		no	yes
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is my prior **informed?**

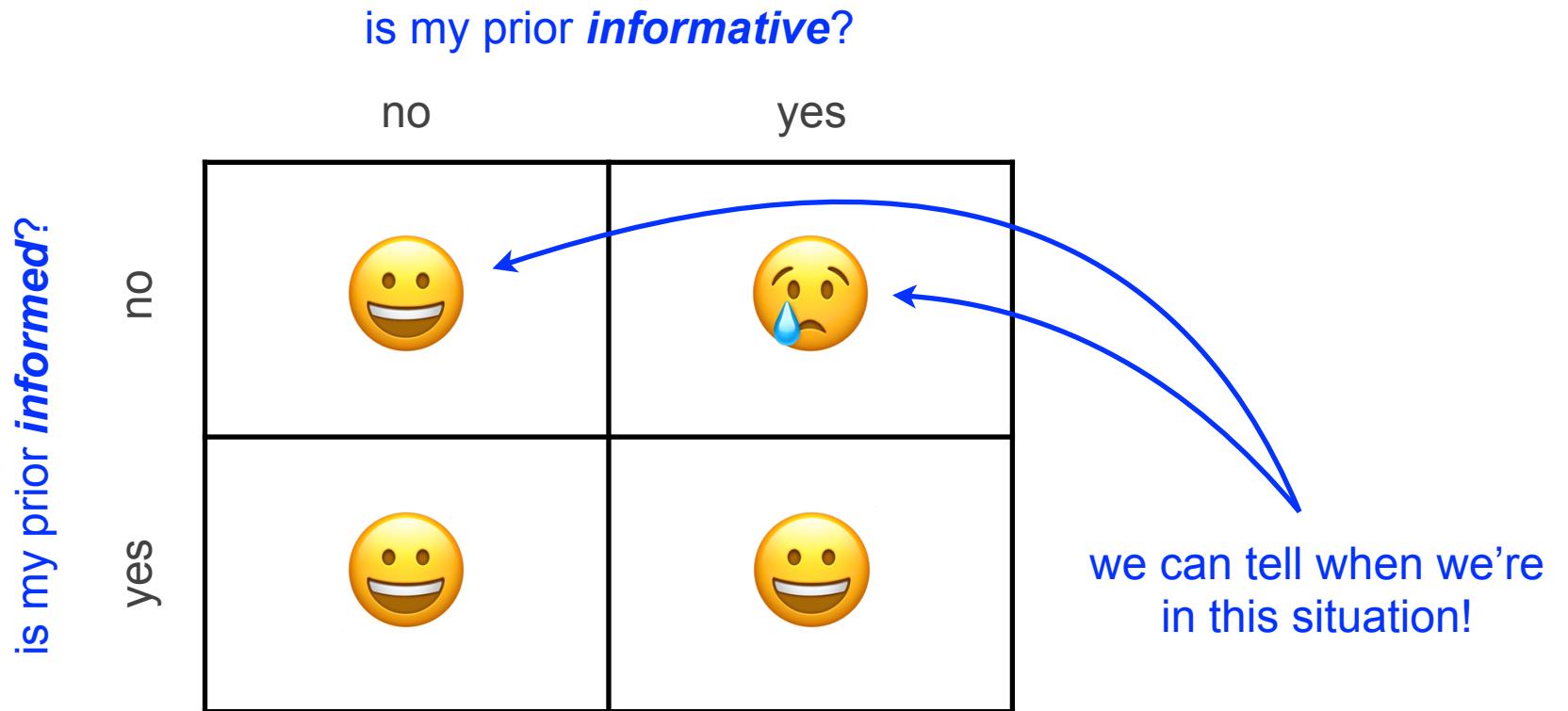
Bayesian Inference

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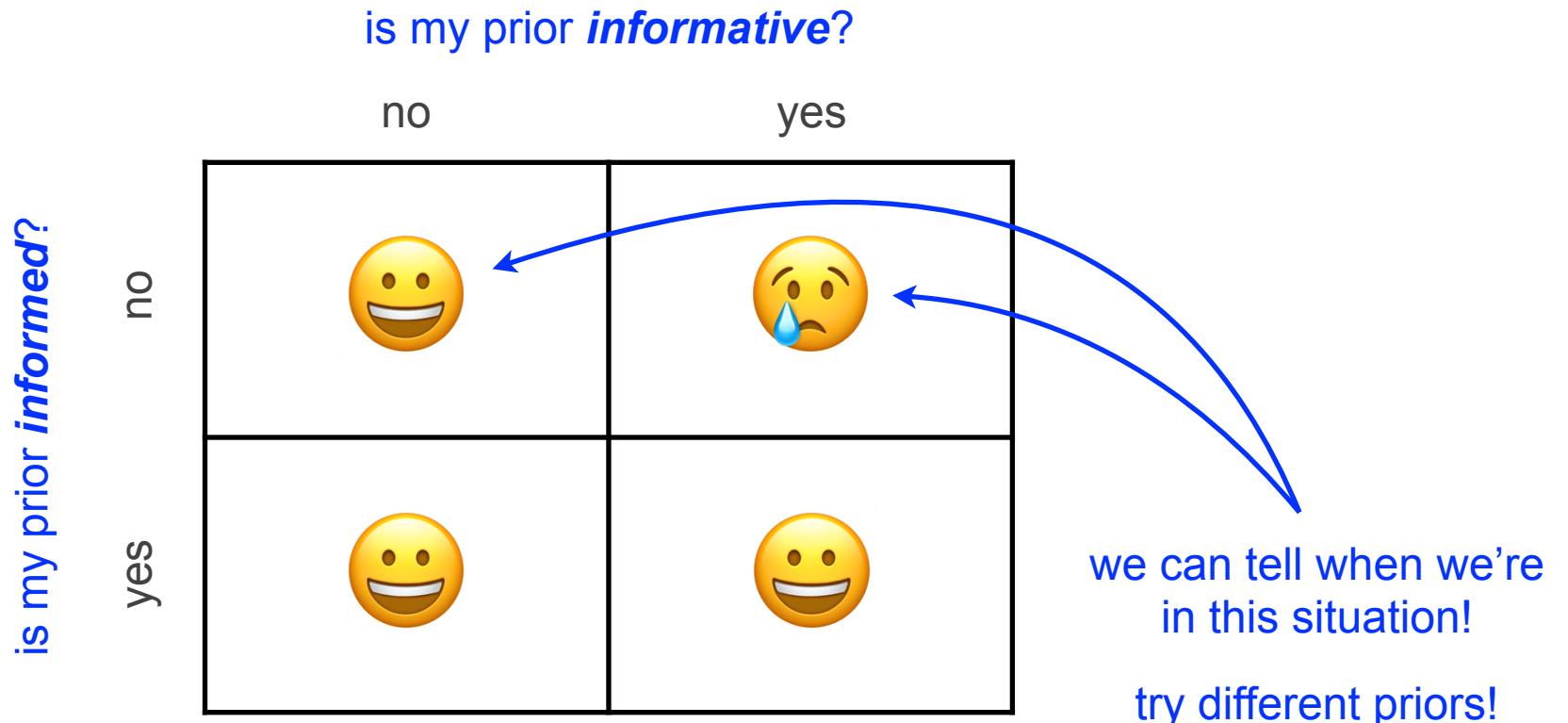
		no	yes
no	no		
	yes		

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Bayesian Inference



Bayesian Inference



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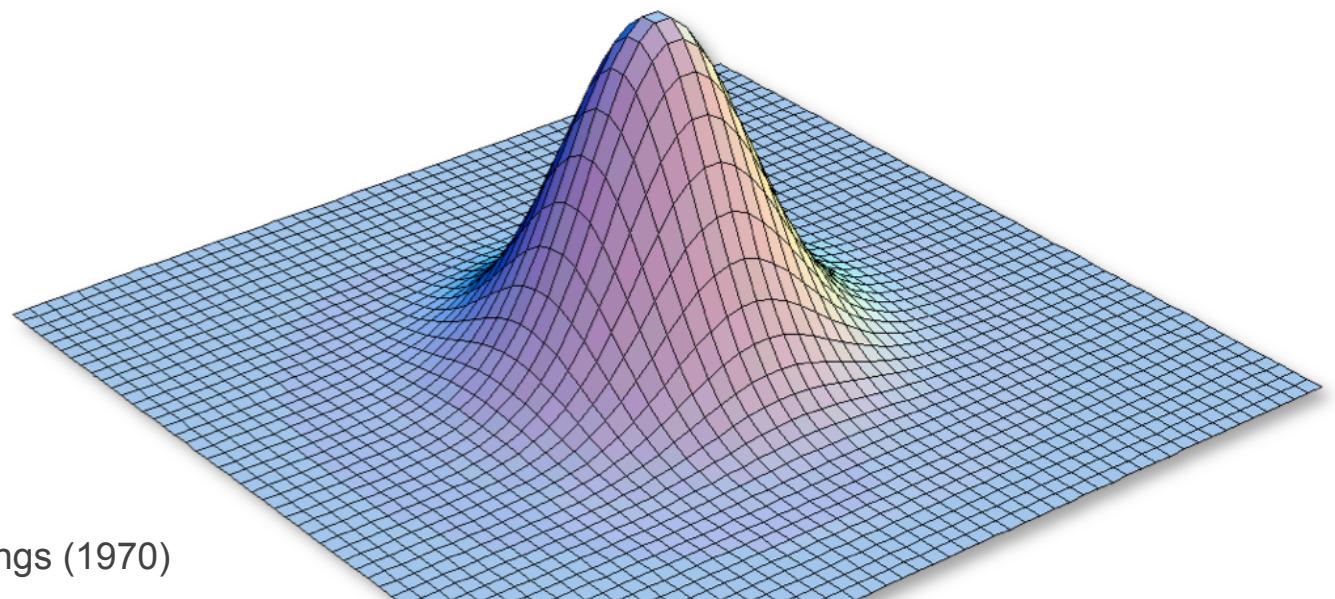
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Approximating the Joint Posterior Probability Density using MCMC

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Programming our MCMC robot...

Our robot parachutes into a random location in the joint posterior density and will explore parameter space by following these simple rules:

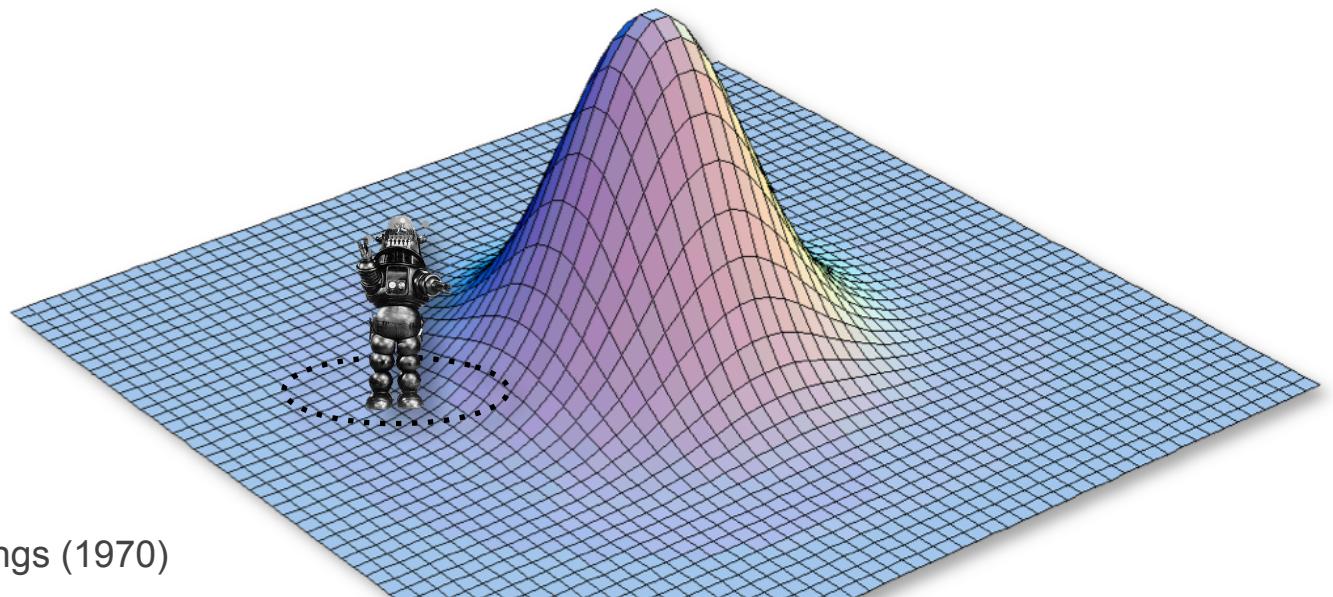


Metropolis et al. (1953); Hastings (1970)

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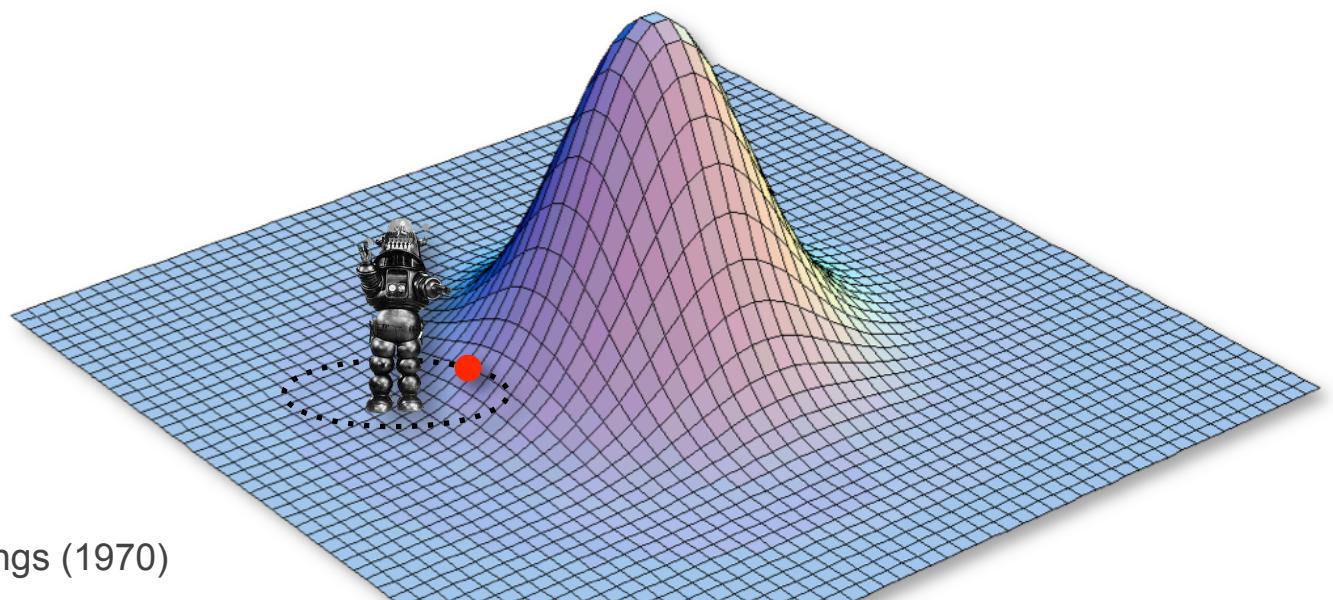
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$$\Pr(\text{Accept}) = 1$$



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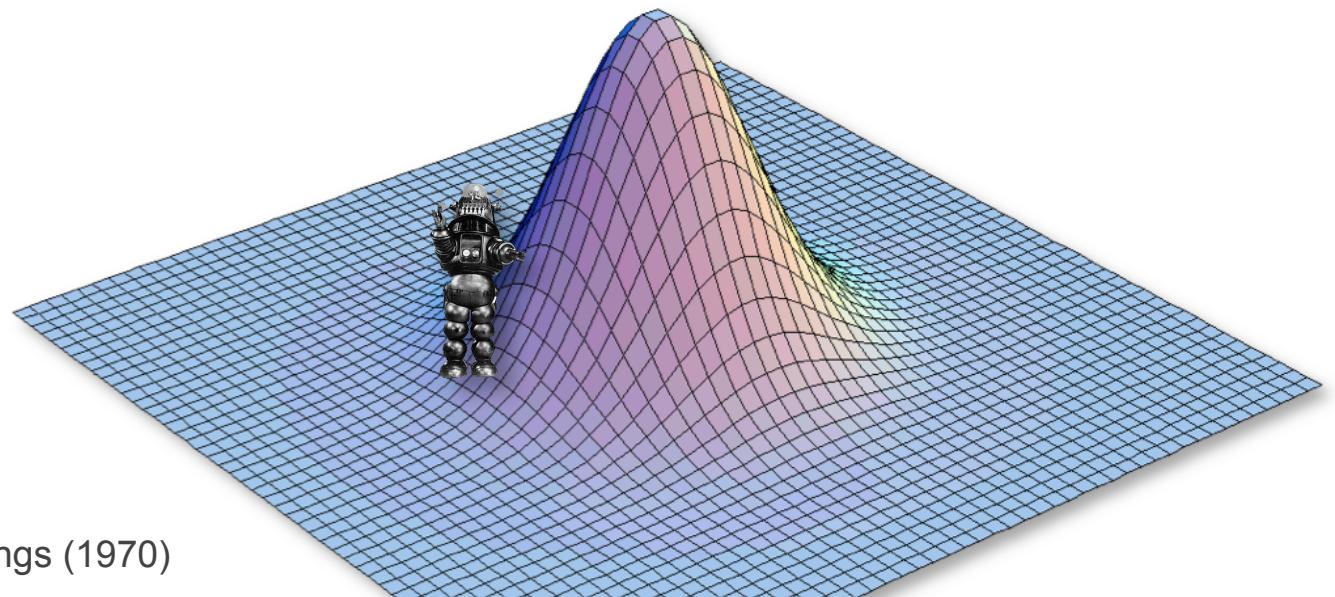
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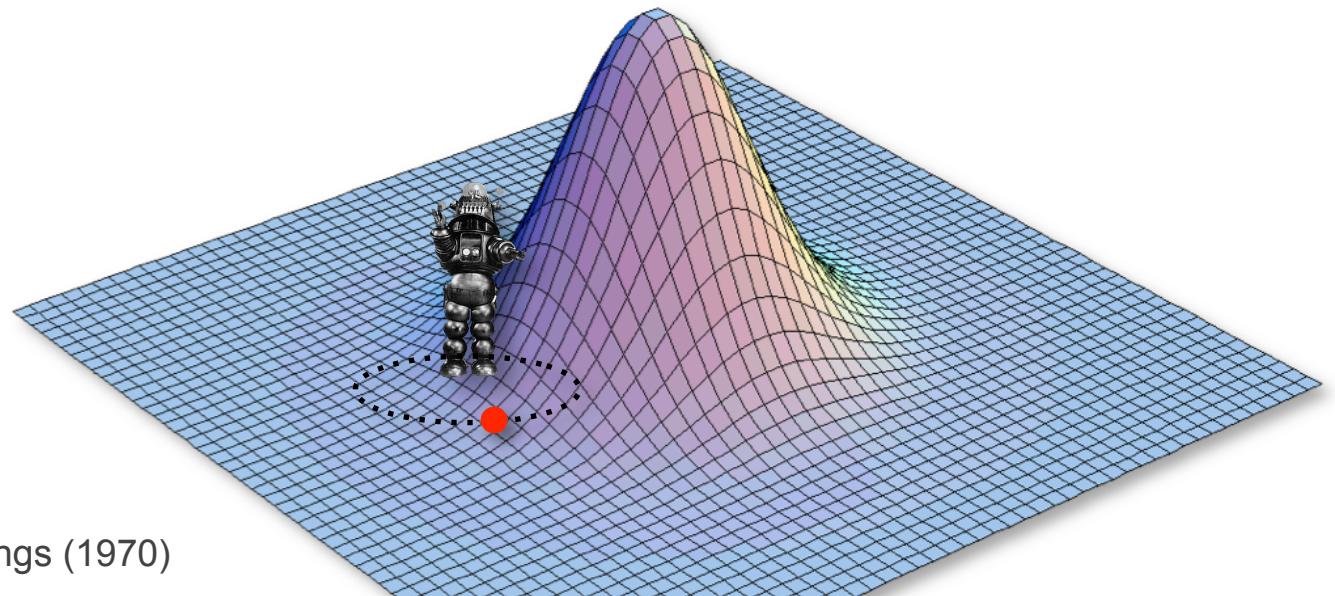
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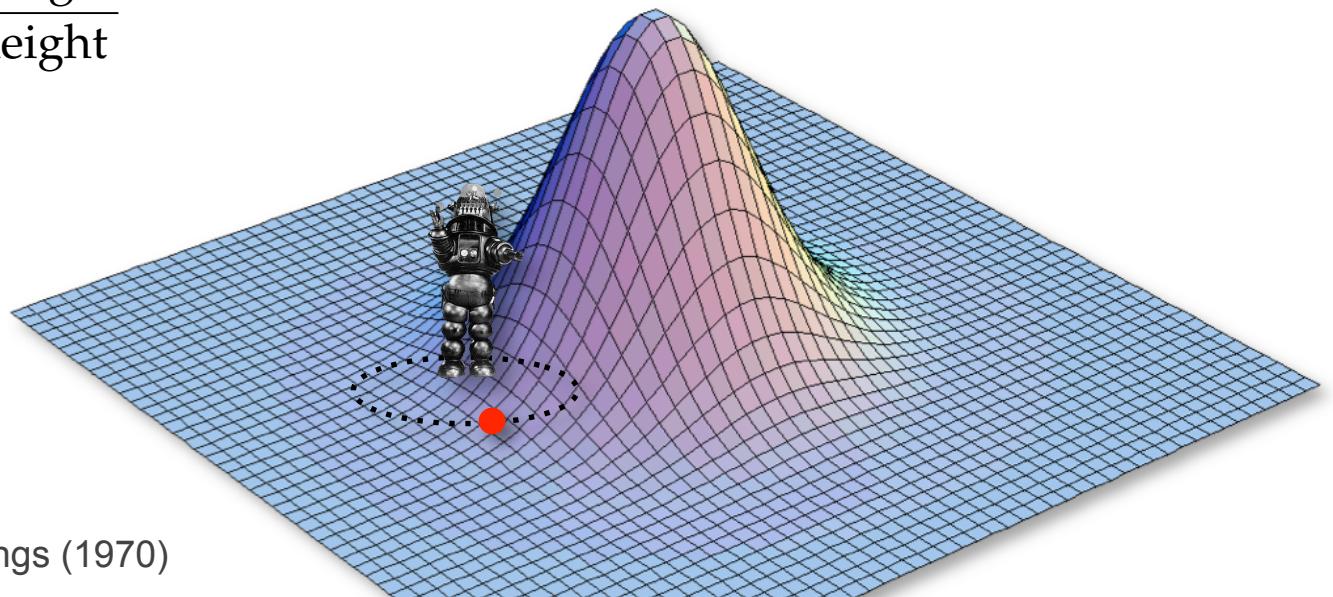
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$$\Pr(\text{Accept}) = \frac{\text{new height}}{\text{old height}}$$



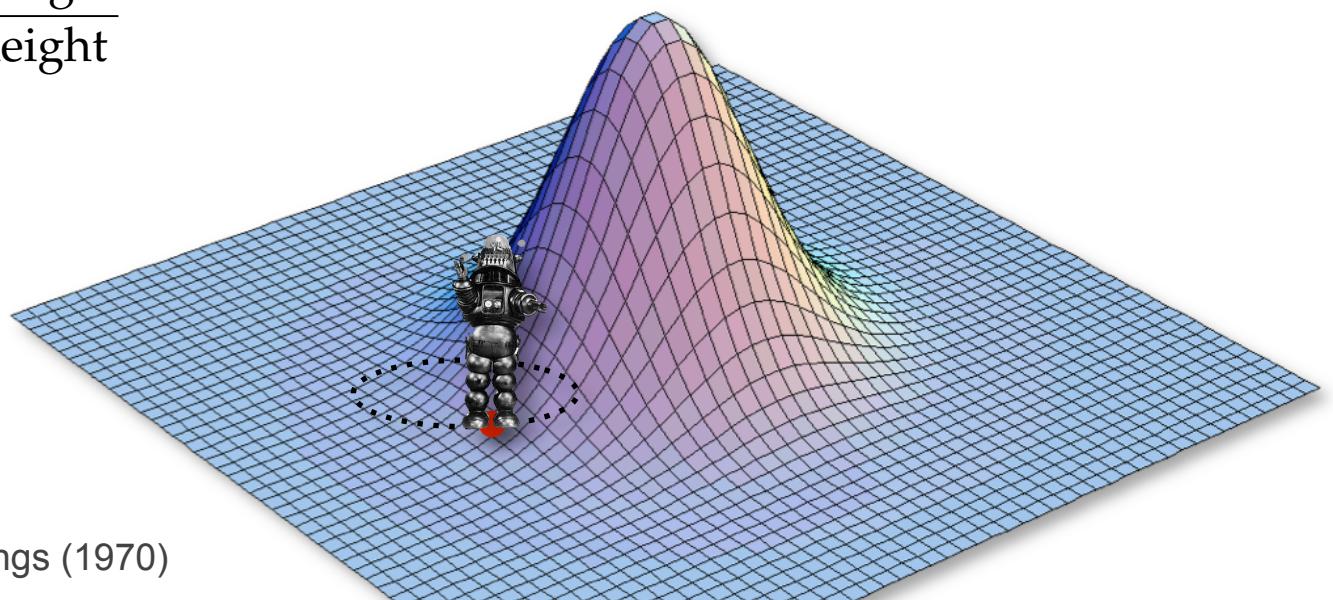
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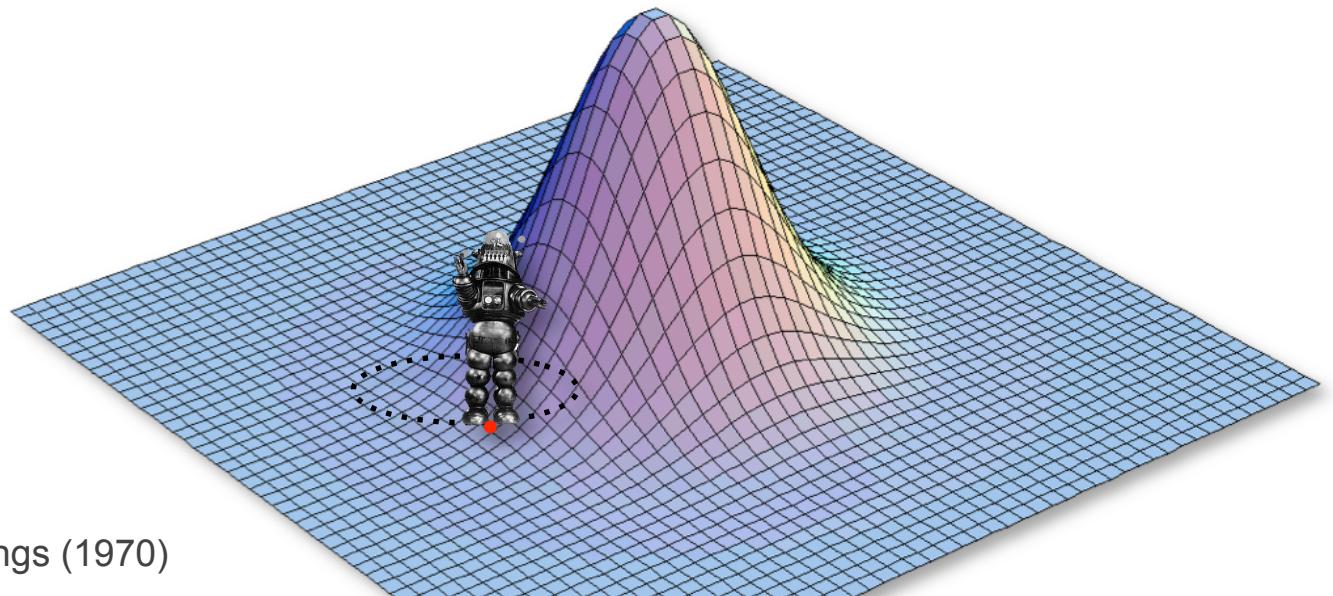


