A Brief Introduction to Bayesian Model Selection and Validation

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CoME, 2022

Outline

I. Model selection

What is the relative fit of the candidate models (hypotheses) to our data?

Bayesian methods for selecting among candidate models (hypotheses)

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II. Model adequacy

What is the <u>absolute</u> fit of the candidate models (hypotheses) to our data?

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III. Model averaging

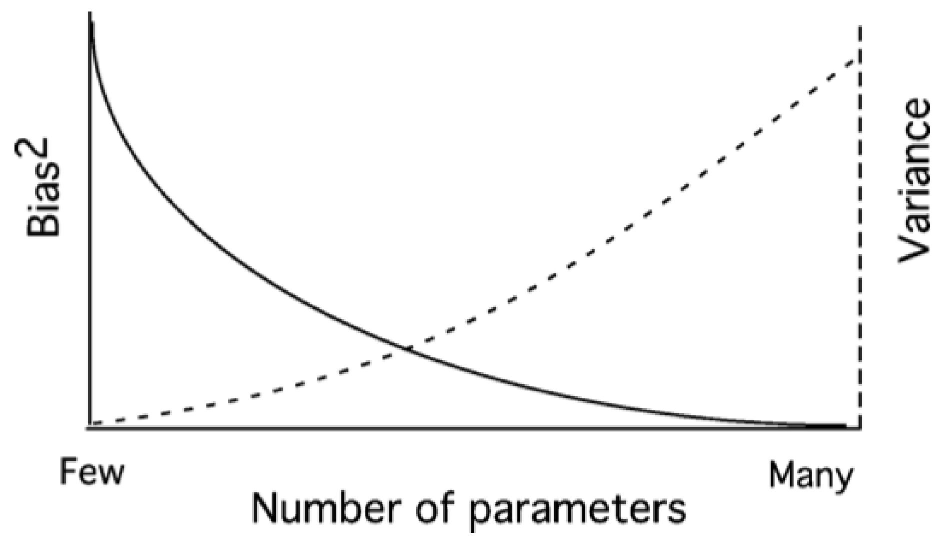
How do we accommodate uncertainty in the choice among candidate models?

Bayesian methods for averaging over candidate models (hypotheses)

Model Specification Issues

Model-based inference is based on the model

All of the parameters of our model (even 'nuisance' parameters) are critical



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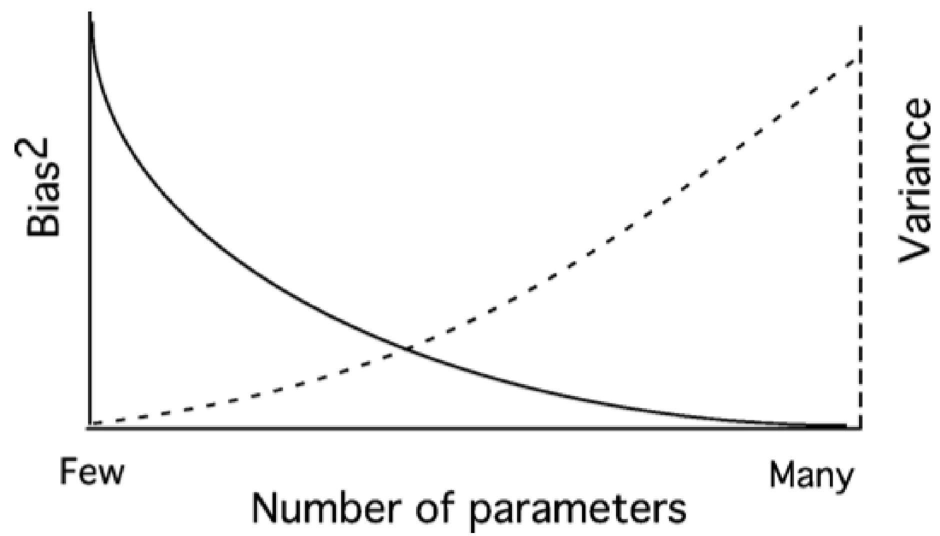