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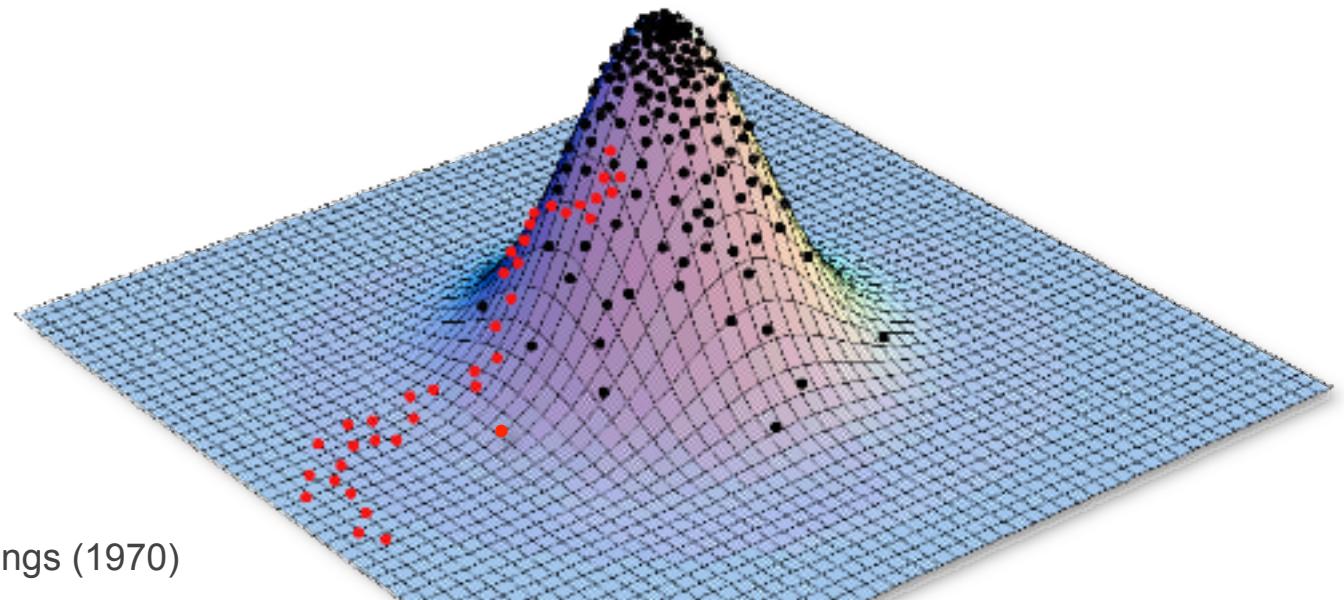


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Metropolis et al. (1953); Hastings (1970)

Approximating the Joint Posterior Probability Density using MCMC

The Metropolis-Hastings algorithm

1. Initialize the chain with some random values for all parameters, including the tree with branch lengths, $\Theta = \{\tau, \nu, \pi, \dots\}$

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# specify a beta prior on x
x ~ dnBeta(1,1)

# place a sliding move on x
moves.append( mvSlide(x, delta = 0.1, weight = 5.0) )
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prior
parameter →

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A code snippet illustrating the Metropolis-Hastings algorithm. The code specifies a beta prior for a parameter x and performs a sliding move on it.

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Annotations:

- A yellow arrow labeled "prior" points to the line `x ~ dnBeta(1,1)`.
- A yellow arrow labeled "proposal weight" points to the line `weight = 5.0`.
- An orange arrow labeled "parameter" points to the variable `x` in the first line of code.

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proposal weight

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```
<scaleOperator scaleFactor="0.75" weight="2">
    <parameter idref="ND5.CP1.kappa"/>
</scaleOperator>
```

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$$R = \min \left[1, \frac{\Pr(X | \theta')}{\Pr(X | \theta)} \times \frac{\Pr(\theta')}{\Pr(\theta)} \times \frac{\Pr(\theta' \rightarrow \theta)}{\Pr(\theta \rightarrow \theta')} \right]$$

likelihood ratio prior ratio proposal ratio

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 - How do we calculate the likelihood for a given parameter value, θ ?

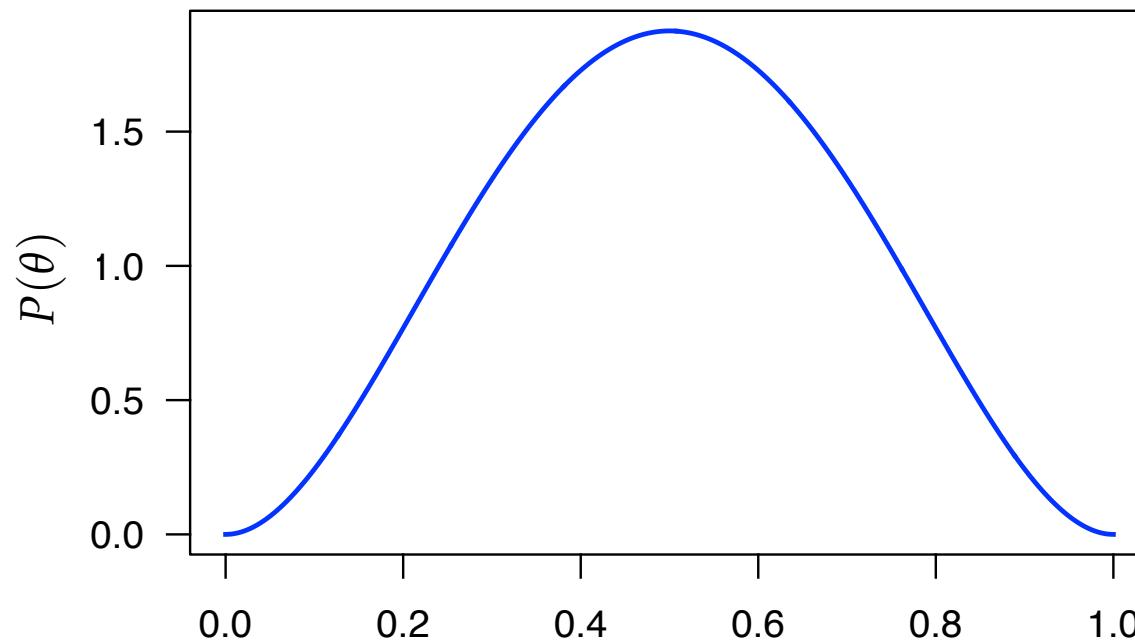
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likelihood ratio prior ratio proposal ratio

Approximating the Joint Posterior Probability Density using MCMC

The prior for each parameter is specified

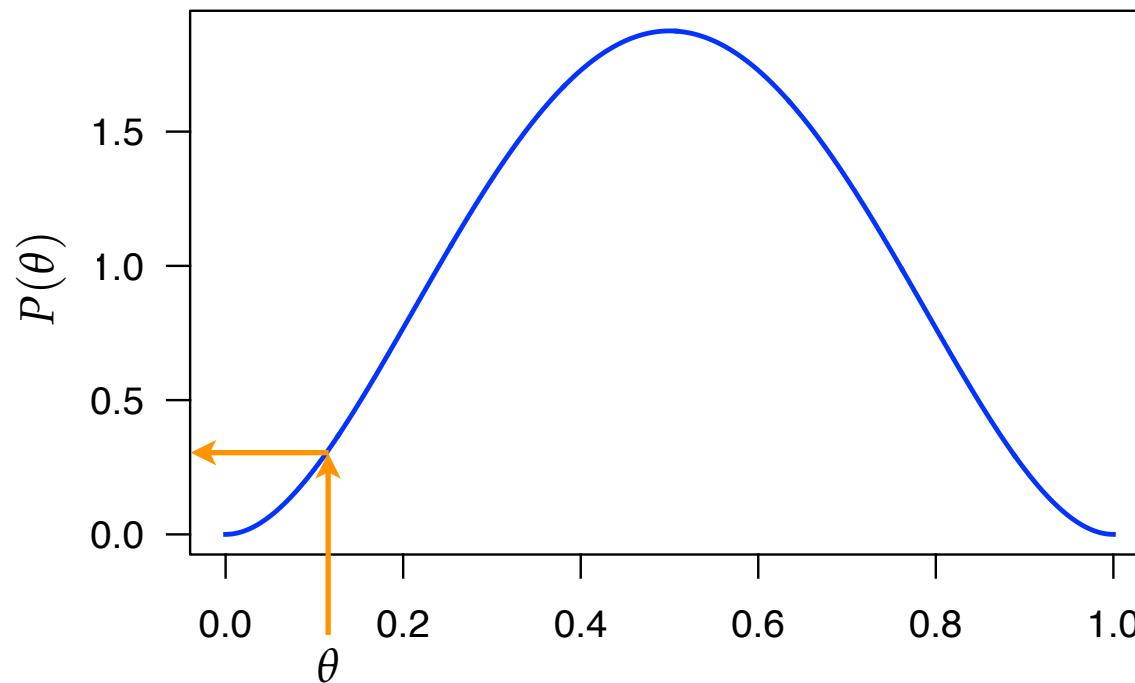
We can just look up the prior probability of a given parameter value



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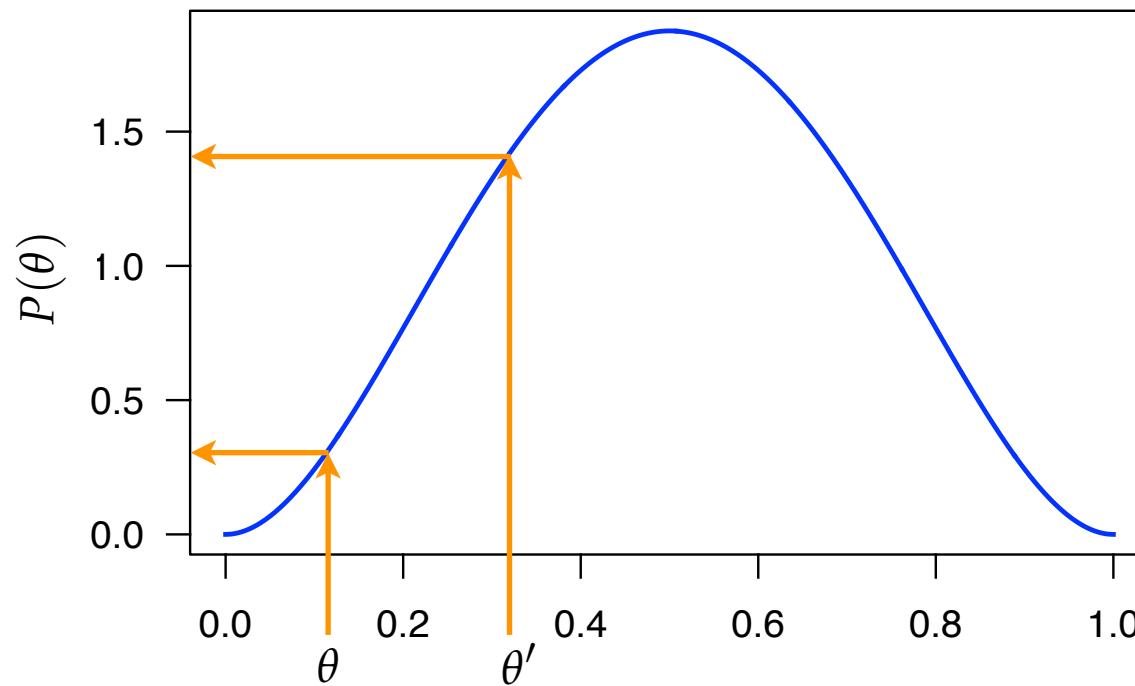
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The prior for each parameter is specified

We can just look up the prior probability of a given parameter value



Approximating the Joint Posterior Probability Density using MCMC

The Metropolis-Hastings algorithm

1. Initialize the chain with some random values for all parameters, including the tree with branch lengths, $\Theta = \{\tau, \nu, \pi, \dots\}$
2. Select a parameter, θ , to update (alter) according to the proposal probabilities
3. Propose a new value, θ' , for the selected parameter via the proposal mechanism
4. Calculate the probability of accepting the proposed change
 - How do we calculate the likelihood for a given parameter value, θ ?
 - How do we calculate the prior for a given parameter value, θ ?

$$R = \min \left[1, \frac{\Pr(X | \theta')}{\Pr(X | \theta)} \times \frac{\Pr(\theta')}{\Pr(\theta)} \times \frac{\Pr(\theta' \rightarrow \theta)}{\Pr(\theta \rightarrow \theta')} \right]$$

likelihood ratio prior ratio proposal ratio

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 - How do we calculate the likelihood for a given parameter value, θ ?
 - How do we calculate the prior for a given parameter value, θ ?
 - How do we calculate the proposal ratio?

$$R = \min \left[1, \frac{\Pr(X | \theta')}{\Pr(X | \theta)} \times \frac{\Pr(\theta')}{\Pr(\theta)} \times \frac{\Pr(\theta' \rightarrow \theta)}{\Pr(\theta \rightarrow \theta')} \right]$$

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likelihood ratio prior ratio

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$$P(\theta' | X) \propto P(X | \theta') P(\theta')$$

$$R = \min \left[1, \frac{\Pr(X | \theta')}{\Pr(X | \theta)} \times \frac{\Pr(\theta')}{\Pr(\theta)} \right]$$

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

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$$R = \min \left[1, \frac{\Pr(X | \theta')}{\Pr(X | \theta)} \times \frac{\Pr(\theta')}{\Pr(\theta)} \right]$$

$$\frac{P(\theta' | X)}{P(\theta | X)} = \frac{P(X | \theta') P(\theta')}{P(X | \theta) P(\theta)}$$

Approximating the Joint Posterior Probability Density using MCMC

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 - How do we calculate the likelihood for a given parameter value, θ ?
 - How do we calculate the prior for a given parameter value, θ ?
 - That means we can explore the posterior probability density without having to compute the marginal likelihood!!

$$R = \min \left[1, \frac{\Pr(X | \theta')}{\Pr(X | \theta)} \times \frac{\Pr(\theta')}{\Pr(\theta)} \right]$$

$$\frac{P(\theta' | X)}{P(\theta | X)} = \frac{P(X | \theta') P(\theta')}{P(X | \theta) P(\theta)}$$

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3. Propose a new value, θ' , for the selected parameter via the proposal mechanism
4. Calculate the probability of accepting the proposed change
5. Generate a uniform random variable, $u \sim \text{Uniform}(0,1)$, accept if $u < R$

$$R = \min \left[1, \frac{\Pr(X | \theta')}{\Pr(X | \theta)} \times \frac{\Pr(\theta')}{\Pr(\theta)} \times \frac{\Pr(\theta' \rightarrow \theta)}{\Pr(\theta \rightarrow \theta')} \right]$$

Approximating the Joint Posterior Probability Density using MCMC

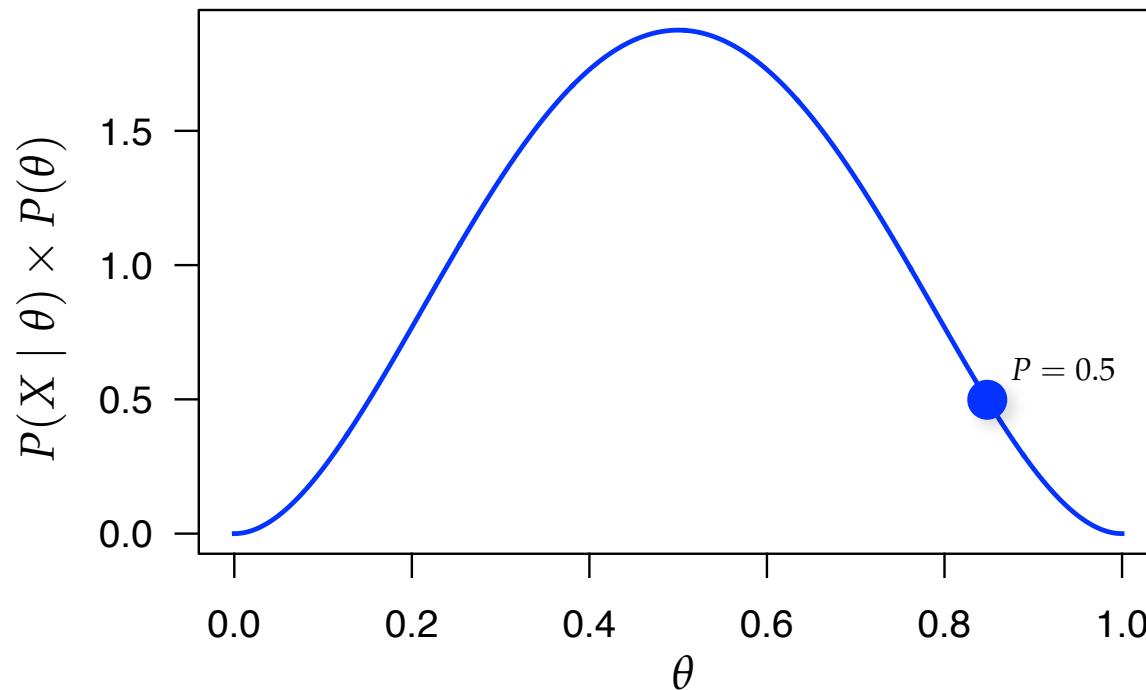
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4. Calculate the probability of accepting the proposed change
5. Generate a uniform random variable, $u \sim \text{Uniform}(0,1)$, accept if $u < R$
6. Repeat steps 2–5 an ‘adequate’ number of times

$$R = \min \left[1, \frac{\Pr(X | \theta')}{\Pr(X | \theta)} \times \frac{\Pr(\theta')}{\Pr(\theta)} \times \frac{\Pr(\theta' \rightarrow \theta)}{\Pr(\theta \rightarrow \theta')} \right]$$

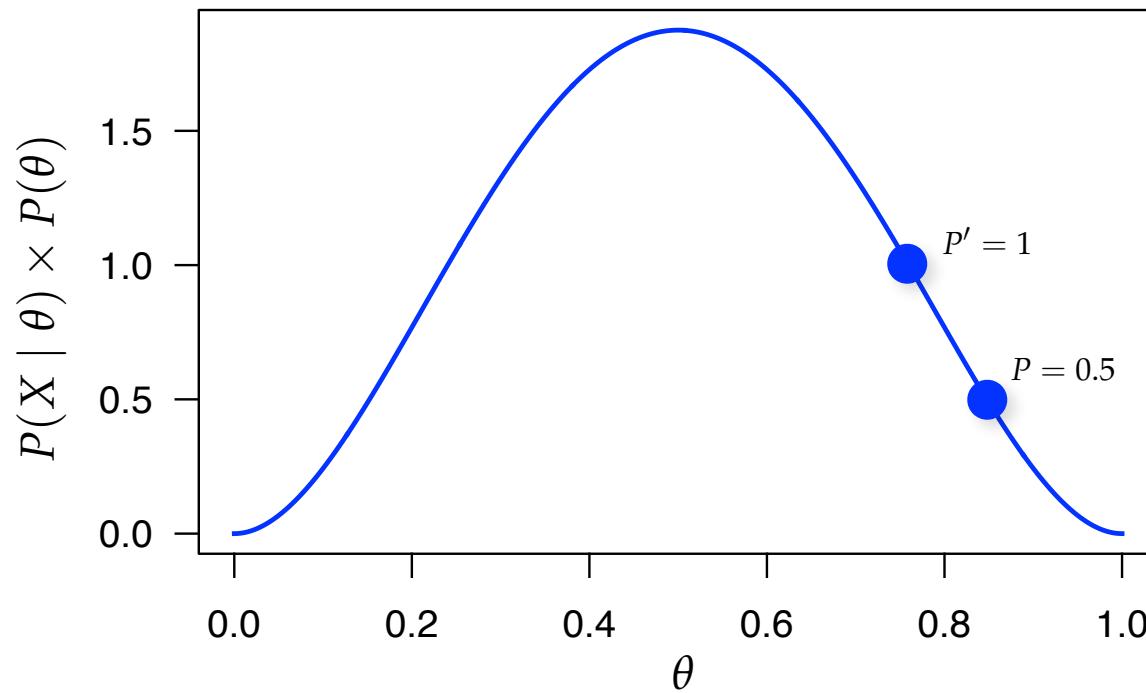
Approximating the Joint Posterior Probability Density using MCMC

The Metropolis-Hastings algorithm



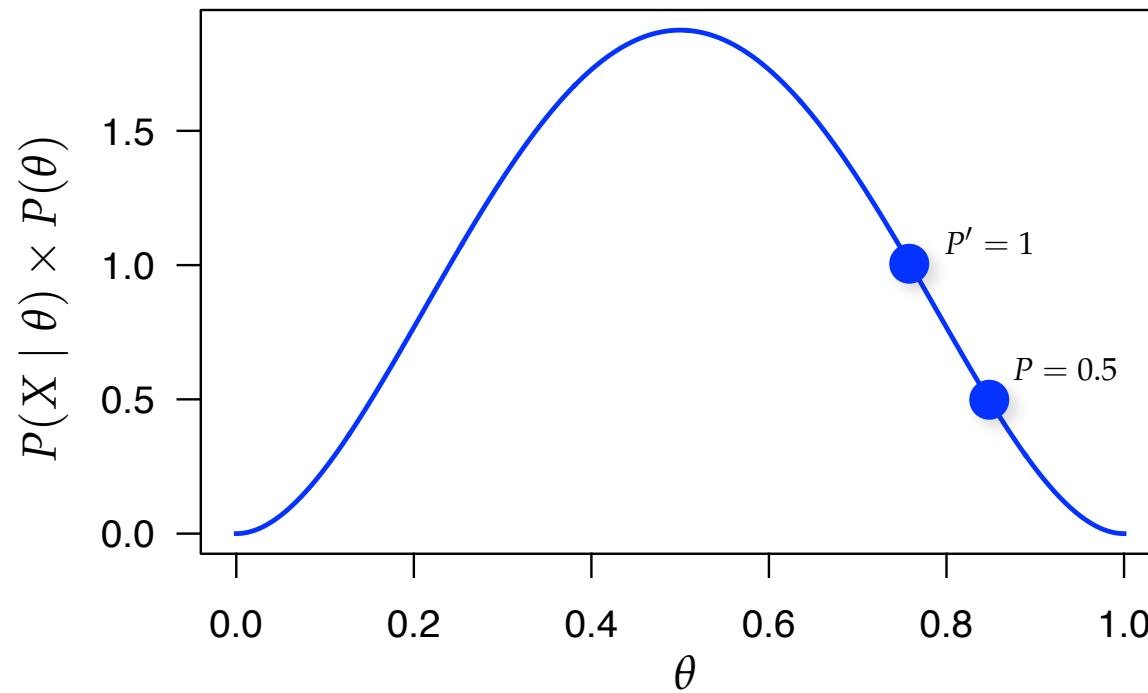
Approximating the Joint Posterior Probability Density using MCMC

The Metropolis-Hastings algorithm



Approximating the Joint Posterior Probability Density using MCMC

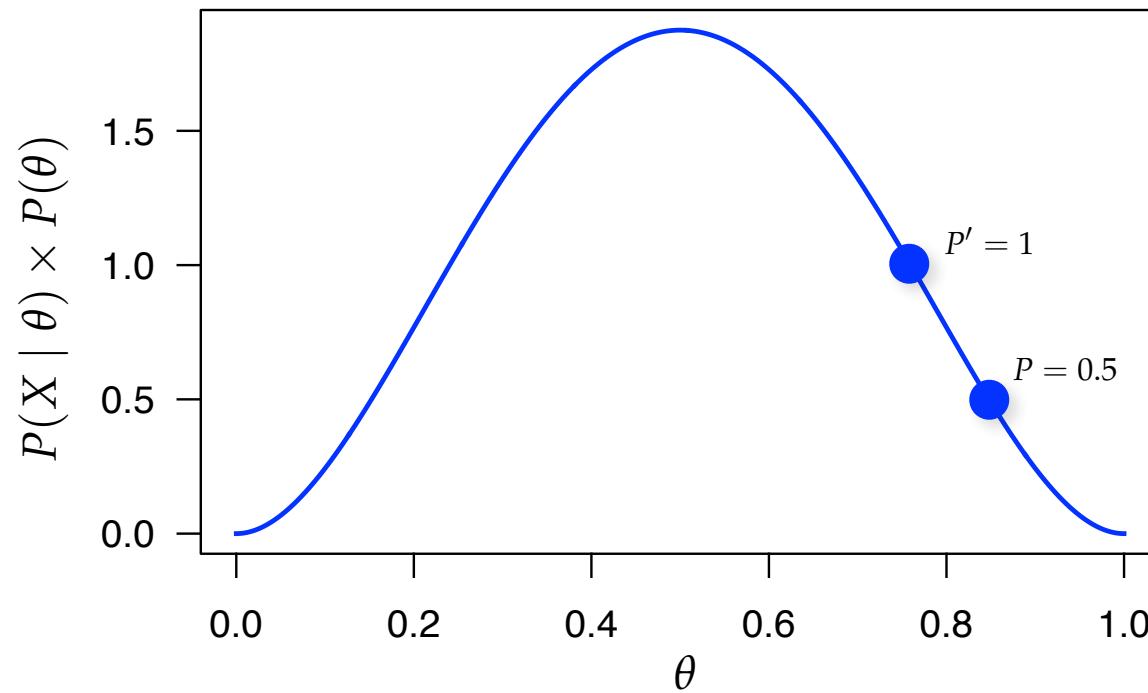
The Metropolis-Hastings algorithm



$$R = \min \left[1, \frac{1}{0.5} \right] = 1$$

Approximating the Joint Posterior Probability Density using MCMC

The Metropolis-Hastings algorithm

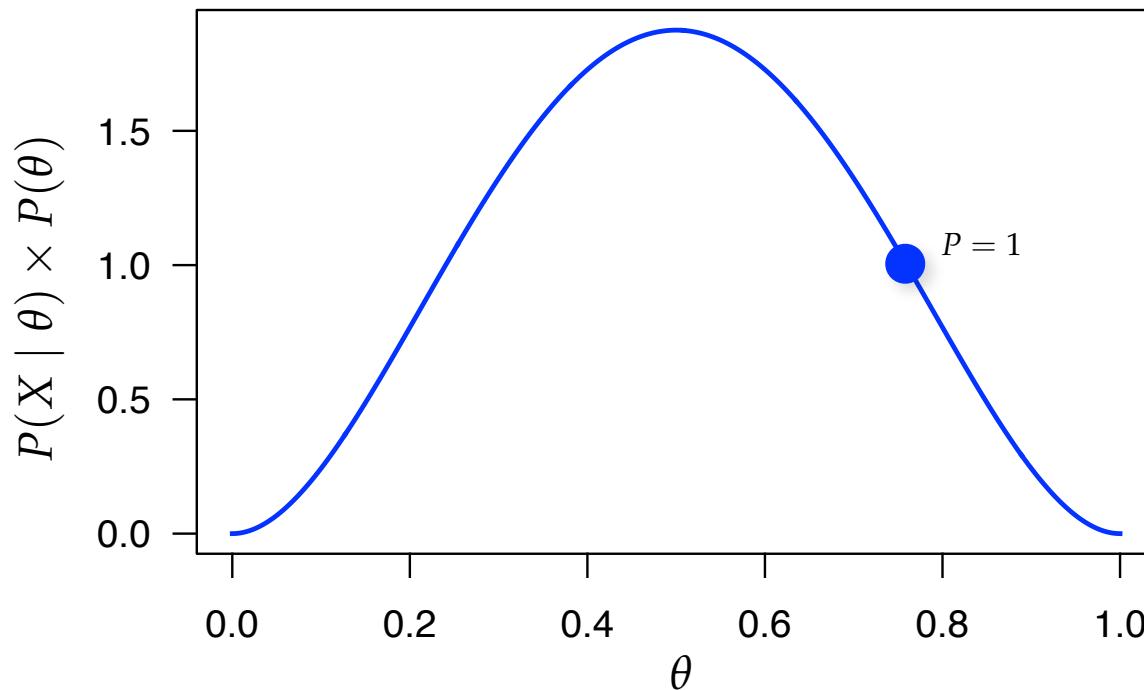


$$R = \min \left[1, \frac{1}{0.5} \right] = 1$$

$$u \sim \text{Uniform}(0, 1), \quad u = 0.983$$

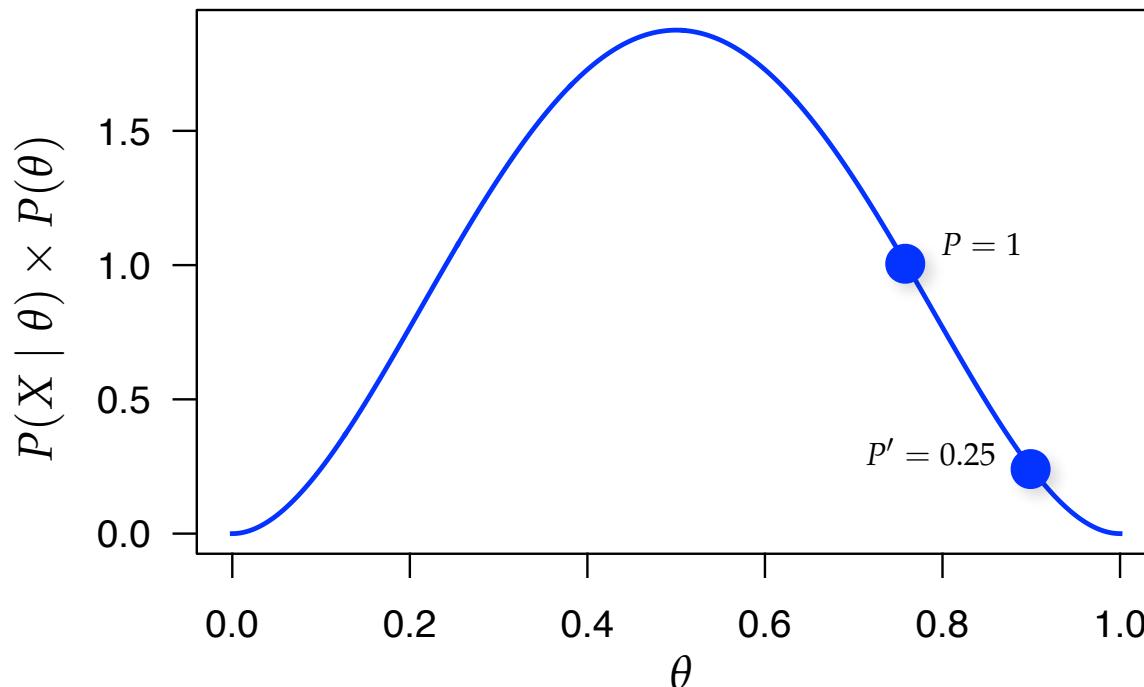
Approximating the Joint Posterior Probability Density using MCMC

The Metropolis-Hastings algorithm



Approximating the Joint Posterior Probability Density using MCMC

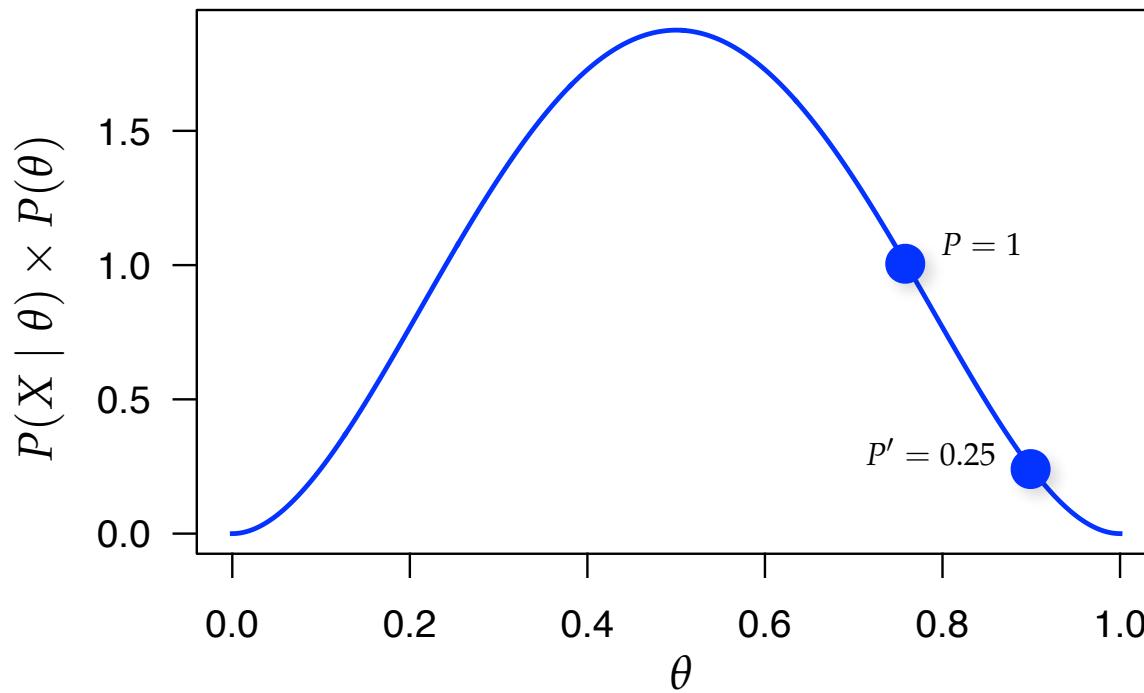
The Metropolis-Hastings algorithm



$$R = \min \left[1, \frac{0.25}{1} \right] = 0.25$$

Approximating the Joint Posterior Probability Density using MCMC

The Metropolis-Hastings algorithm

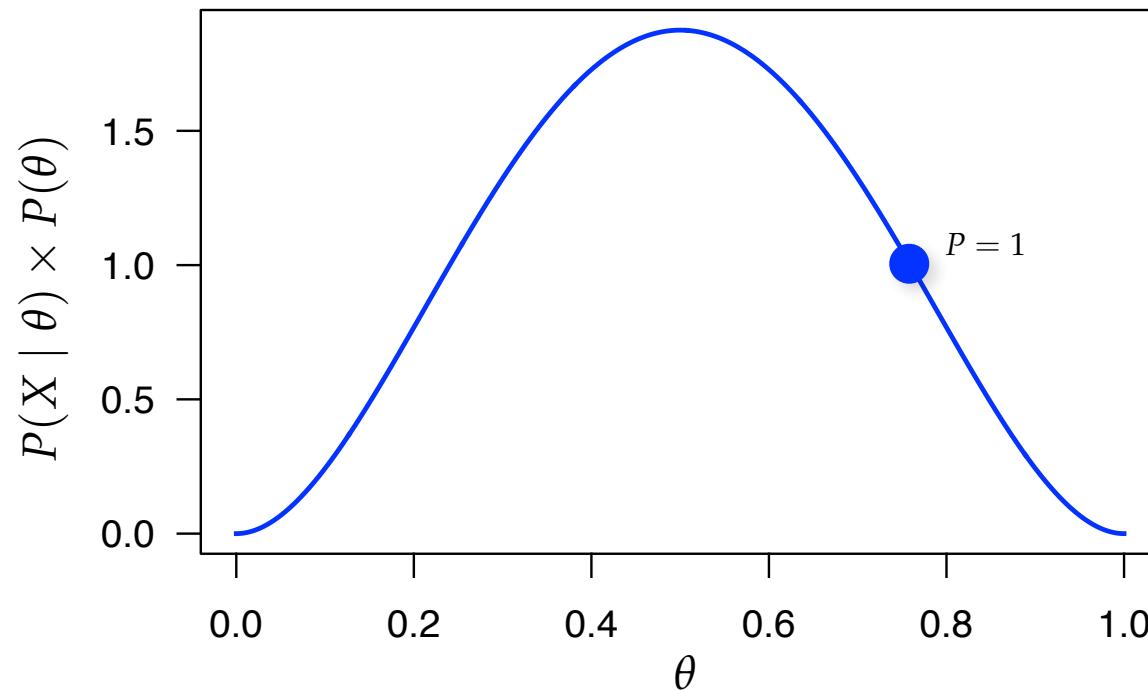


$$R = \min \left[1, \frac{0.25}{1} \right] = 0.25$$

$$u \sim \text{Uniform}(0, 1), \quad u = 0.261$$

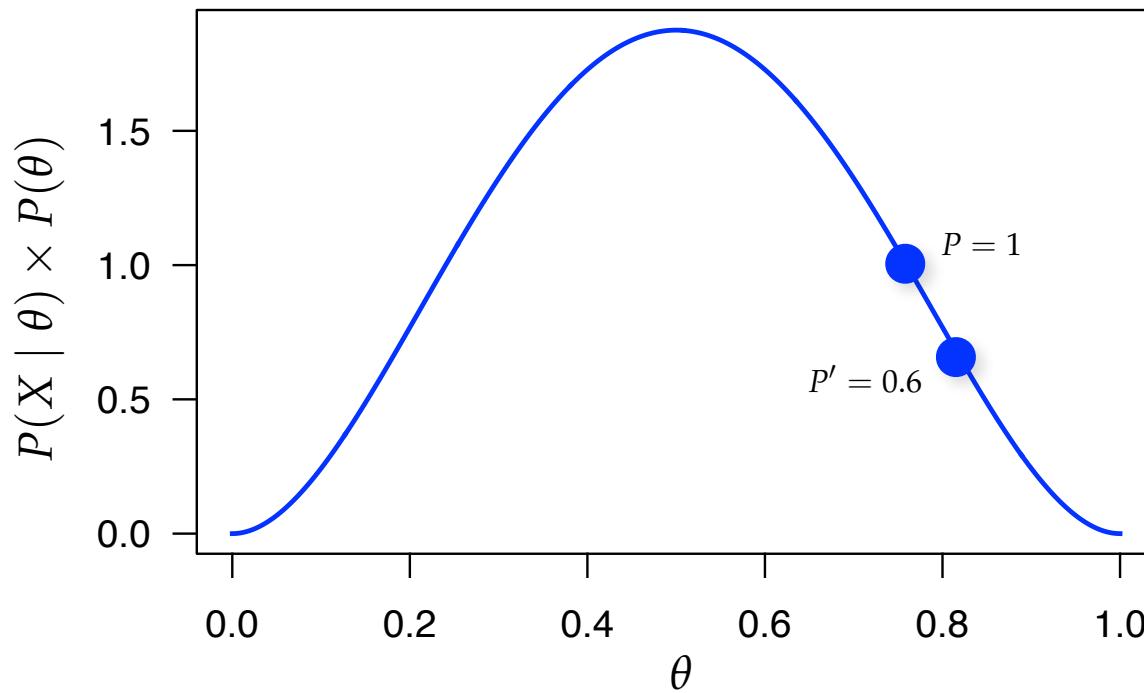
Approximating the Joint Posterior Probability Density using MCMC

The Metropolis-Hastings algorithm



Approximating the Joint Posterior Probability Density using MCMC

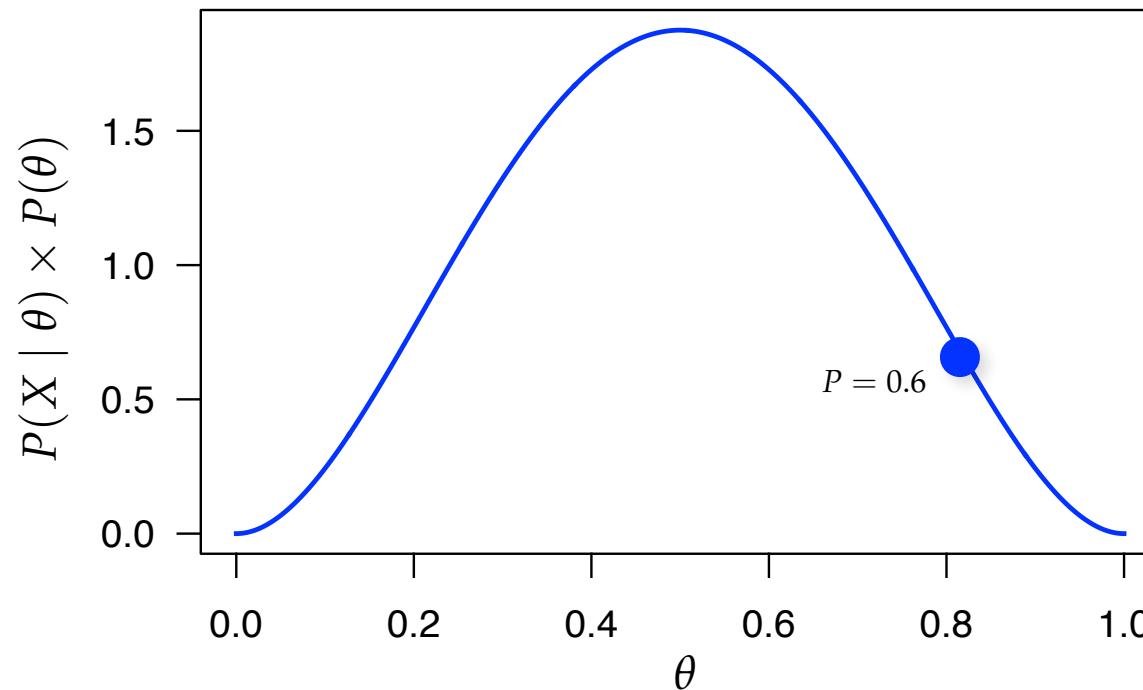
The Metropolis-Hastings algorithm



$$R = \min \left[1, \frac{0.6}{1} \right] = 0.6$$

Approximating the Joint Posterior Probability Density using MCMC

The Metropolis-Hastings algorithm

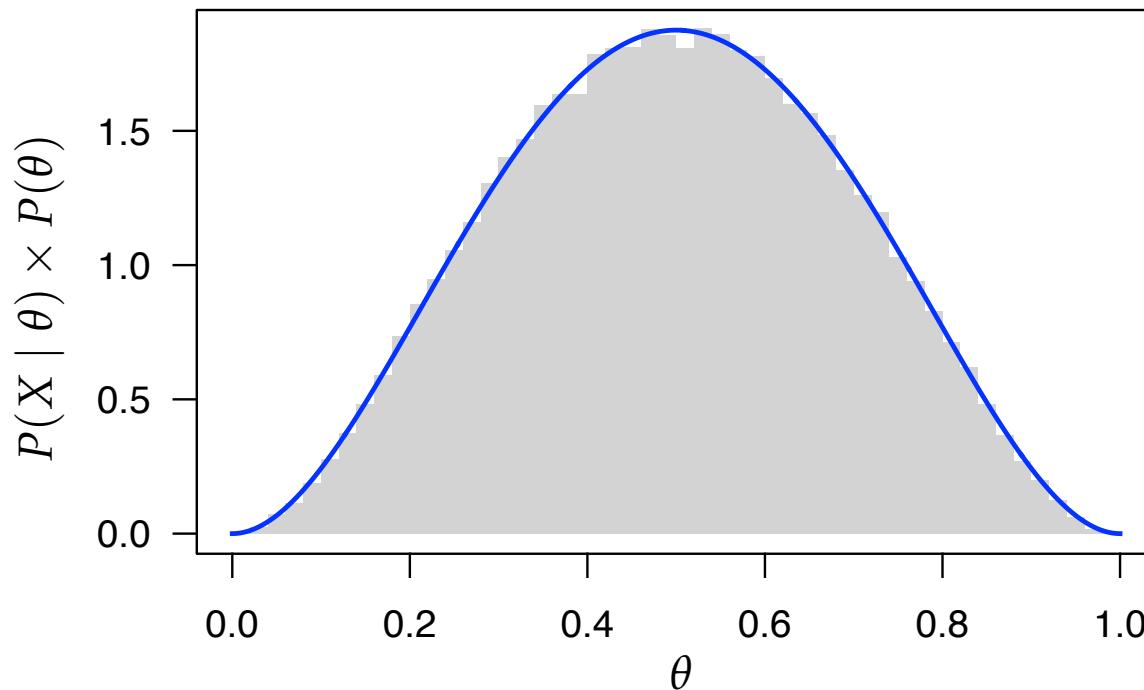


$$R = \min \left[1, \frac{0.6}{1} \right] = 0.6$$

$$u \sim \text{Uniform}(0, 1), \quad u = 0.128$$

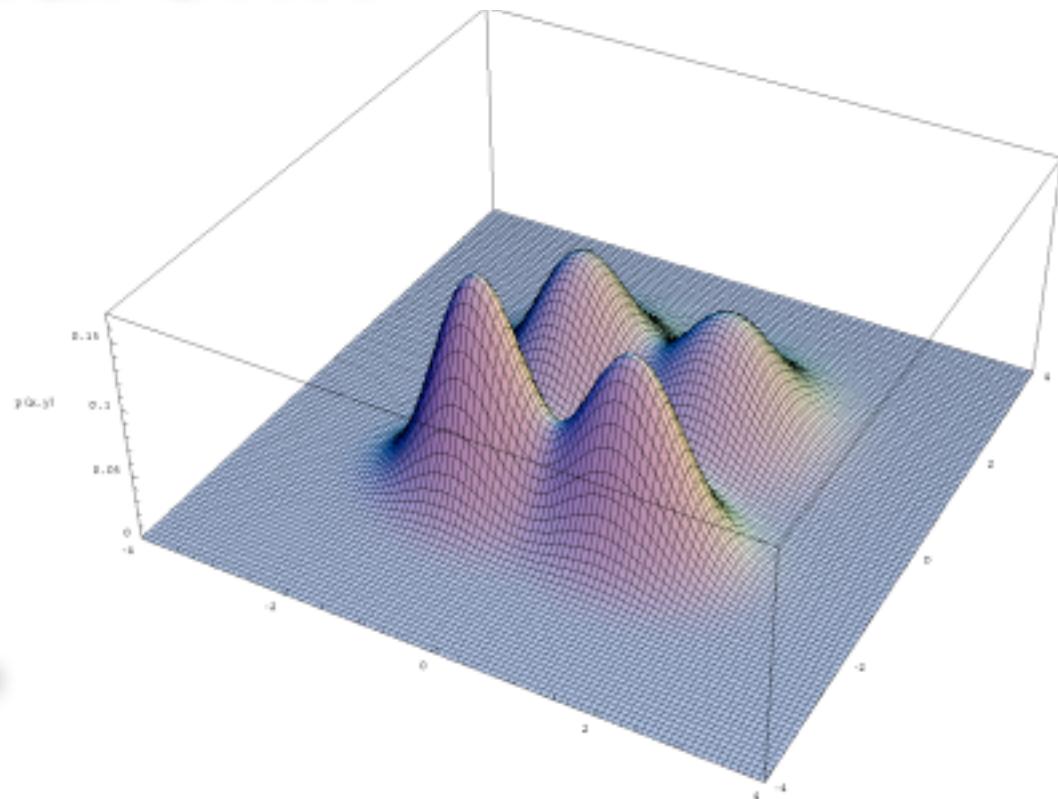
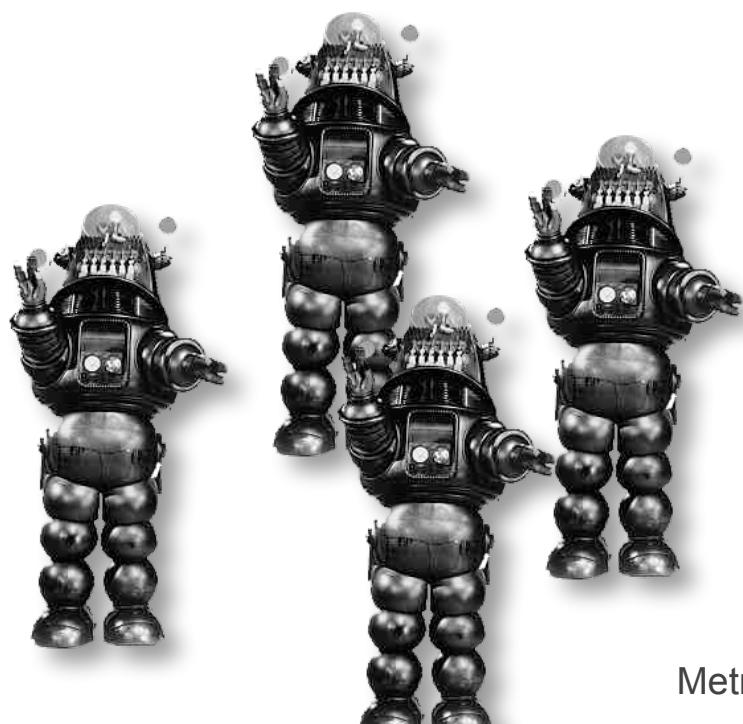
Approximating the Joint Posterior Probability Density using MCMC

The Metropolis-Hastings algorithm



Approximating the Joint Posterior Probability Density using MCMC

Robot Squadron!!



Metropolis et al. (1953); Hastings (1970)

Approximating the Joint Posterior Probability Density using Metropolis-Coupled MCMC

The MC³ algorithm

1. Initialize N independent M-H MCMC chains with random values for all parameters.

Approximating the Joint Posterior Probability Density using Metropolis-Coupled MCMC

The MC³ algorithm

1. Initialize N independent M-H MCMC chains with random values for all parameters.
2. The chains are incrementally heated, such that the first chain is cold (unmodified).
 - posterior of chain i is raised to a power, β_i : the heat of chain $i = 1/(1 + iT)$

chain	temperature
0	0.25
1	
2	
3	

Approximating the Joint Posterior Probability Density using Metropolis-Coupled MCMC

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chain	temperature	
0	0.25	
0	1.00	$\beta_0 = 1/(1 + 0 \cdot 0.25)$
1		
2		
3		

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chain	temperature	
0	0.25	
0	1.00	$\beta_0 = 1/(1 + 0 \cdot 0.25)$
1	0.80	$\beta_1 = 1/(1 + 1 \cdot 0.25)$
2		
3		

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chain	temperature	
0	0.25	
0	1.00	$\beta_0 = 1/(1 + 0 \cdot 0.25)$
1	0.80	$\beta_1 = 1/(1 + 1 \cdot 0.25)$
2	0.67	$\beta_2 = 1/(1 + 2 \cdot 0.25)$
3		

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chain	temperature	
0	0.25	
0	1.00	$\beta_0 = 1/(1 + 0 \cdot 0.25)$
1	0.80	$\beta_1 = 1/(1 + 1 \cdot 0.25)$
2	0.67	$\beta_2 = 1/(1 + 2 \cdot 0.25)$
3	0.57	$\beta_3 = 1/(1 + 3 \cdot 0.25)$

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0	0.25	
0	1.00	$\beta_0 = 1/(1 + 0 \cdot 0.25)$
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2	0.67	$\beta_2 = 1/(1 + 2 \cdot 0.25)$
3	0.57	$\beta_3 = 1/(1 + 3 \cdot 0.25)$

- the incremental heating successively ‘flattens’ the posterior visited by each chain by making the acceptance probability of the i^{th} chain more ‘permissive’:

$$R_i = \min \left[1, \left(\frac{\Pr(X | \theta')}{\Pr(X | \theta)} \times \frac{\Pr(\theta')}{\Pr(\theta)} \right)^{\beta_i} \times \frac{\Pr(\theta' \rightarrow \theta)}{\Pr(\theta \rightarrow \theta')} \right]$$

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0	0.25	
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- this allows heated chains to more readily traverse regions of low probability.

Approximating the Joint Posterior Probability Density using Metropolis-Coupled MCMC