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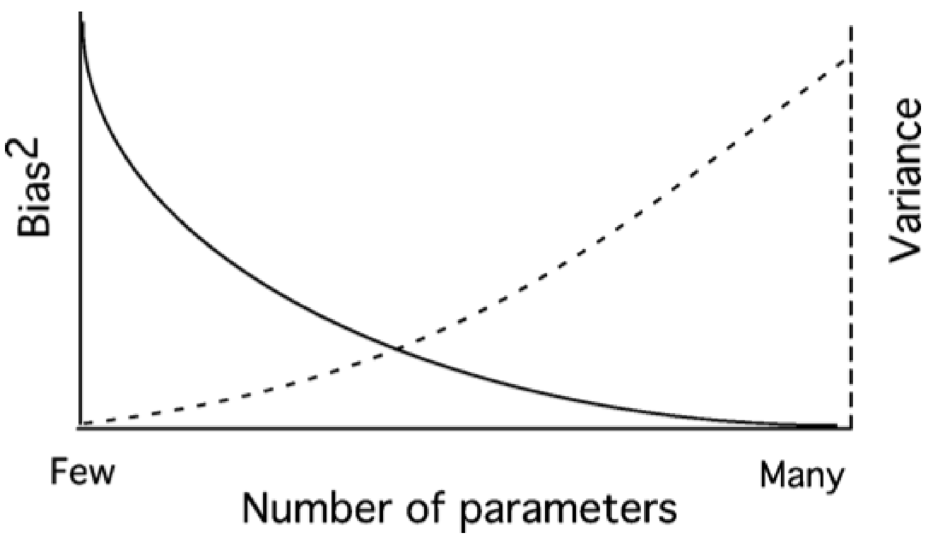

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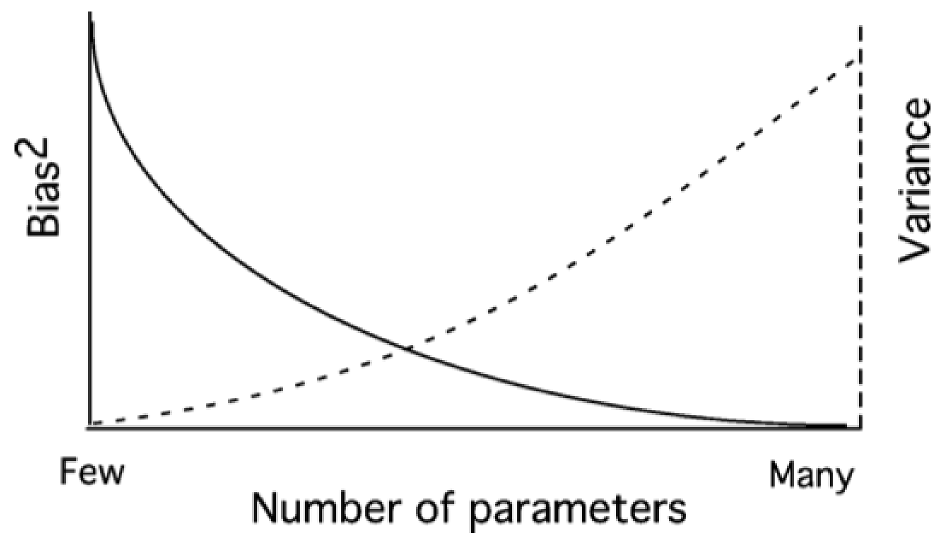
- an over-specified model will inflate the error variance of parameter estimates



Model Selection

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Assessing the fit of our data to competing models is critical and useful:

- we need to identify which model provides the best fit to our data in order to obtain reliable parameter estimates
- comparing the relative fit of two (or more) competing models is how we learn from our data