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0	0.25	
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- this allows heated chains to more readily traverse regions of low probability.
- the degree of incremental heating is controlled by the temperature parameter, T .

Approximating the Joint Posterior Probability Density using Metropolis-Coupled MCMC

The MC³ algorithm

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 - posterior of chain i is raised to a power, β_i : the heat of chain $i = 1/(1 + iT)$

chain	temperature	
	0.25	0.20
0	1.00	1.00
1	0.80	0.83
2	0.67	0.71
3	0.57	0.63

- the incremental heating successively ‘flattens’ the posterior visited by each chain by making the acceptance probability of the i^{th} chain more ‘permissive’:

$$R_i = \min \left[1, \left(\frac{\Pr(X | \theta')}{\Pr(X | \theta)} \times \frac{\Pr(\theta')}{\Pr(\theta)} \right)^{\beta_i} \times \frac{\Pr(\theta' \rightarrow \theta)}{\Pr(\theta \rightarrow \theta')} \right]$$

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chain	temperature		
	0.25	0.20	0.15
0	1.00	1.00	1.00
1	0.80	0.83	0.87
2	0.67	0.71	0.77
3	0.57	0.63	0.69

- the incremental heating successively ‘flattens’ the posterior visited by each chain by making the acceptance probability of the i^{th} chain more ‘permissive’:

$$R_i = \min \left[1, \left(\frac{\Pr(X | \theta')}{\Pr(X | \theta)} \times \frac{\Pr(\theta')}{\Pr(\theta)} \right)^{\beta_i} \times \frac{\Pr(\theta' \rightarrow \theta)}{\Pr(\theta \rightarrow \theta')} \right]$$

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Approximating the Joint Posterior Probability Density using Metropolis-Coupled MCMC

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chain	temperature			
	0.25	0.20	0.15	0.10
0	1.00	1.00	1.00	1.00
1	0.80	0.83	0.87	0.91
2	0.67	0.71	0.77	0.83
3	0.57	0.63	0.69	0.77

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Approximating the Joint Posterior Probability Density using Metropolis-Coupled MCMC

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2. The chains are incrementally heated, such that the first chain is cold (unmodified).
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		temperature				
		chain	0.25	0.20	0.15	0.10
cold chain	0	1.00	1.00	1.00	1.00	1.00
	1	0.80	0.83	0.87	0.91	
	2	0.67	0.71	0.77	0.83	
	3	0.57	0.63	0.69	0.77	

- the incremental heating successively ‘flattens’ the posterior visited by each chain by making the acceptance probability of the i^{th} chain more ‘permissive’:

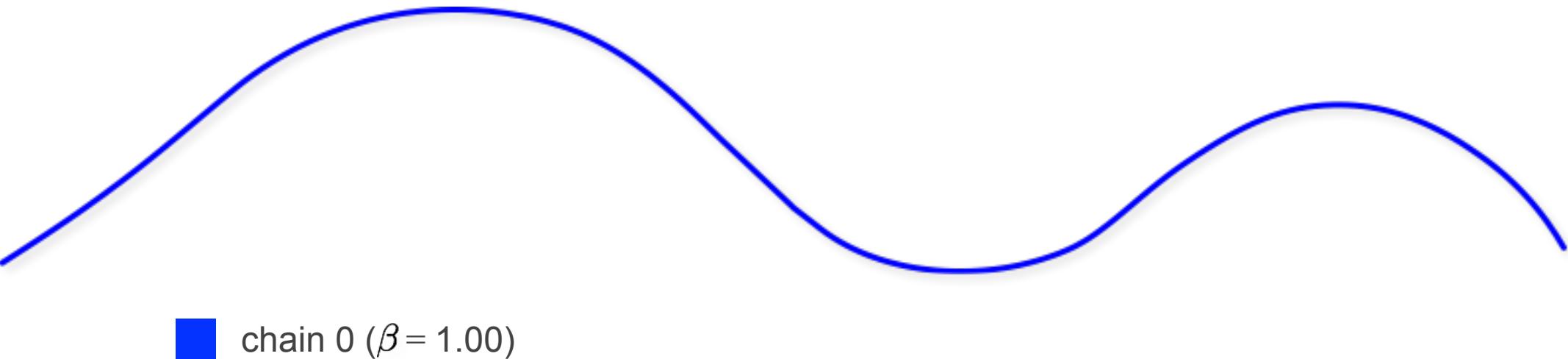
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- this allows heated chains to more readily traverse regions of low probability.
- the degree of incremental heating is controlled by the temperature parameter, T .
- samples are only collected by the ‘cold’ chain (*i.e.*, the undistorted posterior).

Approximating the Joint Posterior Probability Density using Metropolis-Coupled MCMC

The MC³ algorithm

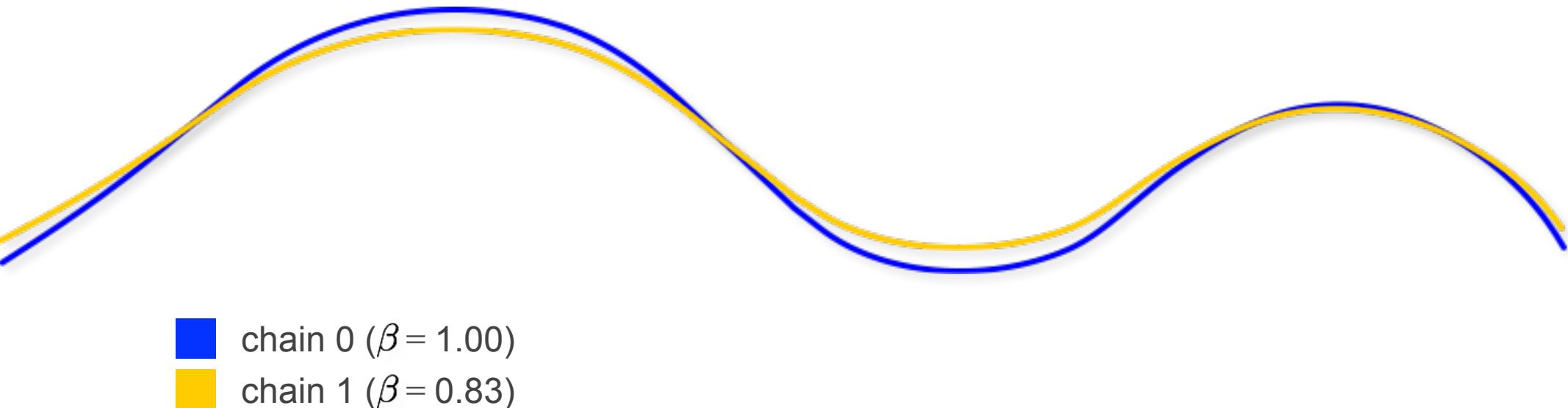
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 - posterior of chain i is raised to a power, β_i : the heat of chain $i = 1/(1 + iT)$
 - the cold chain samples the true posterior, whereas the heated chains sample successively ‘flattened’ distortions of the posterior



Approximating the Joint Posterior Probability Density using Metropolis-Coupled MCMC

The MC³ algorithm

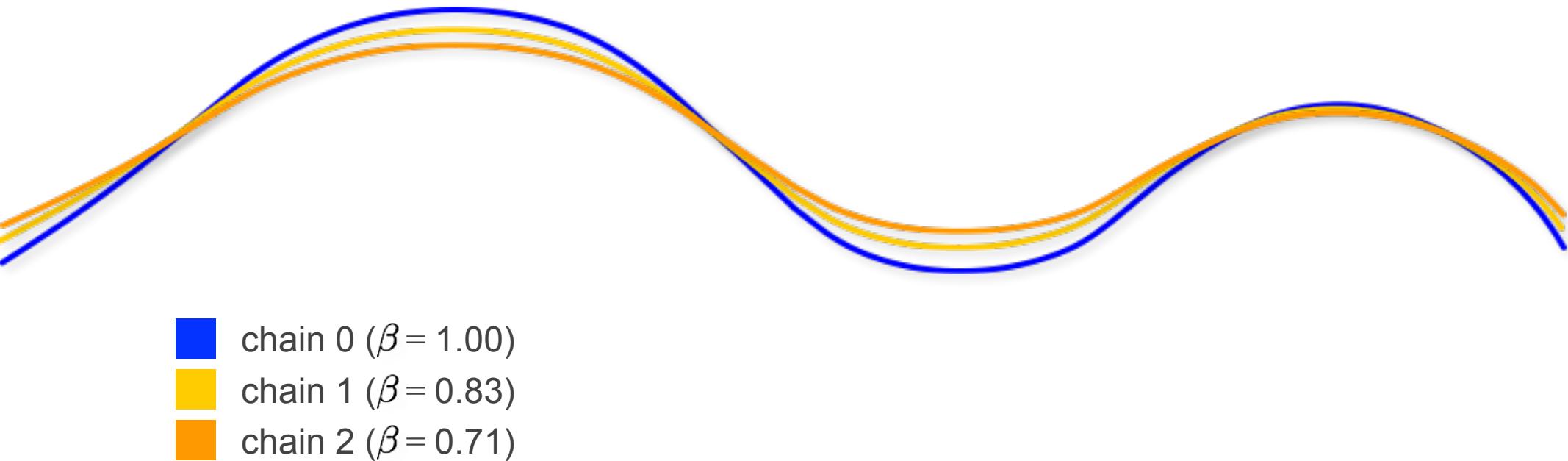
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Approximating the Joint Posterior Probability Density using Metropolis-Coupled MCMC

The MC³ algorithm

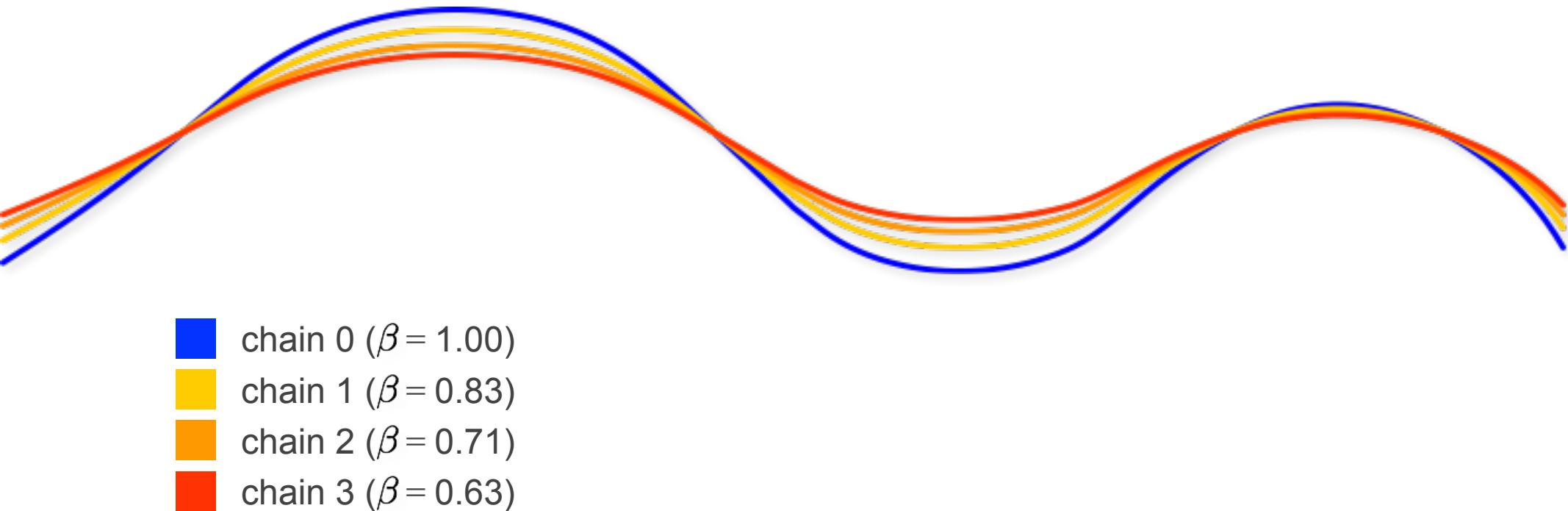
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Approximating the Joint Posterior Probability Density using Metropolis-Coupled MCMC

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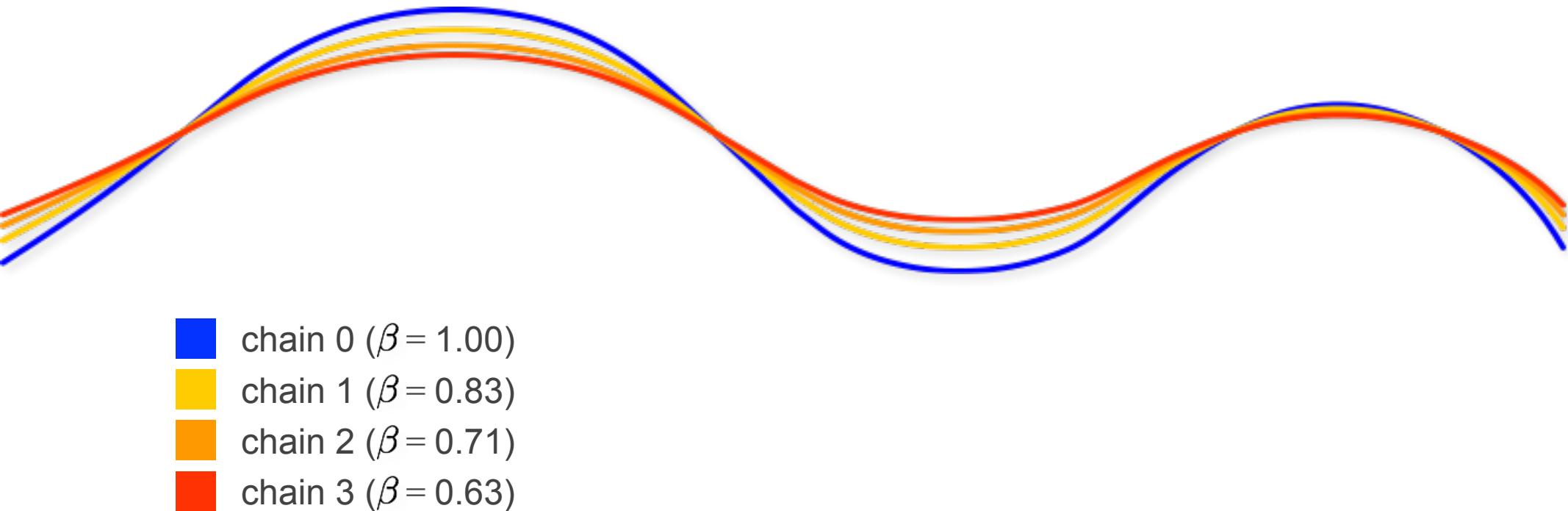
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 - the cold chain samples the true posterior, whereas the heated chains sample successively ‘flattened’ distortions of the posterior



Approximating the Joint Posterior Probability Density using Metropolis-Coupled MCMC

The MC³ algorithm

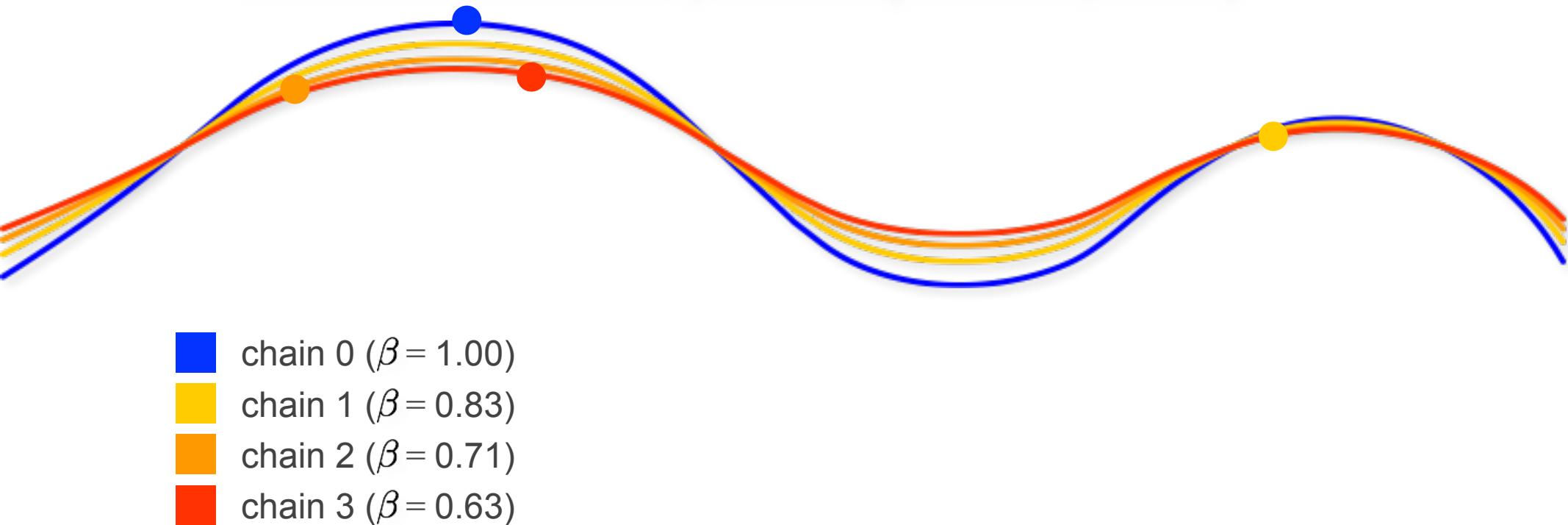
1. Initialize N independent M-H MCMC chains with random values for all parameters.
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 - posterior of chain i is raised to a power, β_i : the heat of chain $i = 1/(1 + iT)$
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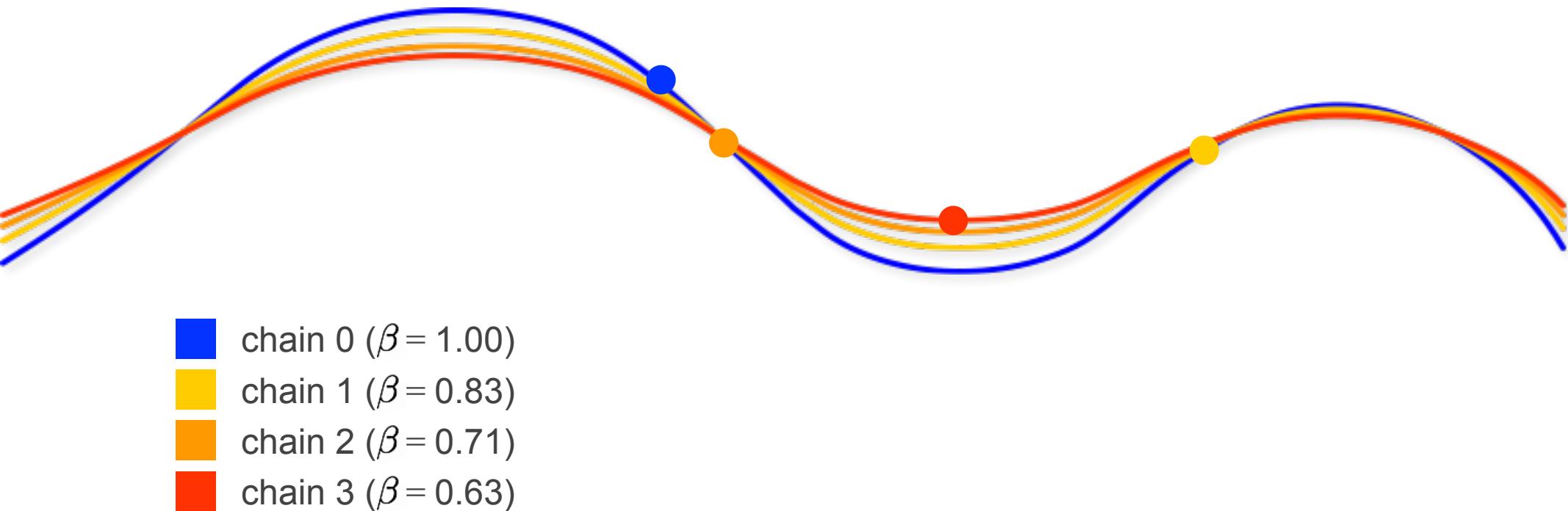
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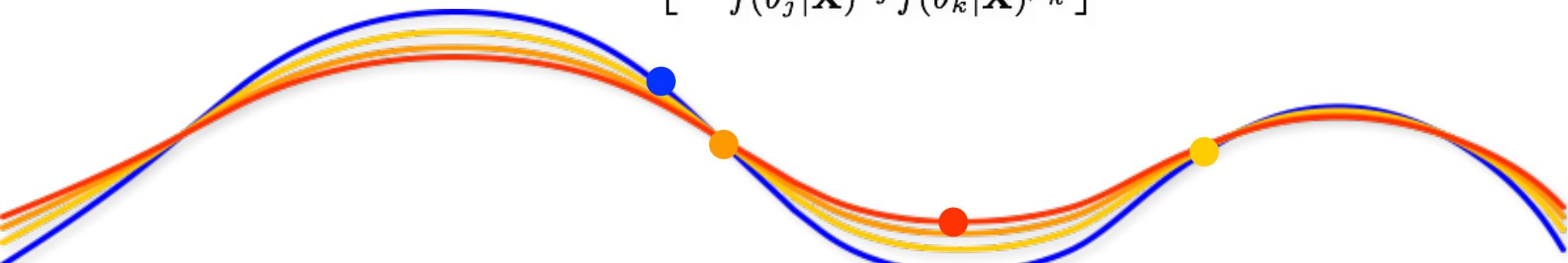


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1. Initialize N independent M-H MCMC chains with random values for all parameters.
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3. At prescribed intervals, two chains are randomly selected to swap.
 - we compute the acceptance probability of swapping the two chains.

$$R = \min \left[1, \frac{f(\theta_k | \mathbf{X})^{\beta_j} f(\theta_j | \mathbf{X})^{\beta_k}}{f(\theta_j | \mathbf{X})^{\beta_j} f(\theta_k | \mathbf{X})^{\beta_k}} \right]$$

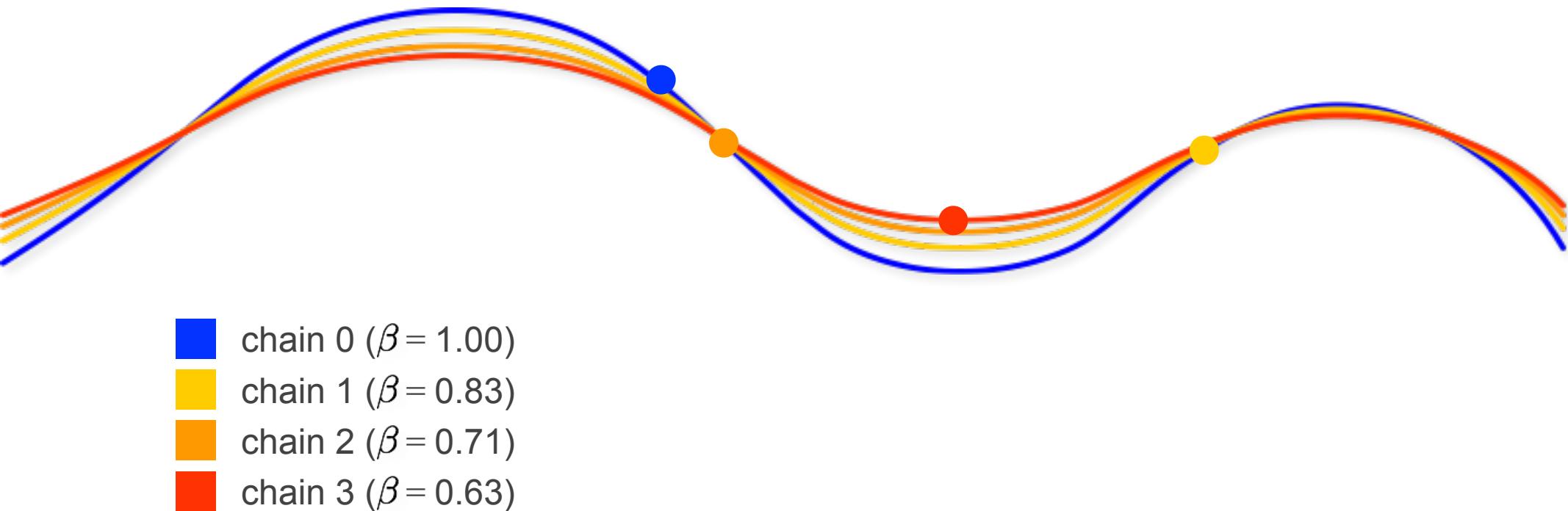


- chain 0 ($\beta = 1.00$)
- chain 1 ($\beta = 0.83$)
- chain 2 ($\beta = 0.71$)
- chain 3 ($\beta = 0.63$)

Approximating the Joint Posterior Probability Density using Metropolis-Coupled MCMC

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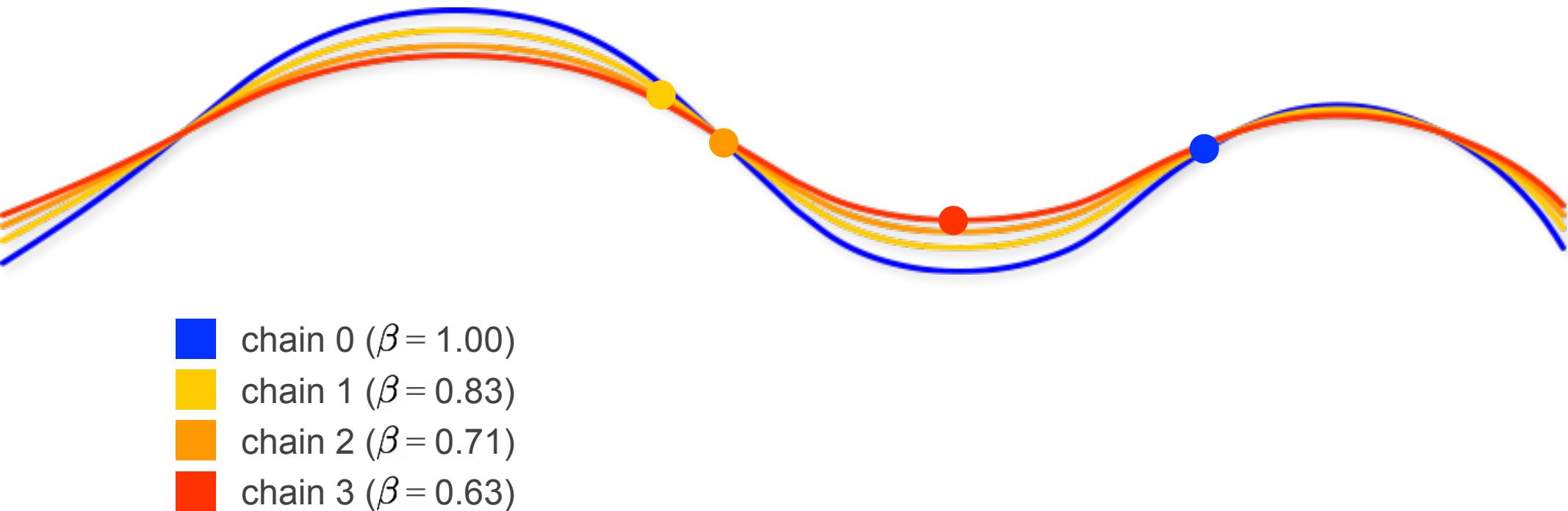
1. Initialize N independent M-H MCMC chains with random values for all parameters.
2. The chains are incrementally heated, such that the first chain is cold (unmodified).
3. At prescribed intervals, two chains are randomly selected to swap.
 - we compute the acceptance probability of swapping the two chains.
 - if accepted, the chains swap positions (and in computer memory)



Approximating the Joint Posterior Probability Density using Metropolis-Coupled MCMC

The MC³ algorithm

1. Initialize N independent M-H MCMC chains with random values for all parameters.
2. The chains are incrementally heated, such that the first chain is cold (unmodified).
3. At prescribed intervals, two chains are randomly selected to swap.
4. Only samples from the cold chain are used to approximate the posterior.



Outline

I. Introduction to Bayesian inference

What is Bayesian inference?

- Deriving Bayes theorem
- Two non-phylogenetic examples
- Bayesian inference of phylogeny

II. The Bayesian hard sell

What's the deal with priors?

Learning to embrace your inner Bayesian

III. Numerical algorithms for Bayesian inference

→ Markov-chain Monte Carlo (MCMC)

- Metropolis-Hastings algorithm
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Summarizing posterior samples

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Samples from the MCMC simulation approximate the joint posterior

The frequency of sampled parameter values provides a valid estimate of the posterior probability of that parameter

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- e.g., the frequency of a sampled clade provides an estimate of its nodal probability

We can query the joint posterior with respect to any individual parameter of interest: the marginal posterior probability

Approximating the Joint Posterior Probability Density using MCMC

Samples from the MCMC simulation approximate the joint posterior

Each row in our log file—with values of all model parameters—is a sample from the *joint* posterior probability density.

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1	-13413.769	1.313	0.166667	0.166667	0.166667	0.166667	0.166667	0.166667	0.166667	0.250000	0.250000	0.250000	0.250000
1000	-10429.772	0.904	0.100364	0.271178	0.057126	0.095681	0.404818	0.070833	0.276201	0.173231	0.228359	0.322209	0.845634
2000	-10420.654	0.980	0.115937	0.254216	0.041309	0.051039	0.455344	0.082157	0.291050	0.181003	0.231042	0.296904	0.670406
3000	-10417.930	0.961	0.137253	0.264348	0.037891	0.056962	0.426295	0.077251	0.291050	0.181003	0.231042	0.296904	0.901480
4000	-10423.816	0.925	0.101065	0.273786	0.035266	0.067623	0.441301	0.080958	0.290603	0.185952	0.231800	0.291644	0.859284
5000	-10425.264	1.002	0.135985	0.259584	0.048509	0.057733	0.430436	0.067753	0.289106	0.189615	0.210373	0.310906	0.671675
6000	-10421.366	0.962	0.119016	0.268203	0.041284	0.062913	0.415543	0.093041	0.281133	0.187367	0.234148	0.297353	0.824395
7000	-10417.840	0.981	0.123308	0.246185	0.032588	0.070686	0.443381	0.083851	0.298478	0.186125	0.221560	0.293837	0.644508
8000	-10420.174	1.058	0.129152	0.263612	0.036846	0.061359	0.424323	0.084708	0.284539	0.192084	0.216456	0.306921	0.691606
9000	-10419.701	0.980	0.101173	0.266573	0.035445	0.072158	0.438826	0.085825	0.285541	0.188378	0.229610	0.296471	0.687021
10000	-10423.917	1.015	0.100312	0.289851	0.045985	0.059364	0.422372	0.082115	0.285505	0.176257	0.228230	0.310007	0.684473
11000	-10418.487	0.945	0.107911	0.270677	0.049322	0.063833	0.421602	0.086655	0.279829	0.188085	0.233921	0.298165	0.860128
12000	-10420.169	0.893	0.115085	0.270950	0.038203	0.070506	0.417478	0.087778	0.288131	0.191473	0.231758	0.288638	0.723312
13000	-10419.081	0.922	0.115323	0.269076	0.036184	0.069919	0.429555	0.079943	0.294340	0.187665	0.227043	0.290952	0.784700
14000	-10423.817	1.030	0.112545	0.254842	0.042601	0.077867	0.436797	0.075348	0.283706	0.189549	0.224014	0.302731	0.615981
15000	-10424.879	0.944	0.131641	0.260134	0.043160	0.069779	0.421550	0.073736	0.296187	0.175620	0.219147	0.309046	0.797970
16000	-10426.143	0.940	0.117469	0.266011	0.056463	0.049593	0.441326	0.069139	0.282578	0.203117	0.231372	0.282933	0.792757
17000	-10421.133	0.978	0.134024	0.277374	0.040419	0.056384	0.416233	0.075565	0.289061	0.187968	0.225825	0.297145	0.767063
18000	-10418.290	0.930	0.104450	0.251683	0.041434	0.063649	0.455528	0.083256	0.287086	0.189510	0.226700	0.296704	0.767072
19000	-10420.052	0.972	0.121227	0.274901	0.037023	0.083743	0.414224	0.068881	0.289061	0.187968	0.225825	0.297145	0.758345
20000	-10425.127	0.955	0.099741	0.277386	0.043745	0.069447	0.433059	0.076622	0.292229	0.197483	0.212827	0.297461	0.645034
21000	-10421.087	0.939	0.105737	0.258514	0.039941	0.094773	0.429045	0.071991	0.292778	0.192129	0.217655	0.297438	0.692877
22000	-10421.805	0.926	0.111237	0.293260	0.047595	0.061320	0.409044	0.077544	0.286897	0.197795	0.222410	0.292899	0.797696
23000	-10422.326	0.943	0.123590	0.240213	0.047236	0.048864	0.453312	0.086786	0.291024	0.187438	0.225934	0.295603	0.851381
24000	-10417.974	0.938	0.123674	0.274369	0.051414	0.065387	0.413009	0.072146	0.291024	0.187438	0.225934	0.295603	0.801620
25000	-10422.454	0.996	0.132415	0.249036	0.036744	0.063052	0.457012	0.061741	0.299053	0.171847	0.226435	0.302665	0.607659
26000	-10424.506	0.892	0.122118	0.235061	0.042240	0.063788	0.462004	0.074790	0.302331	0.170502	0.220011	0.307156	0.812245
27000	-10420.001	0.953	0.128264	0.263415	0.040470	0.058989	0.432138	0.076724	0.279181	0.190422	0.234369	0.296028	0.824956

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1000	-10429.772	0.904	0.100364	0.271178	0.057126	0.095681	0.404818	0.070833	0.276201	0.173231	0.228359	0.322209	0.845634
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13000	-10419.081	0.922	0.115323	0.269076	0.036184	0.069919	0.429555	0.079943	0.294340	0.187665	0.227043	0.290952	0.784700
14000	-10423.817	1.030	0.112545	0.254842	0.042601	0.077867	0.436797	0.075348	0.283706	0.189549	0.224014	0.302731	0.615981
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16000	-10426.143	0.940	0.117469	0.266011	0.056463	0.049593	0.441326	0.069139	0.282578	0.203117	0.231372	0.282933	0.792757
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18000	-10418.290	0.930	0.104450	0.251683	0.041434	0.063649	0.455528	0.083256	0.287086	0.189510	0.226700	0.296704	0.767072
19000	-10420.052	0.972	0.121227	0.274901	0.037023	0.083743	0.414224	0.068881	0.289061	0.187968	0.225825	0.297145	0.758345
20000	-10425.127	0.955	0.099741	0.277386	0.043745	0.069447	0.433059	0.076622	0.292229	0.197483	0.212827	0.297461	0.645034
21000	-10421.087	0.939	0.105737	0.258514	0.039941	0.094773	0.429045	0.071991	0.292778	0.192129	0.217655	0.297438	0.692877
22000	-10421.805	0.926	0.111237	0.293260	0.047595	0.061320	0.409044	0.077544	0.286897	0.197795	0.222410	0.292899	0.797696
23000	-10422.326	0.943	0.123590	0.240213	0.047236	0.048864	0.453312	0.086786	0.291024	0.187438	0.225934	0.295603	0.851381
24000	-10417.974	0.938	0.123674	0.274369	0.051414	0.065387	0.413009	0.072146	0.291024	0.187438	0.225934	0.295603	0.801620
25000	-10422.454	0.996	0.132415	0.249036	0.036744	0.063052	0.457012	0.061741	0.299053	0.171847	0.226435	0.302665	0.607659
26000	-10424.506	0.892	0.122118	0.235061	0.042240	0.063788	0.462004	0.074790	0.302331	0.170502	0.220011	0.307156	0.812245
27000	-10420.001	0.953	0.128264	0.263415	0.040470	0.058989	0.432138	0.076724	0.279181	0.190422	0.234369	0.296028	0.824956

Approximating the Joint Posterior Probability Density using MCMC

Samples from the MCMC simulation approximate the joint posterior

Each column in our log file—with values for a single model parameter—is a sample from the *marginal* posterior probability density.

[ID: 2325481386]													
Gen	LNL	TL	r(A<->C)	r(A<->G)	r(A<->T)	r(C<->G)	r(C<->T)	r(G<->T)	pi(A)	pi(C)	pi(G)	pi(T)	alpha
1	-13413.769	1.313	0.166667	0.166667	0.166667	0.166667	0.166667	0.166667	0.166667	0.250000	0.250000	0.250000	0.250000
1000	-10429.772	0.904	0.100364	0.271178	0.057126	0.095681	0.404818	0.070833	0.276201	0.173231	0.228359	0.322209	0.845634
2000	-10420.654	0.980	0.115937	0.254216	0.041309	0.051039	0.455344	0.082157	0.291050	0.181003	0.231042	0.296904	0.670406
3000	-10417.930	0.961	0.137253	0.264348	0.037891	0.056962	0.426295	0.077251	0.291050	0.181003	0.231042	0.296904	0.901480
4000	-10423.816	0.925	0.101065	0.273786	0.035266	0.067623	0.441301	0.080958	0.290603	0.185952	0.231800	0.291644	0.859284
5000	-10425.264	1.002	0.135985	0.259584	0.048509	0.057733	0.430436	0.067753	0.289106	0.189615	0.210373	0.310906	0.671675
6000	-10421.366	0.962	0.119016	0.268203	0.041284	0.062913	0.415543	0.093041	0.281133	0.187367	0.234148	0.297353	0.824395
7000	-10417.840	0.981	0.123308	0.246185	0.032588	0.070686	0.443381	0.083851	0.298478	0.186125	0.221560	0.293837	0.644508
8000	-10420.174	1.058	0.129152	0.263612	0.036846	0.061359	0.424323	0.084708	0.284539	0.192084	0.216456	0.306921	0.691606
9000	-10419.701	0.980	0.101173	0.266573	0.035445	0.072158	0.438826	0.085825	0.285541	0.188378	0.229610	0.296471	0.687021
10000	-10423.917	1.015	0.100312	0.289851	0.045985	0.059364	0.422372	0.082115	0.285505	0.176257	0.228230	0.310007	0.684473
11000	-10418.487	0.945	0.107911	0.270677	0.049322	0.063833	0.421602	0.086655	0.279829	0.188085	0.233921	0.298165	0.860128
12000	-10420.169	0.893	0.115085	0.270950	0.038203	0.070506	0.417478	0.087778	0.288131	0.191473	0.231758	0.288638	0.723312
13000	-10419.081	0.922	0.115323	0.269076	0.036184	0.069919	0.429555	0.079943	0.294340	0.187665	0.227043	0.290952	0.784700
14000	-10423.817	1.030	0.112545	0.254842	0.042601	0.077867	0.436797	0.075348	0.283706	0.189549	0.224014	0.302731	0.615981
15000	-10424.879	0.944	0.131641	0.260134	0.043160	0.069779	0.421550	0.073736	0.296187	0.175620	0.219147	0.309046	0.797970
16000	-10426.143	0.940	0.117469	0.266011	0.056463	0.049593	0.441326	0.069139	0.282578	0.203117	0.231372	0.282933	0.792757
17000	-10421.133	0.978	0.134024	0.277374	0.040419	0.056384	0.416233	0.075565	0.289061	0.187968	0.225825	0.297145	0.767063
18000	-10418.290	0.930	0.104450	0.251683	0.041434	0.063649	0.455528	0.083256	0.287086	0.189510	0.226700	0.296704	0.767072
19000	-10420.052	0.972	0.121227	0.274901	0.037023	0.083743	0.414224	0.068881	0.289061	0.187968	0.225825	0.297145	0.758345
20000	-10425.127	0.955	0.099741	0.277386	0.043745	0.069447	0.433059	0.076622	0.292229	0.197483	0.212827	0.297461	0.645034
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Approximating the Joint Posterior Probability Density using MCMC

Samples from the MCMC simulation approximate the joint posterior

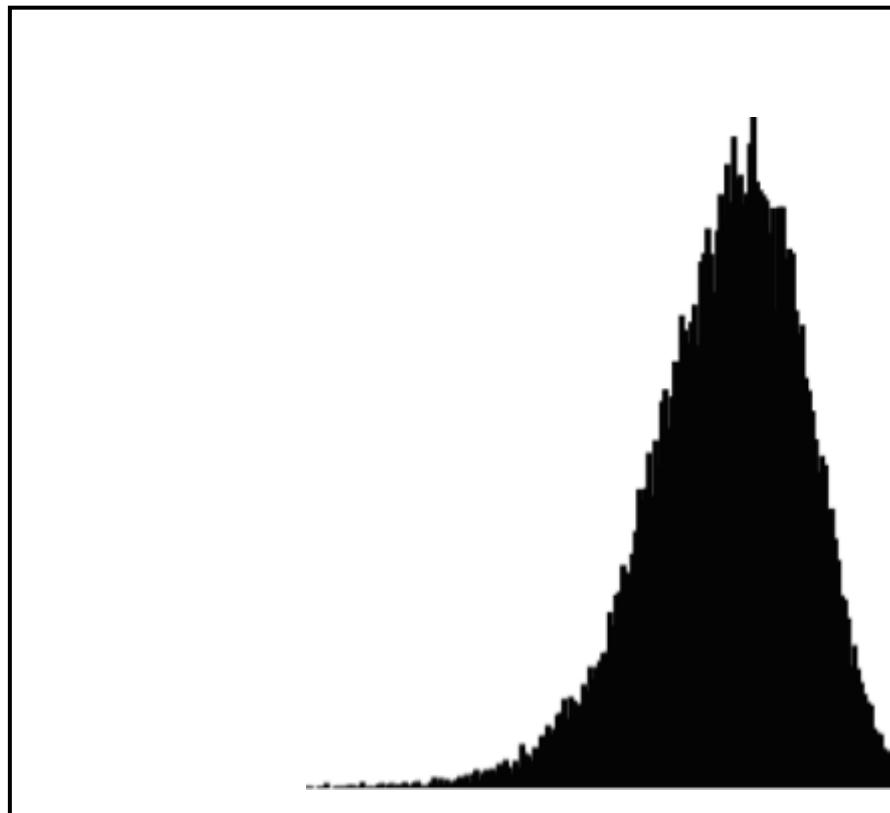
We can query the joint distribution marginally with respect to any parameter.

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Gen	LNL	TL	r(A<->C)	r(A<->G)	r(A<->T)	r(C<->G)	r(C<->T)	r(G<->T)	pi(A)	pi(C)	pi(G)	pi(T)	alpha
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Approximating the Joint Posterior Probability Density using MCMC

Samples from the MCMC simulation approximate the joint posterior

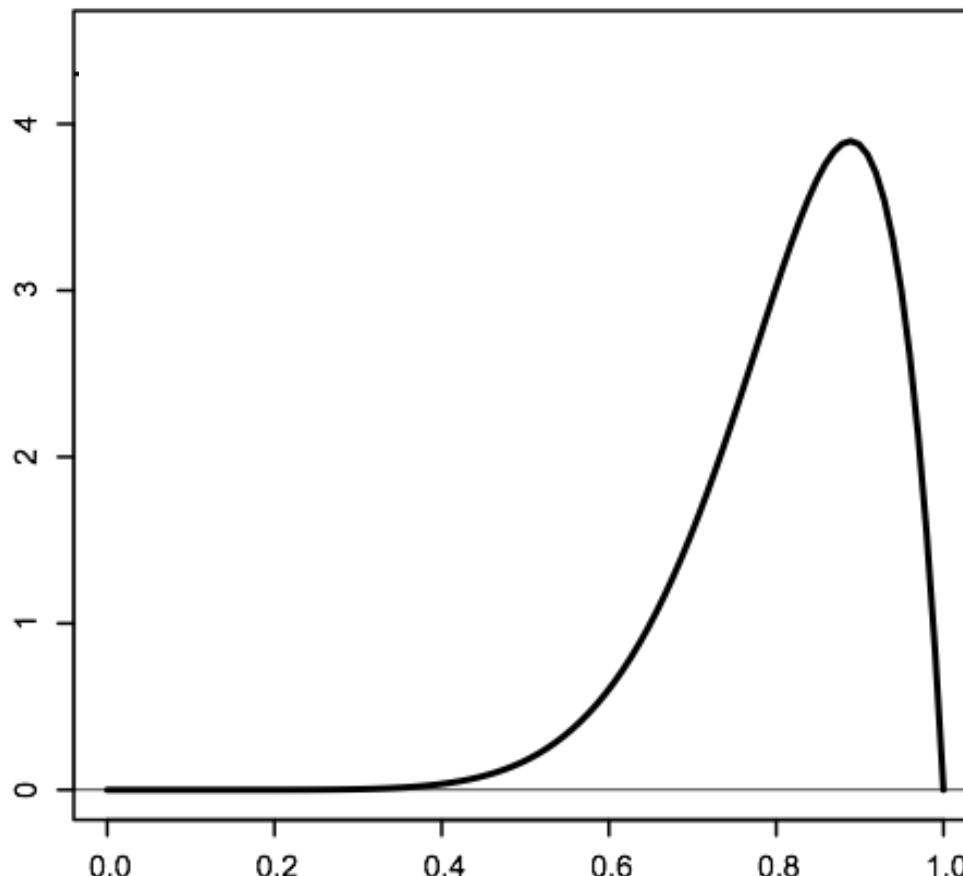
We can do this by simply constructed a histogram for any column in the file
this provides an estimate of its marginal posterior probability density



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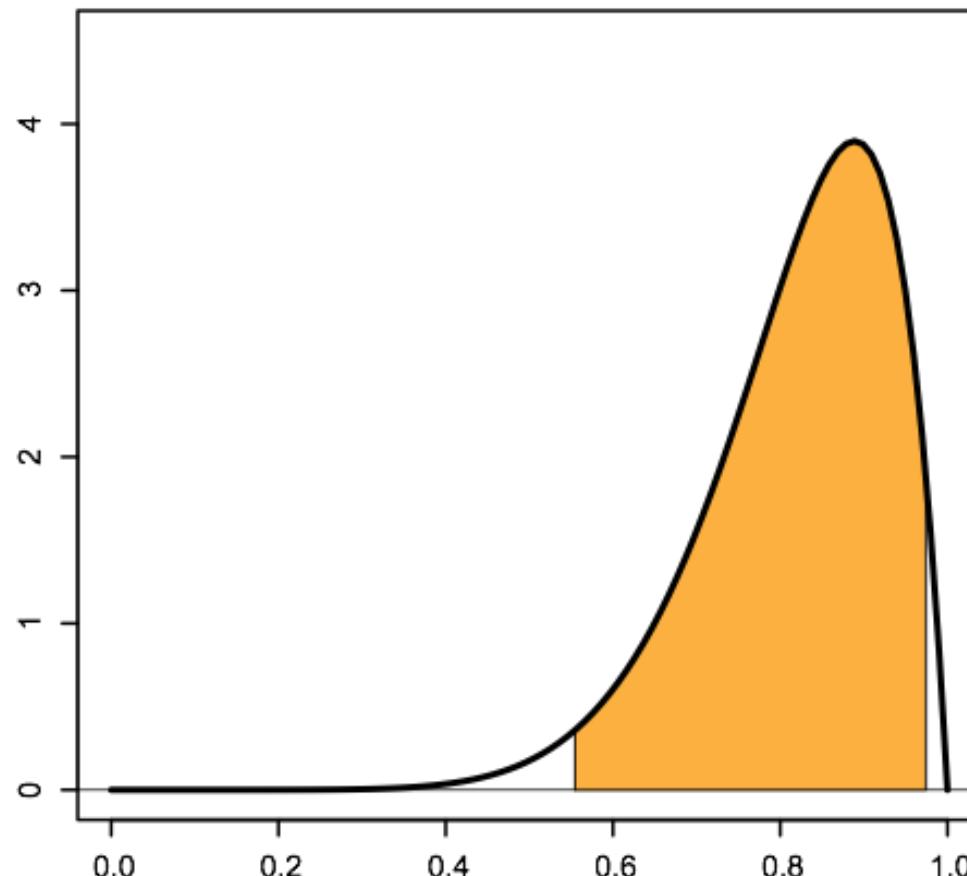
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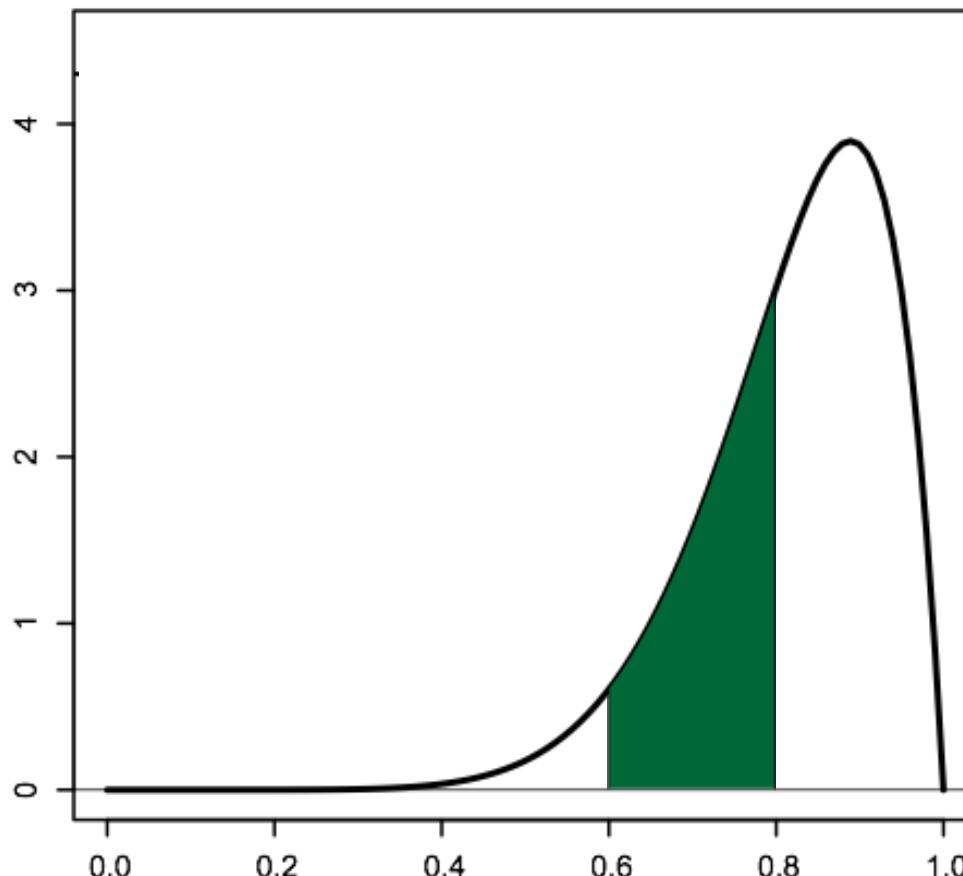
We can easily summarize aspects of the marginal posterior probability density:
e.g., to summarize the 95% credible interval.



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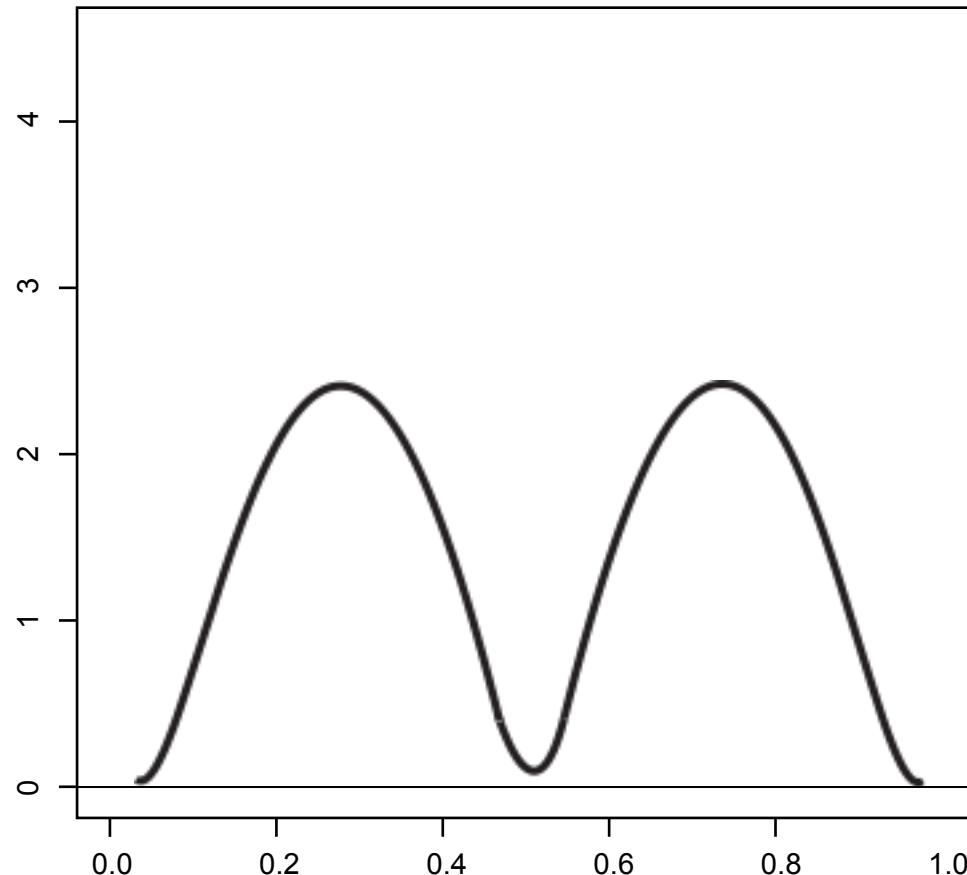
We can easily summarize aspects of the marginal posterior probability density:
e.g., or the probability within some arbitrary interval of interest (0.6–0.8).



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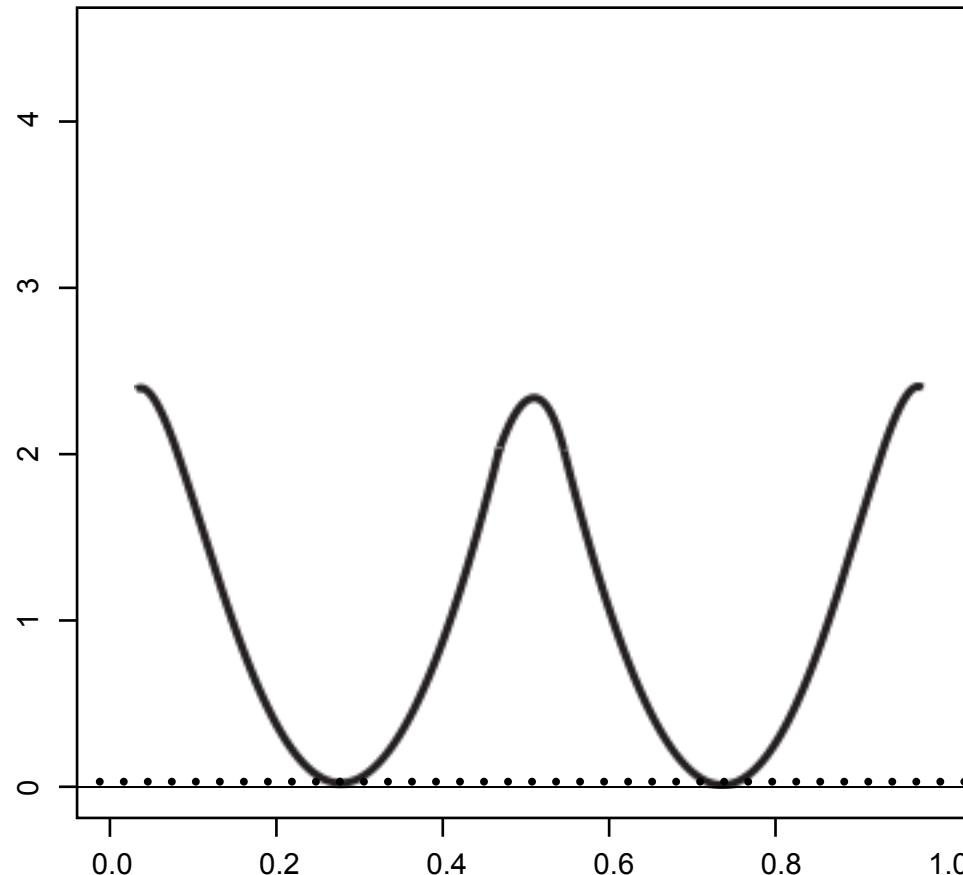
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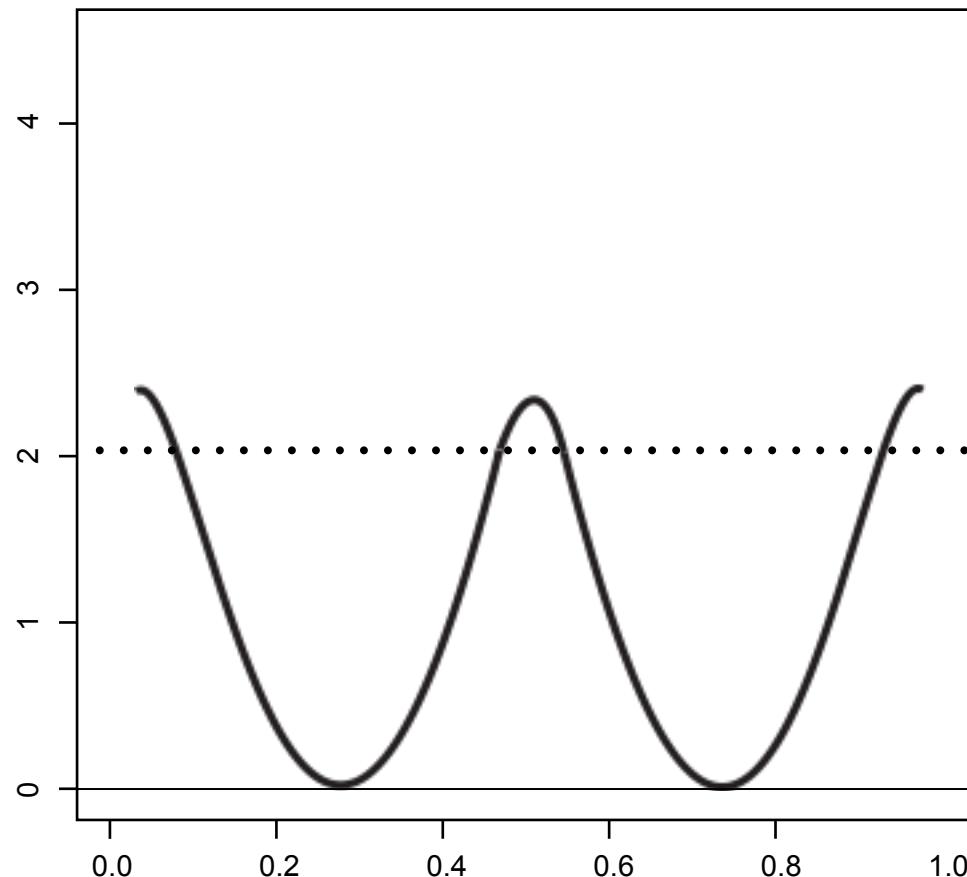
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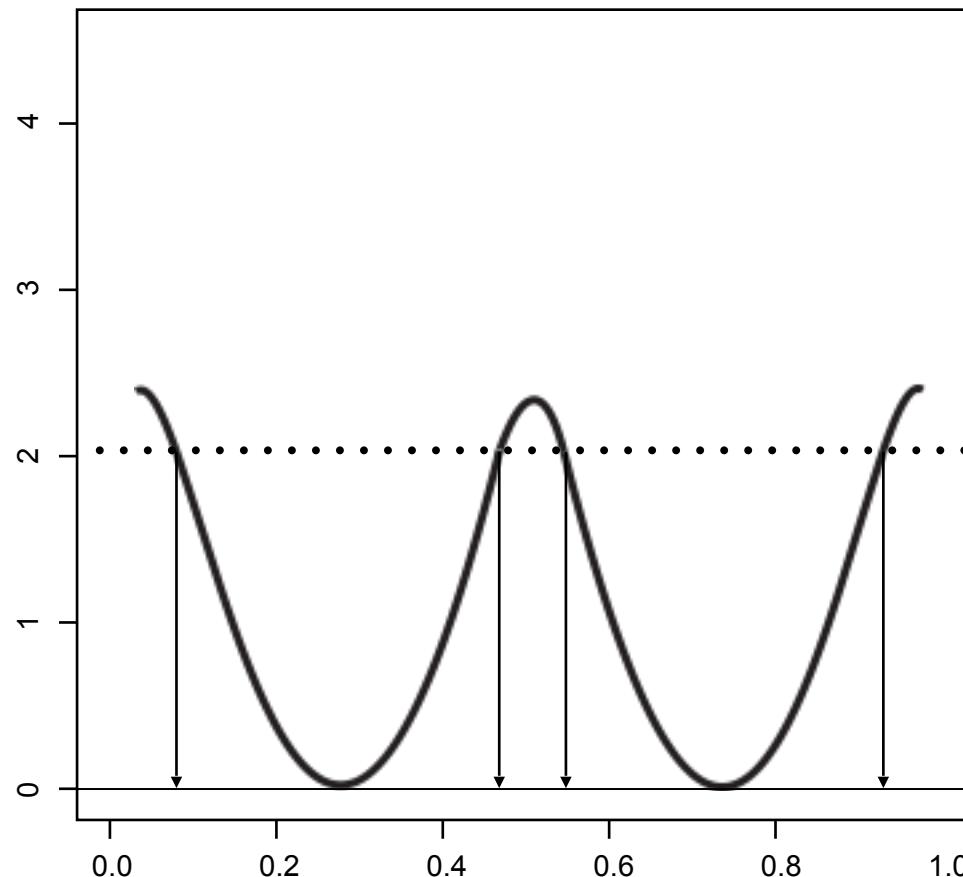
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Outline

I. Introduction to Bayesian inference

What is Bayesian inference?

- Deriving Bayes theorem
- Two non-phylogenetic examples
- Bayesian inference of phylogeny

II. The Bayesian hard sell

What's the deal with priors?

Learning to embrace your inner Bayesian

III. Numerical algorithms for Bayesian inference

Markov-chain Monte Carlo (MCMC)

- Metropolis-Hastings algorithm
- Metropolis-Coupled algorithm

→ Summarizing posterior samples

Outline

IV. Diagnosing MCMC performance

→ Motivation and overview of the basics

V. MCMC Diagnostics

General strategies:

- diagnostics based on single chains
- diagnostics based on multiple, replicate chains

Approximating the Joint Posterior Probability Density using MCMC

MCMC in theory and practice

MCMC in theory...

an appropriately constructed and adequately run chain is guaranteed to provide an arbitrarily precise description of the joint stationary density

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Approximating the Joint Posterior Probability Density using MCMC

MCMC in theory and practice

MCMC in theory...

an appropriately constructed and adequately run chain is guaranteed to provide an arbitrarily precise description of the joint stationary density