Model Selection

Data

sequence
alignment

Model

tree with
branch lengths

substitution
model

Model 1

Inference Method

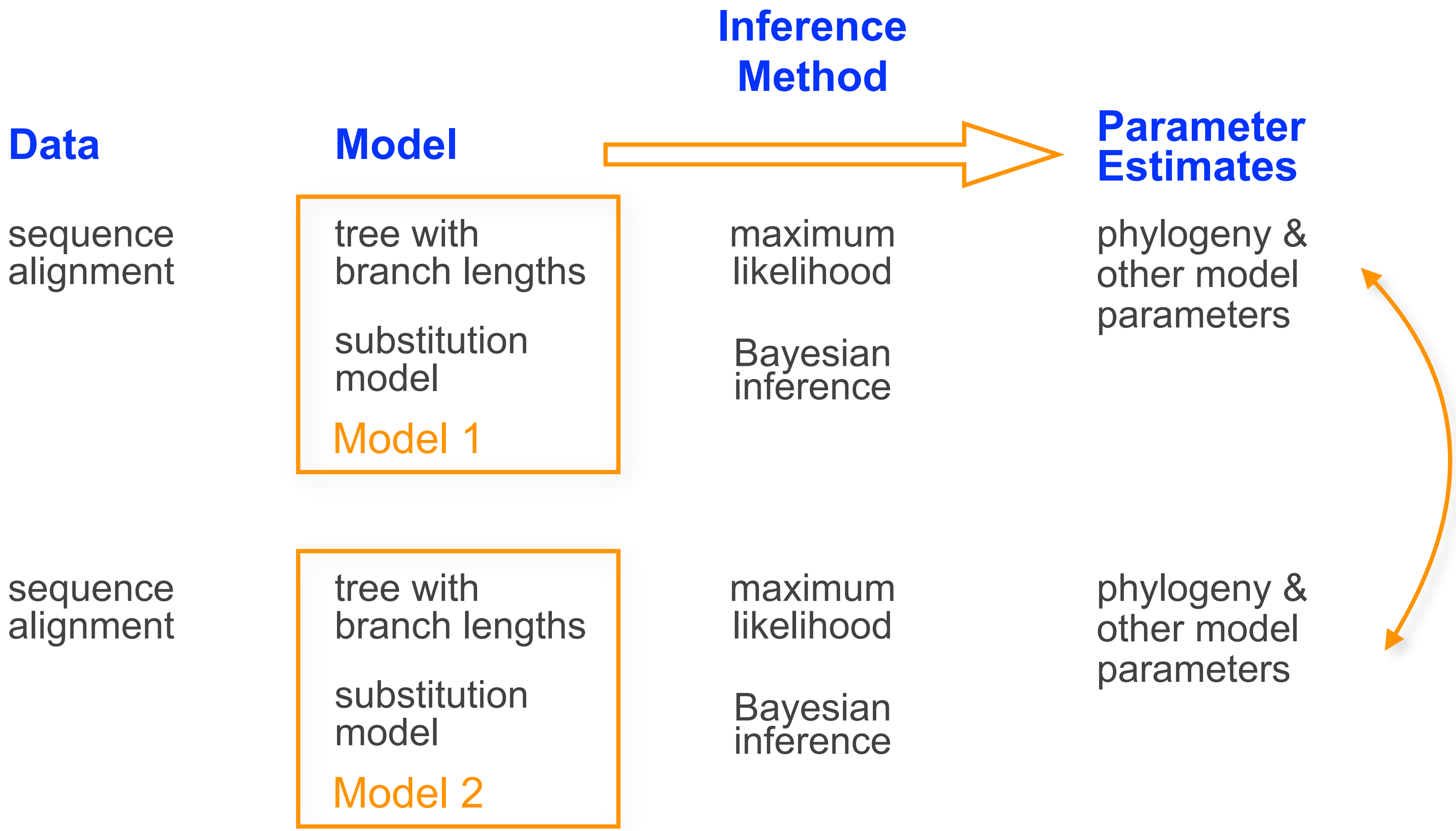
maximum
likelihood

Bayesian
inference

Parameter Estimates

phylogeny &
other model
parameters

Model Selection



Model Selection

Data	Model	Inference Method	Parameter Estimates
sequence alignment	tree with branch lengths substitution model Model 1	maximum likelihood Bayesian inference	phylogeny & other model parameters
sequence alignment	tree with branch lengths substitution model Model 2	maximum likelihood Bayesian inference	phylogeny & other model parameters