MCMC in practice...

although a given sampler may work well in most cases, all samplers will fail in some cases, and is not guaranteed to work for any particular case

Q. When do we know that the MCMC provides an accurate approximation for a given empirical analysis?

A.

NEVER!

Approximating the Joint Posterior Probability Density using MCMC

MCMC performance

It is not sufficient to merely be deeply concerned about MCMC performance...
you need to be **completely obsessed** about it!

Approximating the Joint Posterior Probability Density using MCMC

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Approximating the Joint Posterior Probability Density using MCMC

MCMC performance

It is not sufficient to merely be deeply concerned about MCMC performance...
you need to be **completely obsessed** about it!
for **any** Bayesian inference based on MCMC
particularly for complex models/inference problems



WE
ARE
HERE



WE
SHOULD
BE HERE



I'LL
BE
HERE

careless

careful

paranoid

Approximating the Joint Posterior Probability Density using MCMC

Markov Chain Monte Carlo Convergence Diagnostics: A Comparative Review

Mary Kathryn COWLES and Bradley P. CARLIN

A critical issue for users of Markov chain Monte Carlo (MCMC) methods in applications is how to determine when it is safe to stop sampling and use the samples to estimate characteristics of the distribution of interest. Research into methods of computing theoretical convergence bounds holds promise for the future but to date has yielded relatively little of practical use in applied work. Consequently, most MCMC users address the convergence problem by applying diagnostic tools to the output produced by running their samplers. After giving a brief overview of the area, we provide an expository review of 13 convergence diagnostics, describing the theoretical basis and practical implementation of each. We then compare their performance in two simple models and conclude that all of the methods can fail to detect the sorts of convergence failure that they were designed to identify. We thus recommend a combination of strategies aimed at evaluating and accelerating MCMC sampler convergence, including applying diagnostic procedures to a small number of parallel chains, monitoring autocorrelations and cross-correlations, and modifying parameterizations or sampling algorithms appropriately. We emphasize, however, that it is not possible to say with certainty that a finite sample from an MCMC algorithm is representative of an underlying stationary distribution.

KEY WORDS: Autocorrelation; Gibbs sampler; Metropolis-Hastings algorithm.

Approximating the Joint Posterior Probability Density using MCMC

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...under simulation, all MCMC diagnostics may fail to detect the exact problems that they were specifically designed to identify...

...therefore, it is critical to use a combination of tools to detect MCMC failure

a finite sample from an MCMC algorithm is representative of an underlying stationary distribution.

KEY WORDS: Autocorrelation; Gibbs sampler; Metropolis-Hastings algorithm.

Outline

IV. Diagnosing MCMC performance

→ Motivation and overview of the basics

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Assessing MCMC Performance: Two Main Issues

1. Convergence

Has the chain (robot) successfully targeted the stationary distribution?

Assessing MCMC Performance: Two Main Issues

1. Convergence

Has the chain (robot) successfully targeted the stationary distribution?

2. Mixing

Is the chain (robot) efficiently integrating over the joint posterior probability?

Assessing MCMC Performance: Based on Single Chains

1. Convergence diagnostics

Time-series plots of parameter estimates

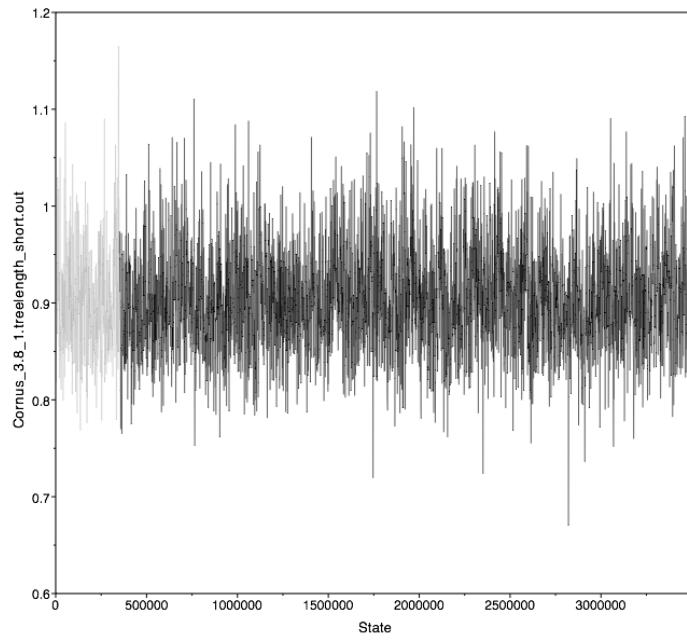
Continuous parameters (e.g., substitution rates)

- some parameters are more reliable than others
- steps may occur!

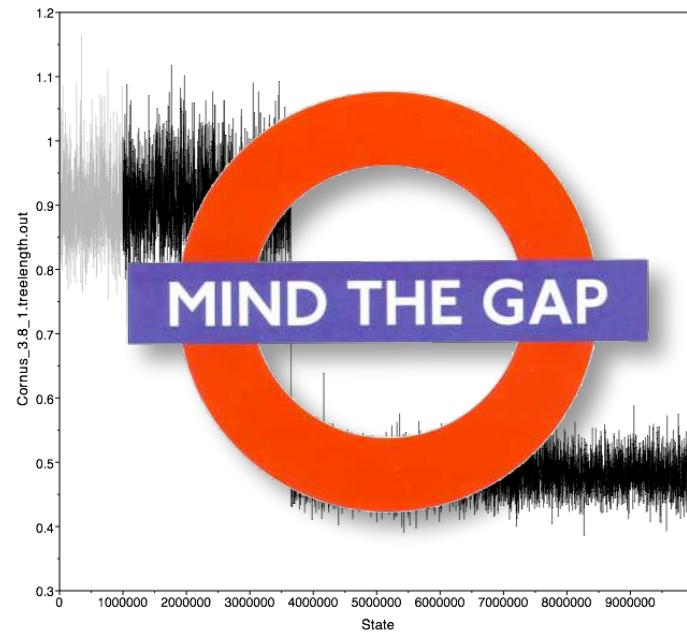
Assessing MCMC Performance: Based on Single Chains

Example: Tracer plots of tree-length at two stages of a single MrBayes run

all looks good...



until it doesn't



fast*

InL

base freq.

sub. rates

ASRV

TL

slow*

topology

*somewhat data-set dependent

Assessing MCMC Performance: Based on Single Chains

1. Convergence diagnostics

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Continuous parameters (e.g., substitution rates)

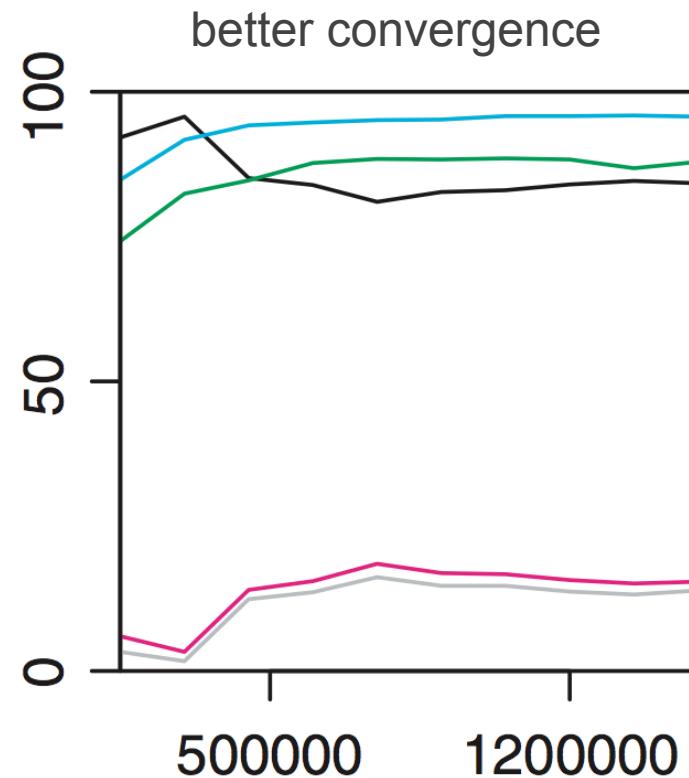
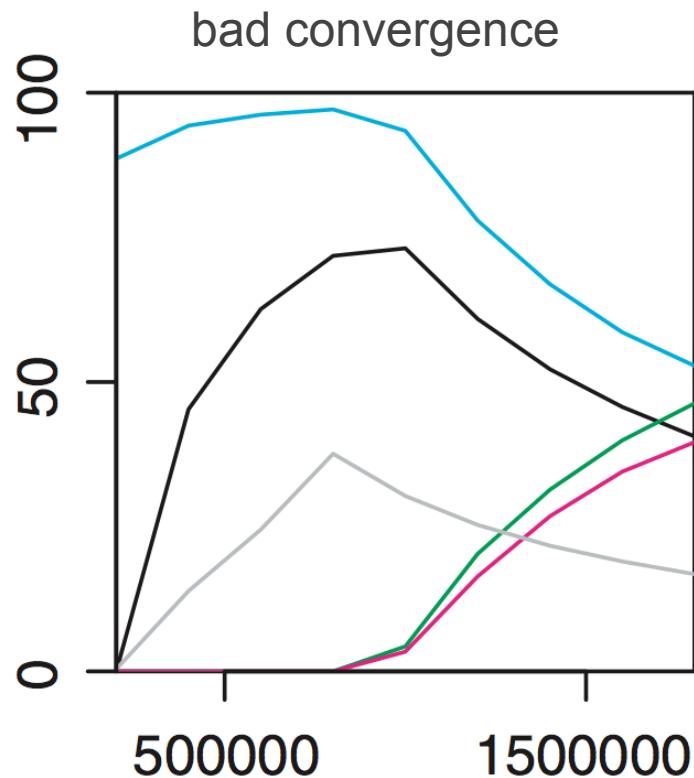
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Discrete parameters (e.g., bi-partitions)

- some parameters are more reliable than others
- steps may occur!

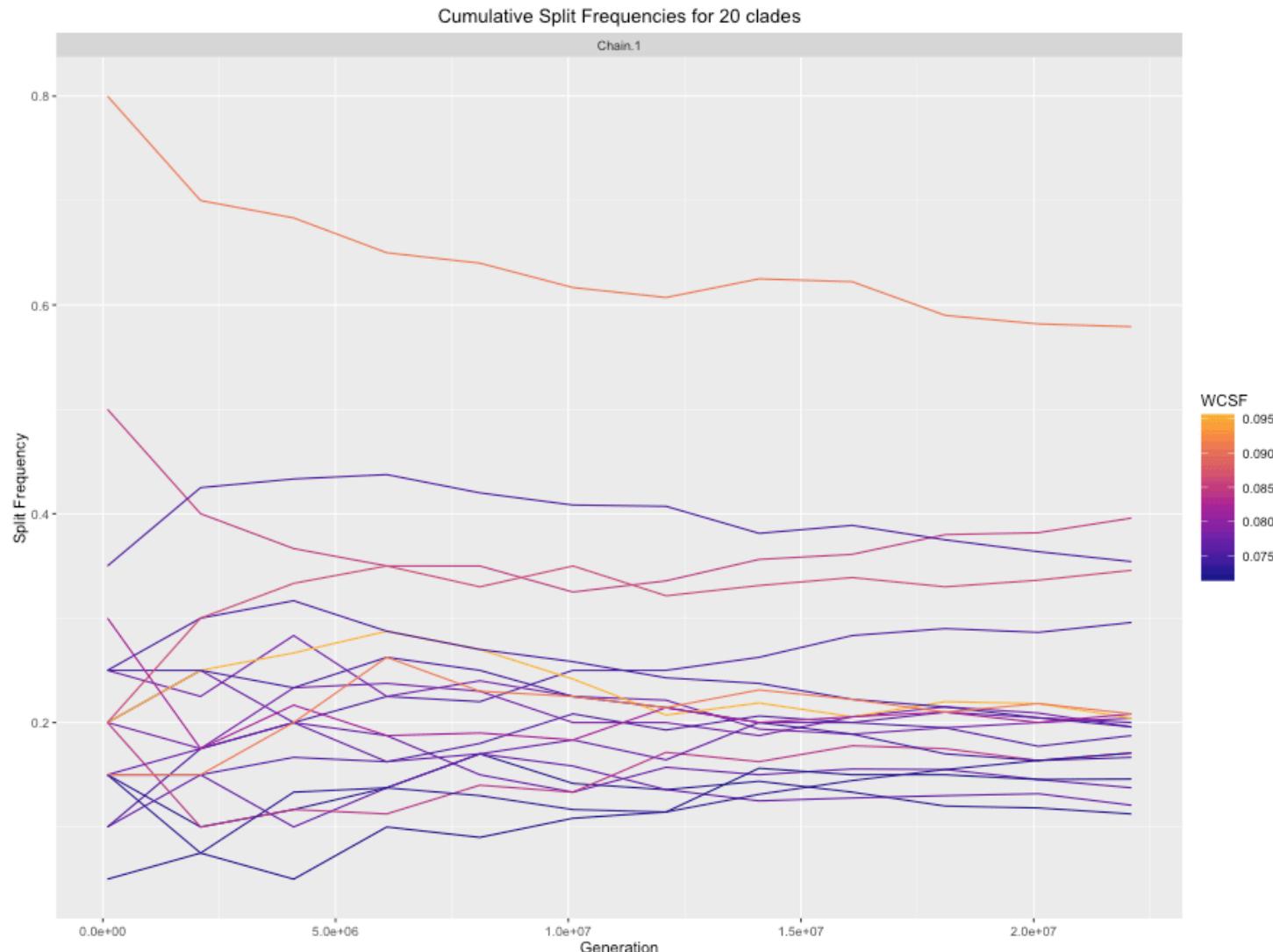
Assessing MCMC Performance: Based on Single Chains

Example: AWTY plots of cumulative bi-partition frequency of 5 nodes



Assessing MCMC Performance: Based on Single Chains

Example: **RWTY** plots of cumulative bi-partition frequency of 20 nodes



Assessing MCMC Performance: Based on Single Chains

1. Convergence diagnostics

Time-series plots of parameter estimates

Assessing MCMC Performance: Based on Single Chains

1. Convergence diagnostics

Time-series plots of parameter estimates

Geweke diagnostic (coda)

Continuous or discrete parameters

- A test for equality of the means of the first and last part of a Markov chain (by default the first 10% and the last 50%)

Assessing MCMC Performance: Based on Single Chains

1. Convergence diagnostics

Time-series plots of parameter estimates

Geweke diagnostic (coda)

Continuous or discrete parameters

- A test for equality of the means of the first and last part of a Markov chain (by default the first 10% and the last 50%)
- If the samples are drawn from the stationary distribution, the two means should equal and Geweke's statistic has an asymptotically standard normal distribution

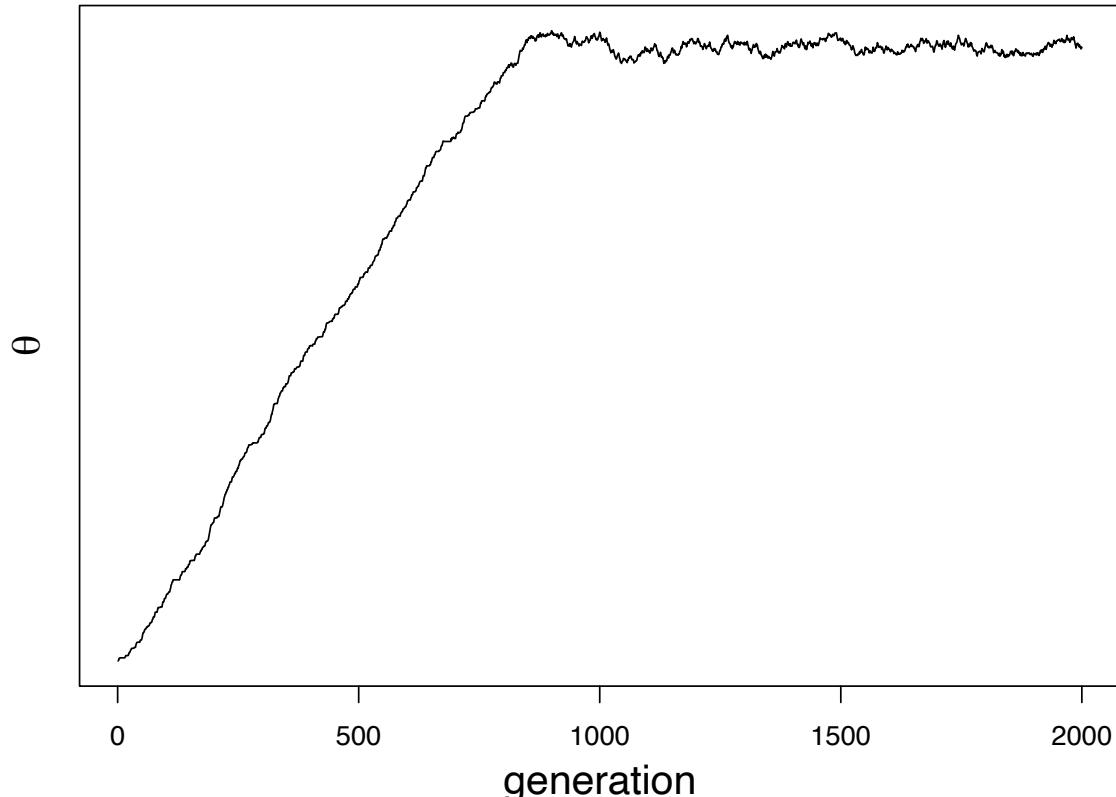
Assessing MCMC Performance: Based on Single Chains

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Continuous or discrete parameters



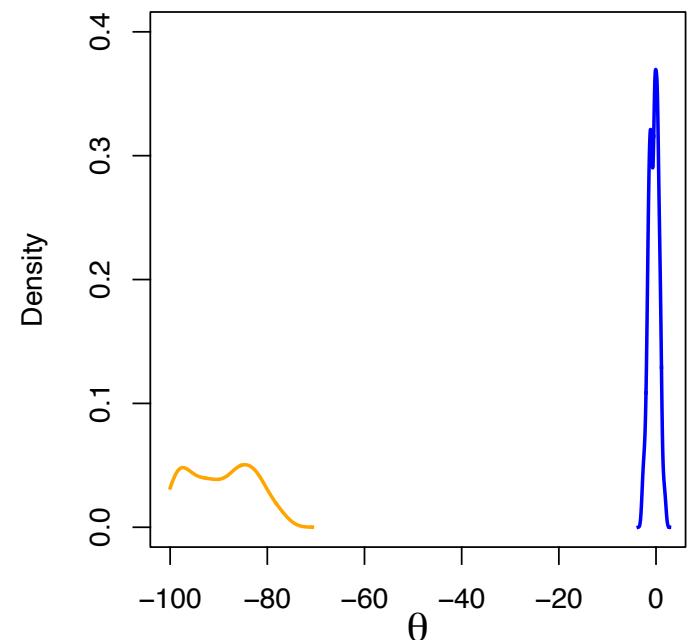
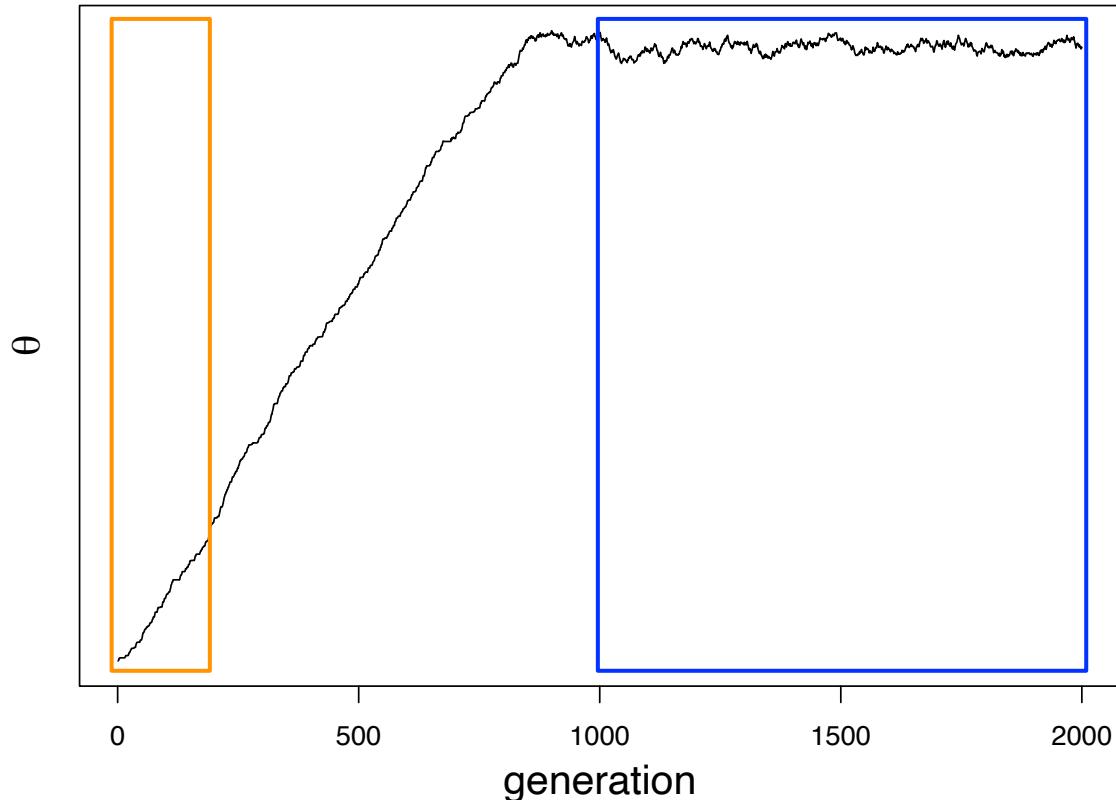
Assessing MCMC Performance: Based on Single Chains

1. Convergence diagnostics

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Geweke (1992)

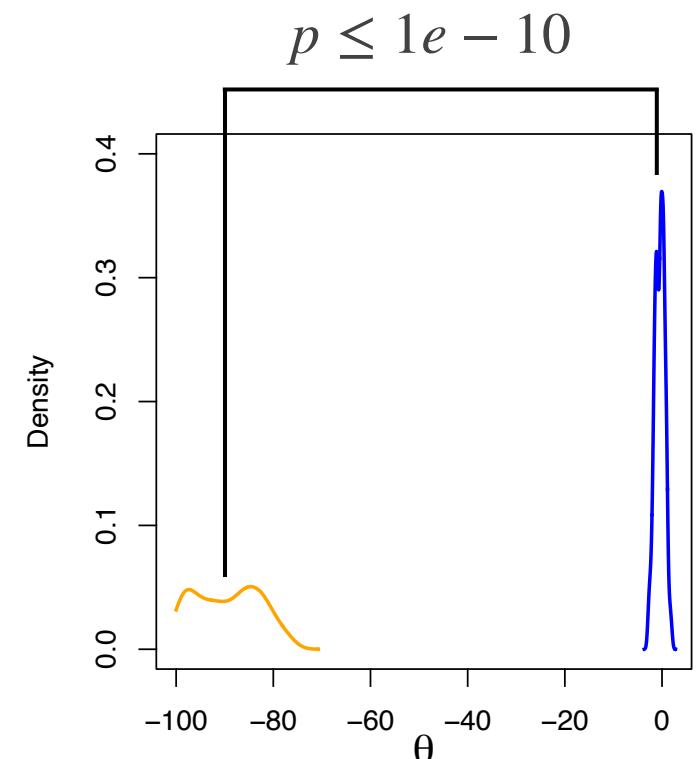
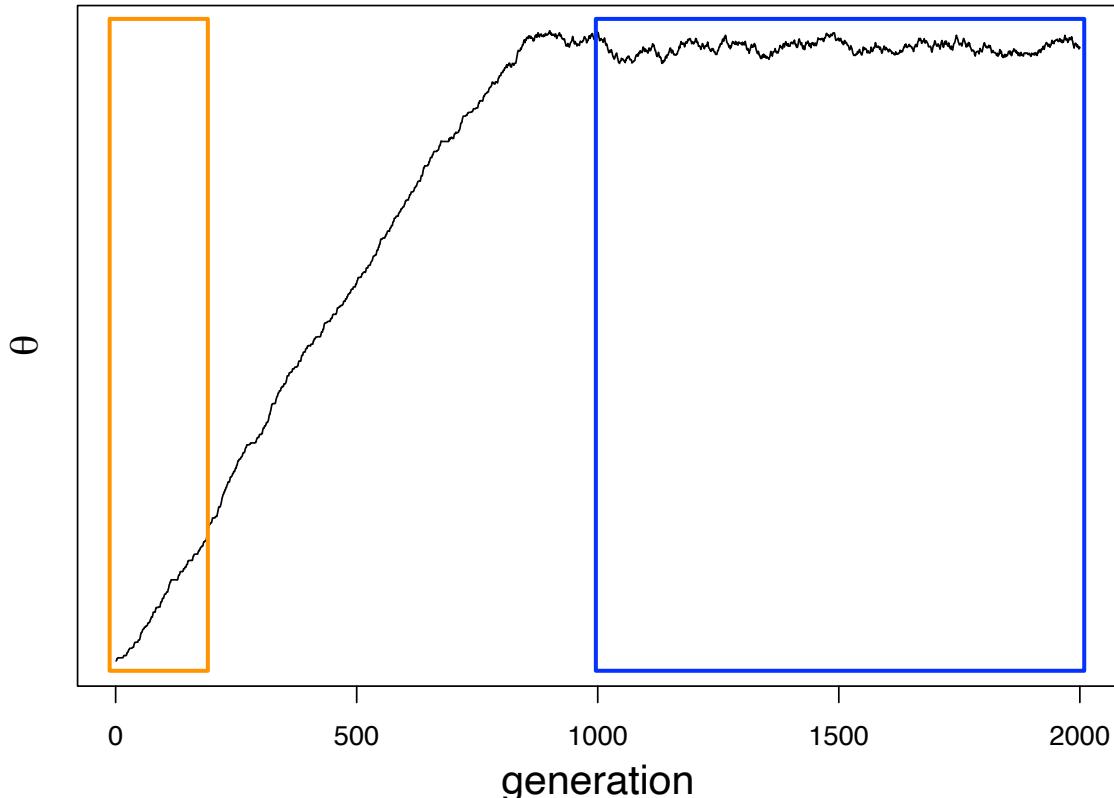
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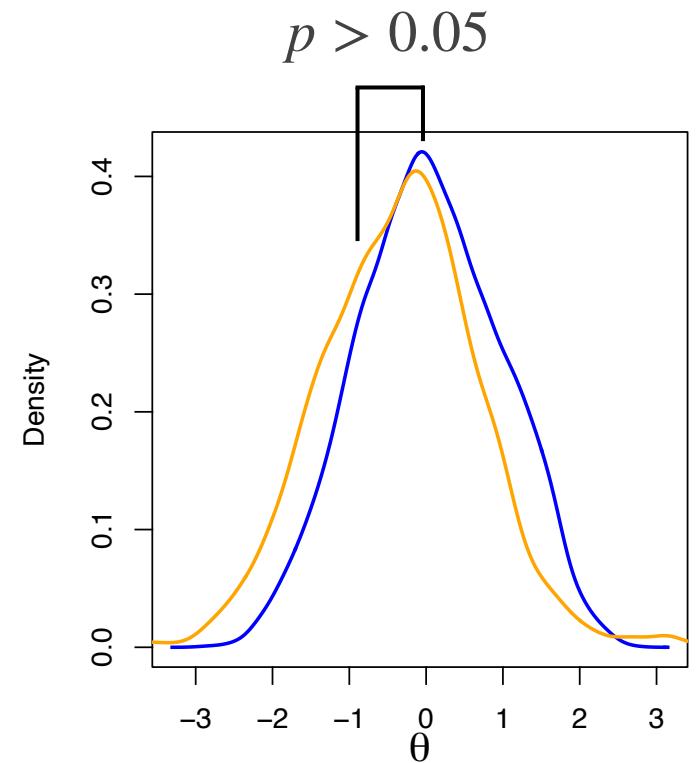
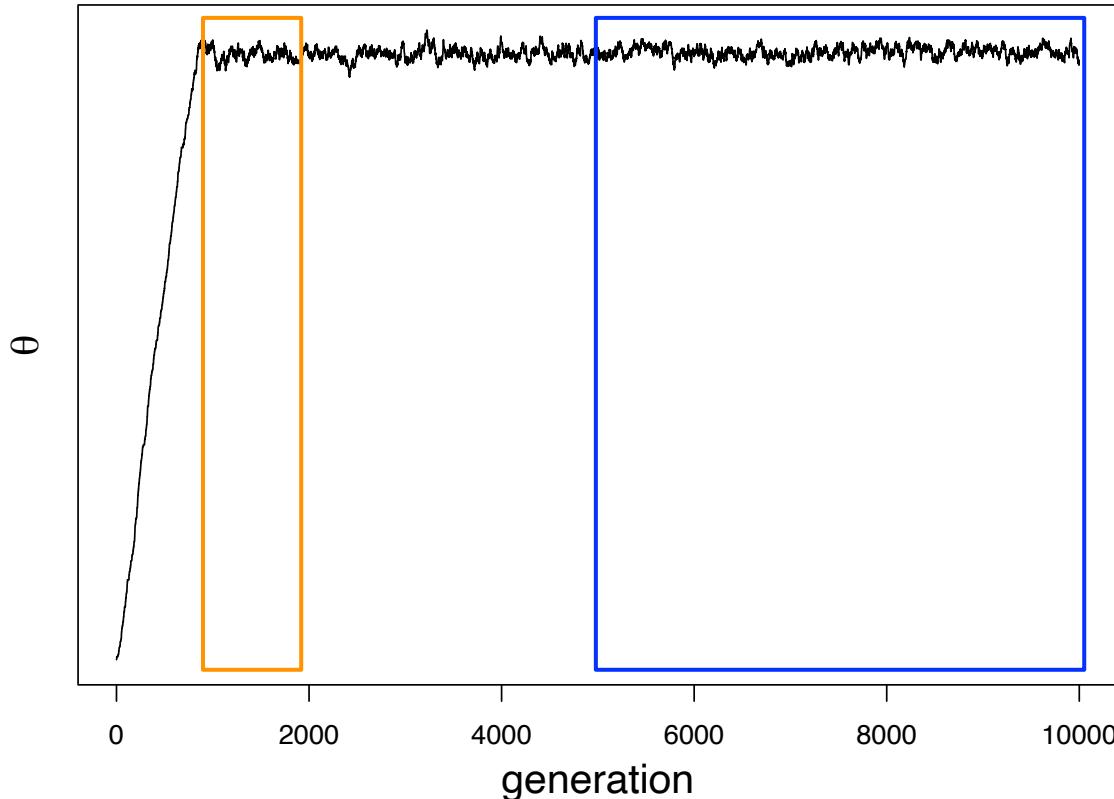
Assessing MCMC Performance: Based on Single Chains

1. Convergence diagnostics

Time-series plots of parameter estimates

Geweke diagnostic (coda)

Continuous or discrete parameters



Geweke (1992)

Assessing MCMC Performance: Based on Single Chains

1. Convergence diagnostics

Time-series plots of parameter estimates

Geweke diagnostic (coda)

(many others)

Assessing MCMC Performance: Based on Single Chains

2. Mixing diagnostics

Assessing MCMC Performance: Based on Single Chains

2. Mixing diagnostics

Form of the time-series plots of parameter estimates

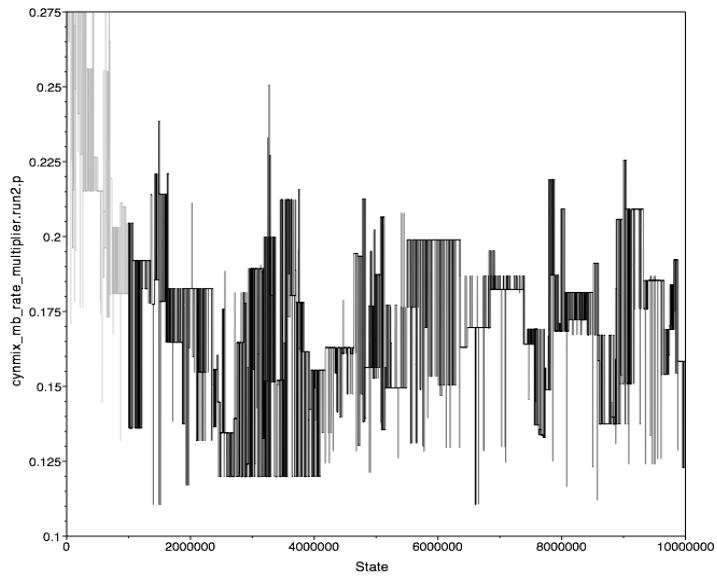
Continuous parameters (e.g., substitution rates)

- warm and fuzzy caterpillars

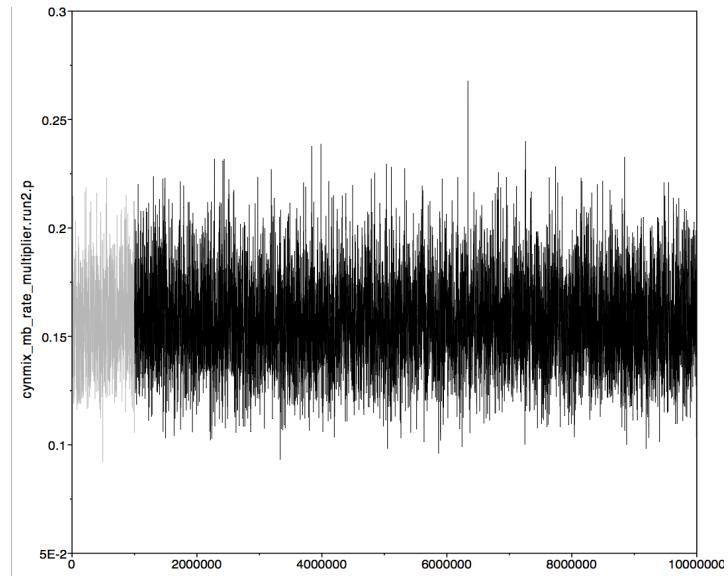
Assessing MCMC Performance: Based on Single Chains

Example: Tracer plots of relative-rate multipliers from two MrBayes runs

bad mixing



better mixing



Assessing MCMC Performance: Based on Single Chains

Example: Tracer plots of relative-rate multipliers from two MrBayes runs

bad mixing



better mixing



Assessing MCMC Performance: Based on Single Chains

2. Mixing diagnostics

Form of the time-series plots of parameter estimates

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- warm and fuzzy caterpillars

Acceptance rates of parameter updates

Continuous and discrete parameters

- rates should ideally fall in the ~20–70% range

Assessing MCMC Performance: Based on Single Chains

Example: Tracer plots of relative-rate multipliers from two MrBayes runs

bad mixing



better mixing



Acceptance rates for the moves in the "cold" chain of run 1:

With prob. Chain accepted changes to
13.61 % param. 1 (revmat) with Dirichlet proposal

.

.

.

0.04 % param. 34 (rate multiplier) Dirichlet proposal
6.59 % param. 35 (topology and branch lengths) TBR
14.06 % param. 35 (topology and branch lengths) LOCAL

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Assessing MCMC Performance: Based on Single Chains

2. Mixing diagnostics

Form of the time-series plots of parameter estimates

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- to increase acceptance rates, decrease scale of tuning parameter (and vice versa)

The diagram illustrates the mapping of R code parameters to MCMC tuning components. A black rectangular box contains R code. Three orange arrows point from labels above the box to specific parts of the code:

- A horizontal arrow labeled "parameter" points to the first line of code: `# specify a beta prior on x`.
- An arrow labeled "prior distribution" points to the line: `x ~ dnBeta(1,1)`.
- An arrow labeled "tuning parameter" points to the line: `moves.append(mvSlide(x, delta = 0.1, weight = 5.0))`.
- An arrow labeled "proposal weight" points to the same line as the tuning parameter, specifically to the `weight = 5.0` part.

```
# specify a beta prior on x
x ~ dnBeta(1,1)

# place a sliding move on x
moves.append( mvSlide(x, delta = 0.1, weight = 5.0) )
```

Assessing MCMC Performance: Based on Single Chains

2. Mixing diagnostics

Form of the time-series plots of parameter estimates

Continuous parameters (e.g., substitution rates)

- warm and fuzzy caterpillars

Acceptance rates of parameter updates

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```
# burn the chain in  
mymcmc.burnin(generations = 1000, tuningInterval = 100)
```



adjust tuning parameters

Assessing MCMC Performance: Based on Single Chains

2. Mixing diagnostics

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Form of the marginal posterior probability densities

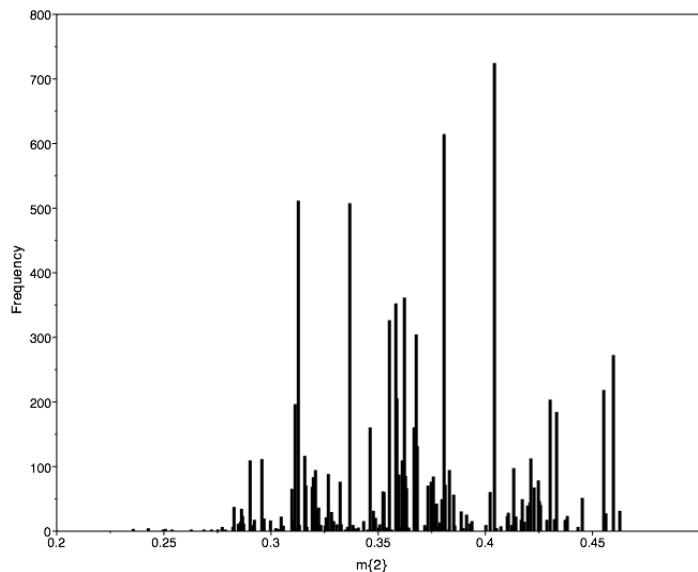
Continuous parameters (e.g., substitution rates)

- beware of porcupine roadkill!

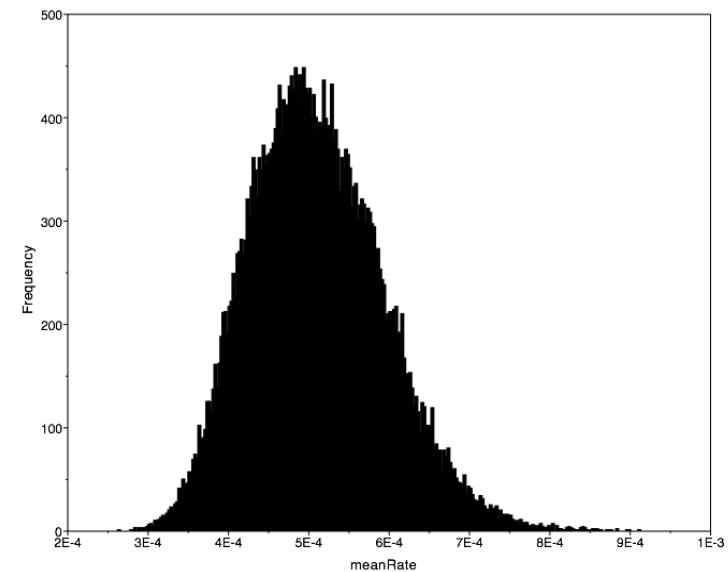
Assessing MCMC Performance: Based on Single Chains

Example: Tracer plots of relative-rate multipliers from two MrBayes runs

bad mixing



better mixing



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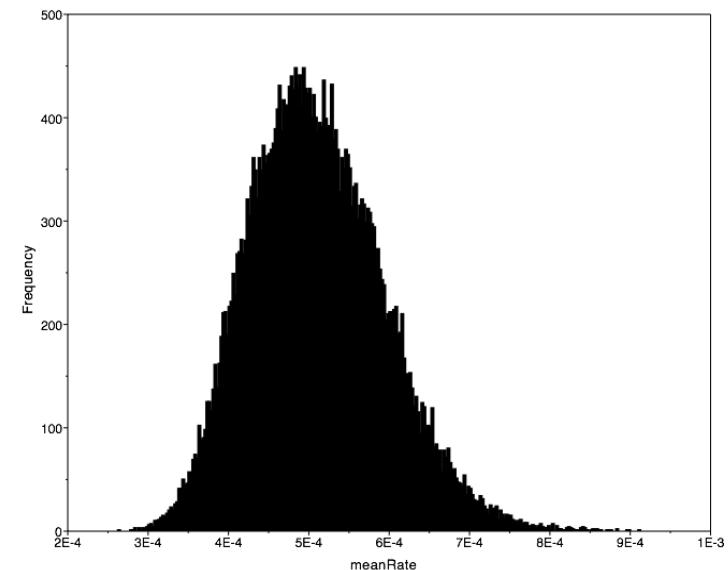
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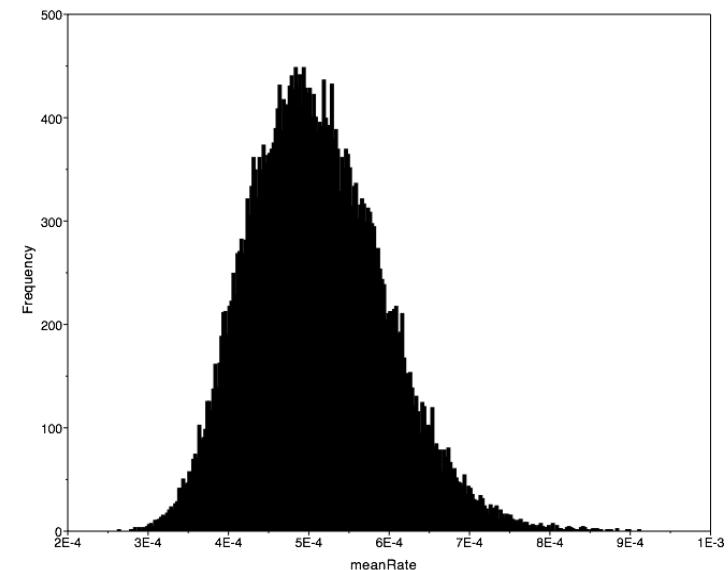
Assessing MCMC Performance: Based on Single Chains

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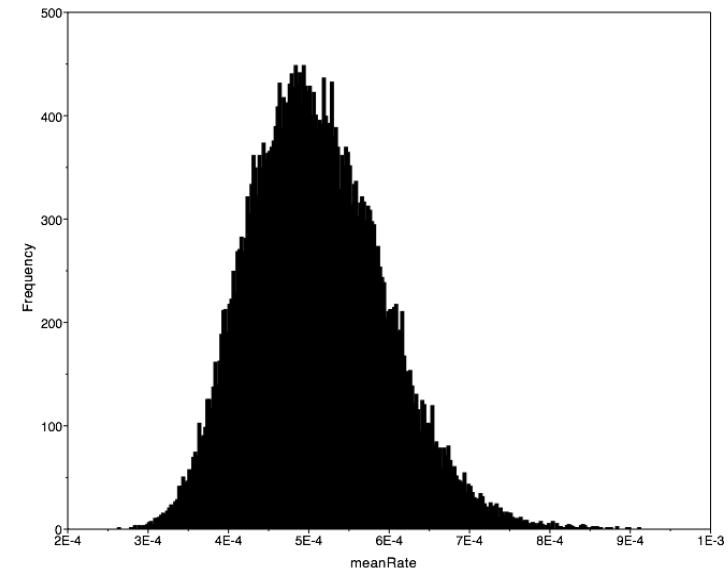
Assessing MCMC Performance: Based on Single Chains

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Assessing MCMC Performance: Based on Single Chains

2. Mixing diagnostics

Form of the time-series plots of parameter estimates

Continuous parameters (e.g., substitution rates)

- warm and fuzzy caterpillars

Acceptance rates of parameter updates

Continuous and discrete parameters

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Form of the marginal posterior probability densities

Continuous parameters (e.g., substitution rates)

- beware of porcupine roadkill!

Assessing MCMC Performance: Based on Single Chains

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qualitative
diagnostics

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qualitative
diagnostics

Autocorrelation time (ACT) of parameter samples

Effective sample size (ACT) of parameter samples

quantitative
diagnostics

Assessing MCMC Performance: Based on Single Chains

2. Mixing diagnostics

Autocorrelation time (ACT) of parameter samples

Assessing MCMC Performance: Based on Single Chains

2. Mixing diagnostics

Autocorrelation time (ACT) of parameter samples

The lag (number of cycles) it takes for autocorrelation in parameter values to break down.

Assessing MCMC Performance: Based on Single Chains

2. Mixing diagnostics

Autocorrelation time (ACT) of parameter samples

The lag (number of cycles) it takes for autocorrelation in parameter values to break down.

Effective Sample Size (ESS) diagnostic

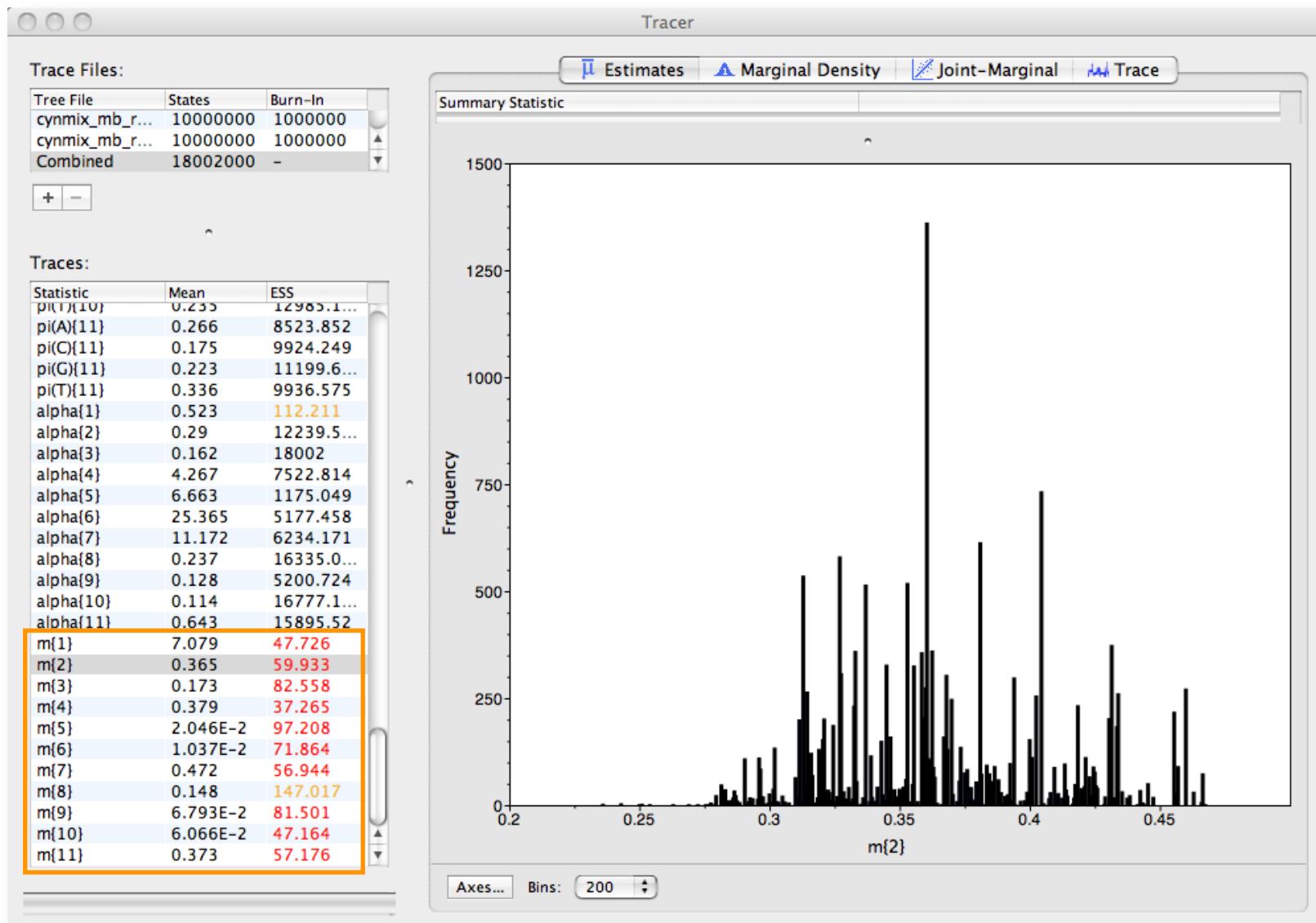
Continuous or discrete parameters

- number of samples/autocorrelation time (ACT)

Assessing MCMC Performance: Based on Single Chains

Example: ESS values for relative-rate multipliers from two MrBayes runs

poor mixing



Outline

IV. Diagnosing MCMC performance

Motivation and overview of the basics

V. MCMC Diagnostics

General strategies:

- 
- diagnostics based on single chains
 - diagnostics based on multiple, replicate chains

Outline

IV. Diagnosing MCMC performance

Motivation and overview of the basics

V. MCMC Diagnostics

General strategies:

- diagnostics based on single chains
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Assessing MCMC Performance: Diagnostics Based on Multiple Runs

Compare estimates from multiple independent chains

Assessing MCMC Performance: Diagnostics Based on Multiple Runs

Compare estimates from multiple independent chains

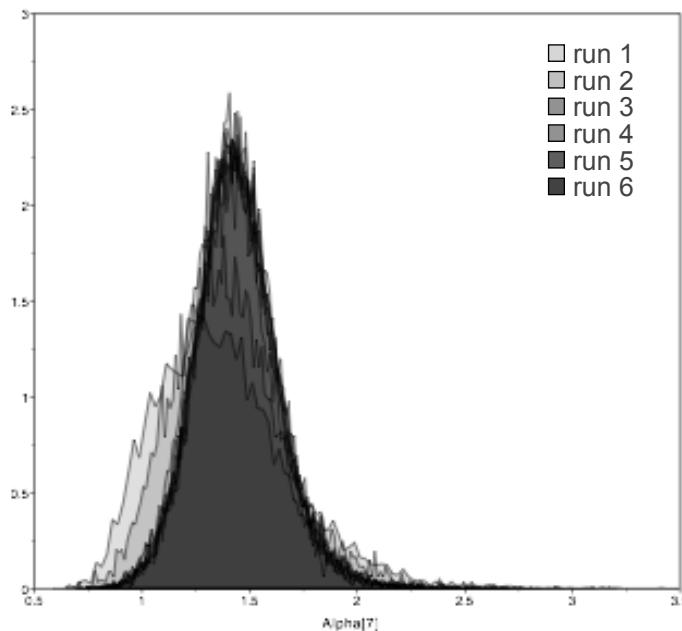
Form of the marginal posterior densities for all parameters

Continuous parameters

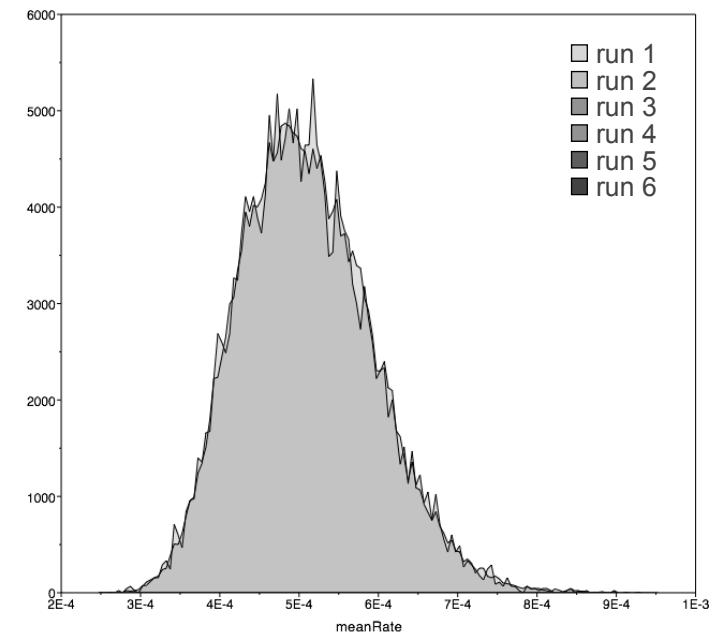
Assessing MCMC Performance: Diagnostics Based on Multiple Runs

Example: Tracer plots of marginal densities from multiple runs

bad convergence



better convergence



Parameter estimates from replicate independent MCMC analyses should be effectively identical.

Assessing MCMC Performance: Diagnostics Based on Multiple Runs

Compare estimates from multiple independent chains

Form of the marginal posterior densities for all parameters

Continuous parameters

PSRF (Gelman–Rubin) diagnostic

Continuous and discrete parameters

1. Run $m \geq 2$ chains of length $2c$ from overdispersed starting values.
2. Calculate the within-chain and between-chain variance.
3. Calculate the PSRF.

Assessing MCMC Performance: Diagnostics Based on Multiple Runs

Example: PSRF values for relative-rate multipliers from two MrBayes runs

bad convergence		95% Cred. Interval					
Parameter		Mean	Variance	Lower	Upper	Median	PSRF *
TL{all}		4.921609	2.998138	2.836000	7.295000	5.056000	9.084
kappa{4,5}		3.095696	0.054125	2.667623	3.587024	3.085271	1.000
alpha{5}		1.006544	0.087721	0.606472	1.738482	0.950093	1.000
pinvar{1}		0.307396	0.009357	0.095913	0.471070	0.316173	1.000
m{1}		0.264226	0.009315	0.146502	0.421870	0.244468	5.507
m{2}		0.040919	0.000227	0.022205	0.065884	0.037425	5.279
m{3}		2.721453	7.157157	0.039001	5.544253	5.030560	69.564
m{4}		2.125810	3.568002	0.199137	4.044249	3.917338	150.012
m{5}		0.188768	0.004373	0.109303	0.295129	0.170624	5.749

better convergence		95% Cred. Interval					
Parameter		Mean	Variance	Lower	Upper	Median	PSRF *
TL{all}		0.073893	0.000034	0.063000	0.086000	0.074000	1.000
kappa{2,3}		3.236308	0.366904	2.199024	4.587719	3.190195	1.000
m{1}		1.285838	0.028345	0.980634	1.630387	1.278161	1.000
m{2}		1.423906	0.015507	1.182596	1.664627	1.423610	1.000
m{3}		0.589346	0.005341	0.453175	0.736459	0.587617	1.001

Assessing MCMC Performance: Diagnostics Based on Multiple Runs

Compare estimates from multiple independent chains

Form of the marginal posterior densities for all parameters

- Continuous parameters

- PSRF (Gelman–Rubin) diagnostic

- Continuous and discrete parameters

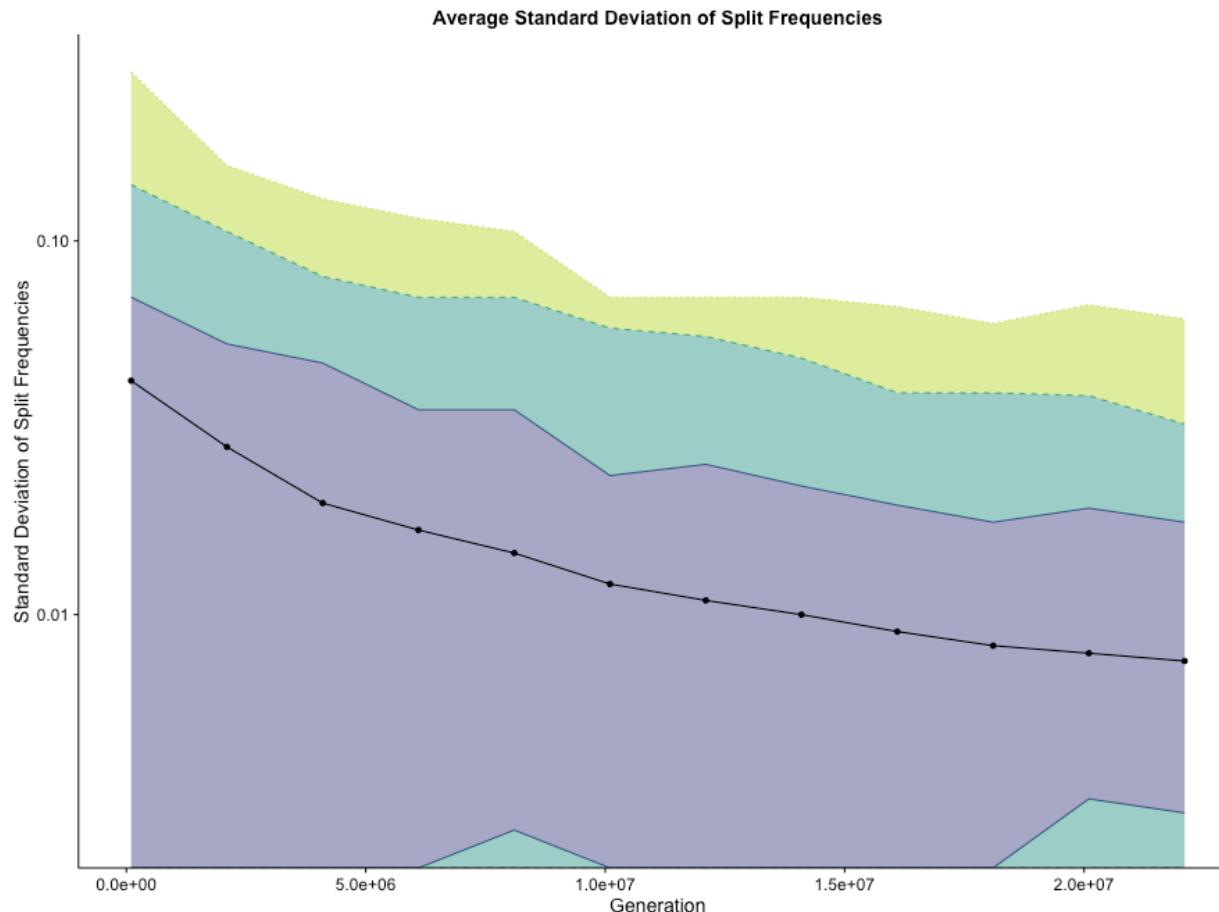
Comparing independent samples of trees

- ASDSF: similarity of trees sampled by paired, independent chains

Assessing MCMC Performance: Diagnostics Based on Multiple Runs

Example: ASDSF

The overall similarity of the trees sampled by two independent, simultaneous MCMC analyses



Assessing MCMC Performance: Diagnostics Based on Multiple Runs

Compare estimates from multiple independent chains

Form of the marginal posterior densities for all parameters

- Continuous parameters

- PSRF (Gelman–Rubin) diagnostic

- Continuous and discrete parameters

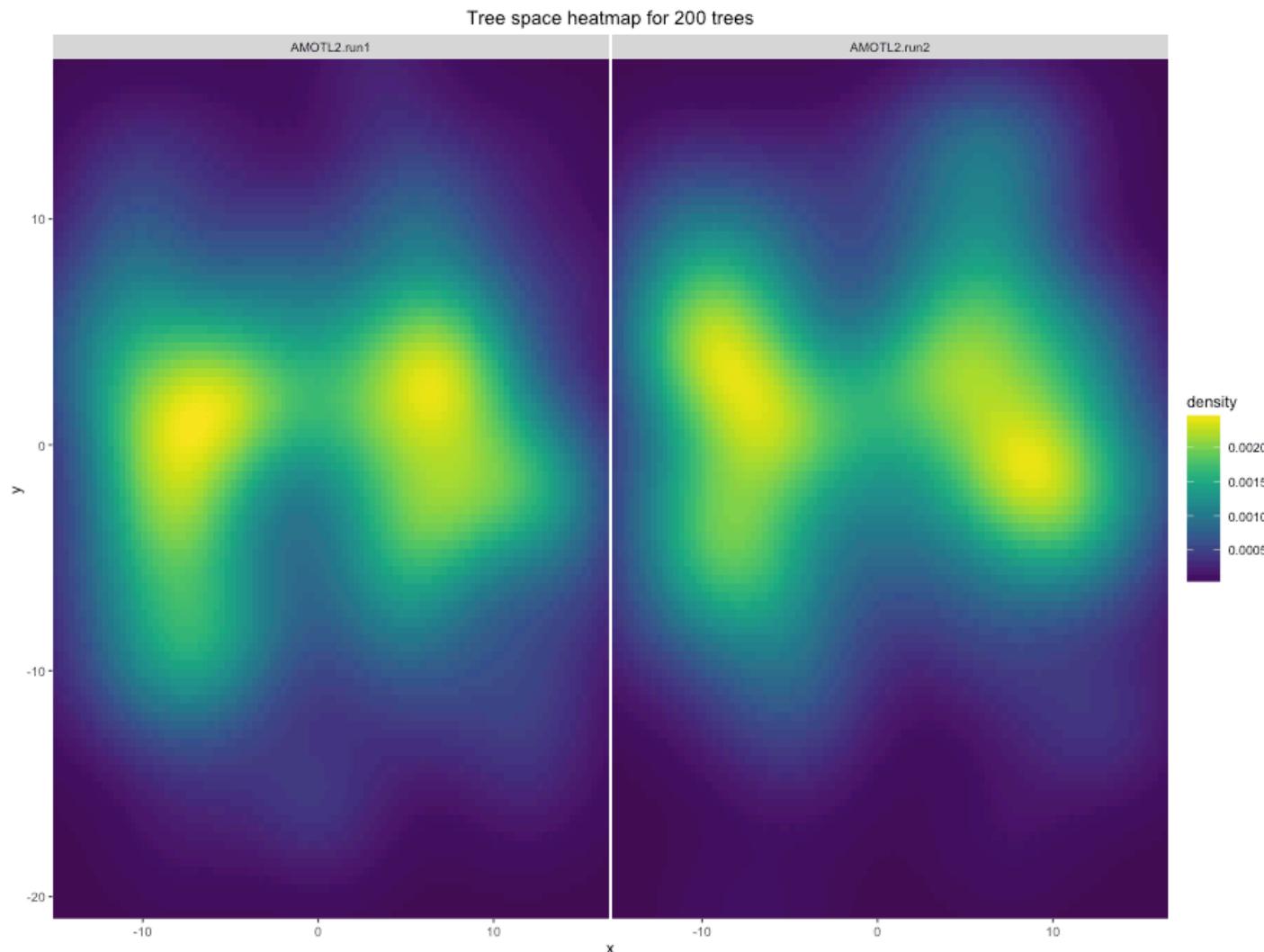
Comparing independent samples of trees

- ASDSF: similarity of trees sampled by paired, independent chains

- Treespace visualization

Assessing MCMC Performance: Diagnostics Based on Multiple Runs

Example: Visualizing treespace with RWTY



Assessing MCMC Performance: Diagnostics Based on Multiple Runs

Compare estimates from multiple independent chains

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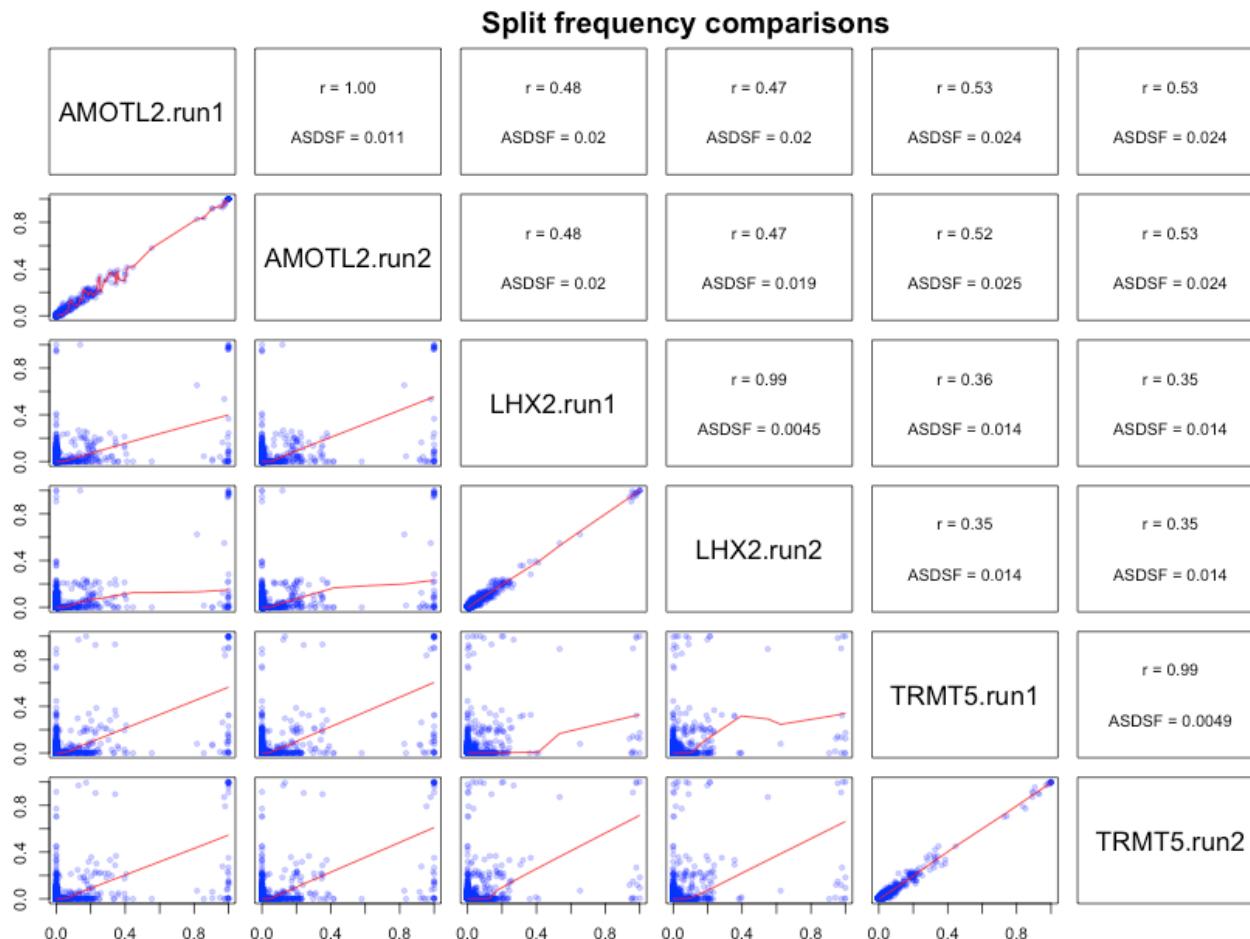
- ASDSF: similarity of trees sampled by paired, independent chains

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- Split frequencies among runs

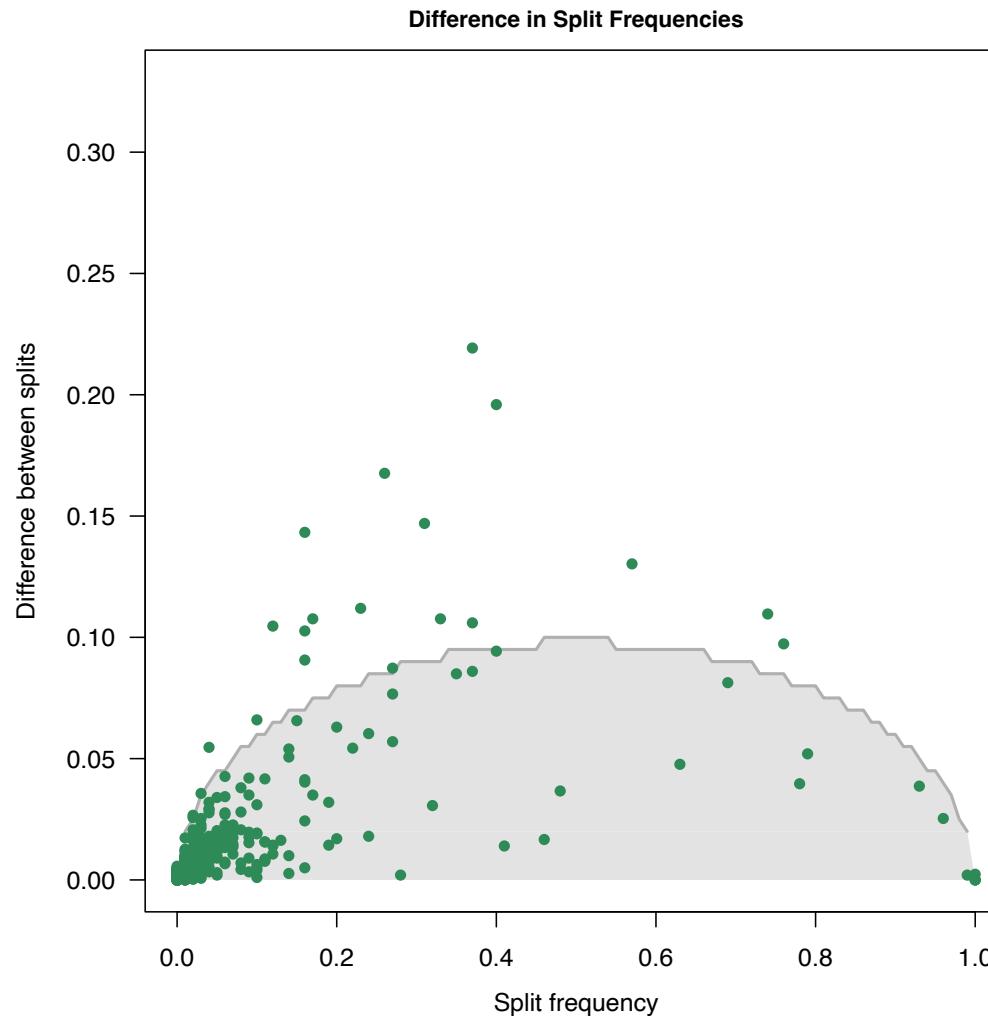
Assessing MCMC Performance: Diagnostics Based on Multiple Runs

Example: Comparing split frequencies among chains



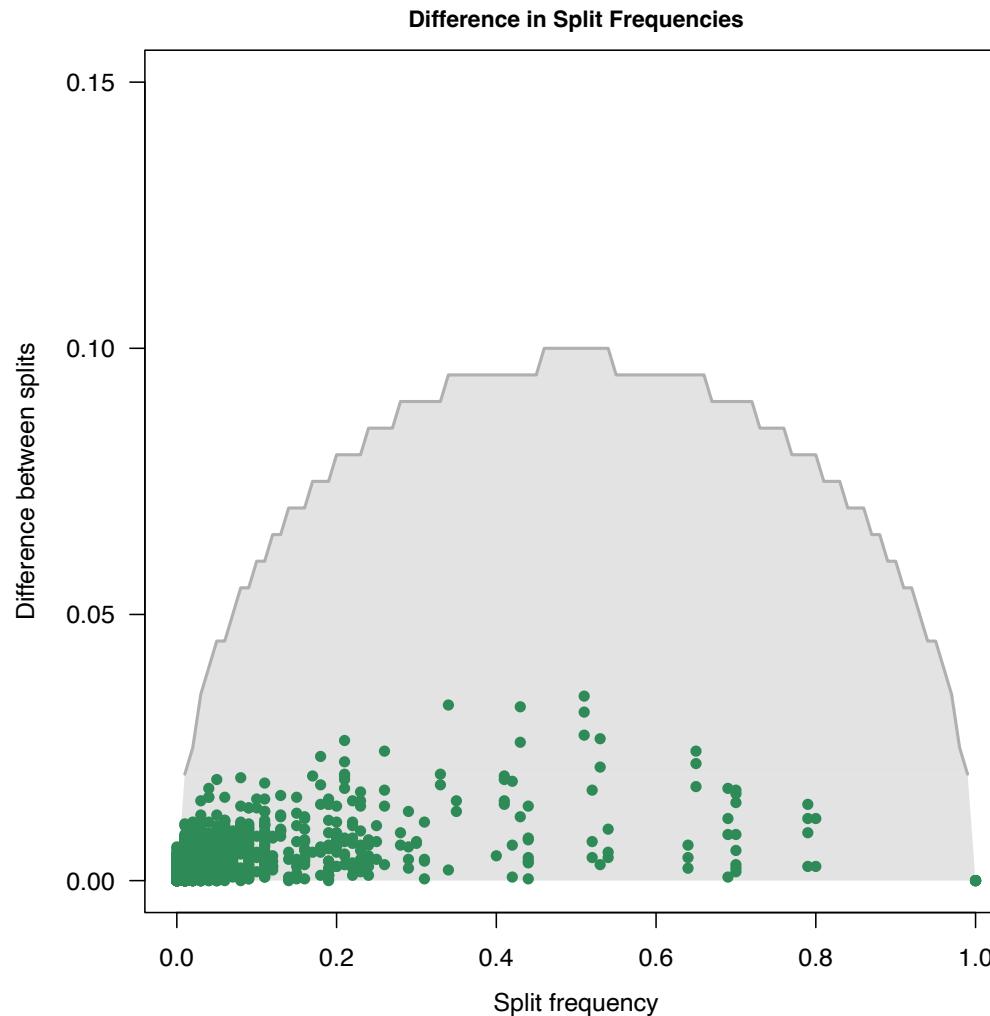
Assessing MCMC Performance: Diagnostics Based on Multiple Runs

Example: Testing for equality of split frequencies among chains



Assessing MCMC Performance: Diagnostics Based on Multiple Runs

Example: Testing for equality of split frequencies among chains



Summary: Some General Strategies for Assessing MCMC Performance

1. When do you need to assess MCMC performance?

ALWAYS

2. When should you assess the performance of individual runs?

ALWAYS

3. Which diagnostics should you use to assess individual runs?

ALL that are relevant for the models/parameters you are estimating under

4. When is a single run sufficient to assess MCMC performance?

NEVER

Summary: Some General Strategies for Assessing MCMC Performance

5. When should you use Metropolis-Coupling?

Whenever you cannot be certain that standard MCMC is adequate
i.e., **ALWAYS** (and be wary of programs where it is not possible)

6. When should you perform multiple independent MCMC runs?

ALWAYS (and be wary of pseudo-independence)

7. Which diagnostics should you use to assess multiple runs?

ALL that are relevant for the models/parameters you are estimating under

8. How many independent MCMC runs are sufficient?

AS MANY AS POSSIBLE (*i.e.*, as many as you think your data/problem deserve)

9. How long should you run each MCMC analysis?

AS LONG AS POSSIBLE (*i.e.*, as long as you think your data/problem deserve)

Summary: Some General Strategies for Assessing MCMC Performance

Tracer

<https://github.com/beast-dev/tracer/releases/latest>

RWTY

<https://github.com/danlwarren/RWTY>

convenience

<https://revbayes.github.io/tutorials/convergence/>