Model comparison is critical for obtaining unbiased parameter estimates

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Model comparison is critical for obtaining unbiased parameter estimates

Model comparison is the means by which we test hypotheses about our data

Model Selection: Bayesian Methods

Bayes factors

The marginal likelihood is the weighted sum over the possible discrete parameter values:

$$\overbrace{P(\theta_i \mid \mathbf{X})}^{\text{posterior probability}} = \frac{\overbrace{P(\mathbf{X} \mid \theta_i)}^{\text{likelihood}}\overbrace{P(\theta_i)}^{\text{prior}}}{\underbrace{\sum_{j=1}^{N} P(\mathbf{X} \mid \theta_j) P(\theta_j)}_{\text{marginal likelihood}}}$$

Model Selection: Bayesian Methods

Bayes factors

The marginal likelihood is the weighted sum over the possible discrete parameter values:

$$\overbrace{\Pr[\text{Biased} \mid \text{⚃}, \text{⚅}]}^{\text{posterior probability}} = \frac{\overbrace{\Pr[\text{⚃}, \text{⚅} \mid \text{Biased}]}^{\text{likelihood}} \times \overbrace{\Pr[\text{Biased}]}^{\text{prior probability}}}{\underbrace{\Pr[\text{⚃}, \text{⚅} \mid \text{Biased}] \times \Pr[\text{Biased}] + \Pr[\text{⚃}, \text{⚅} \mid \text{Fair}] \times \Pr[\text{Fair}]}_{\text{marginal likelihood}}}$$

Model Selection: Bayesian Methods

Bayes factors

The marginal likelihood is the weighted integral over the possible continuous parameter values:

$$\overbrace{P(\theta \mid \mathbf{X})}^{\text{posterior probability}} = \frac{\overbrace{P(\mathbf{X} \mid \theta)}^{\text{likelihood}}\overbrace{P(\theta)}^{\text{prior}}}{\underbrace{\int_\theta P(\mathbf{X} \mid \theta) P(\theta) d\theta}_{\text{marginal likelihood}}}$$

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More generally, the marginal likelihood does not depend on any particular parameter values:

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$$P(\mathbf{X}) = \int_\theta P(\mathbf{X} \mid \theta) P(\theta) d\theta$$

Model Selection: Bayesian Methods

Bayes factors

What it *does* depend on are the model and priors (the “full Bayesian model”), M_i

$$\overbrace{P(\theta \mid \mathbf{X}, M_i)}^{\text{posterior probability}} = \frac{\overbrace{P(\mathbf{X} \mid \theta, M_i)}^{\text{likelihood}}\overbrace{P(\theta \mid M_i)}^{\text{prior}}}{\underbrace{P(\mathbf{X} \mid M_i)}_{\text{marginal likelihood}}}$$

Model Selection: Bayesian Methods

Bayes factors

Bayesian model comparison is based on the *average* fit of the model to the data

- the marginal likelihood is the likelihood of the data under the model averaged over the joint prior probability of the model parameters

More complex models are automatically penalized by virtue of the corresponding priors

- model comparison is (intentionally) sensitive to the assumed priors

Model Selection: Bayesian Methods

Bayes factors

Bayes factors are computed based on the marginal likelihoods of competing models:

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- models are preferred by virtue of their relative ability to predict the data
- $BF_{01} > 1$ supports model M_0, $BF_{01} < 1$ supports model M_1

BF_{01}	$2\ln BF_{01}$	Support for model M_0
1 to 3	0 to 2	Not worth more than a bare mention
3 to 20	2 to 6	Positive
20 to 150	6 to 10	Strong
> 150	> 10	Very strong

Model Selection: Bayesian Methods

Bayes factors

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Nasty properties of Bayes factors for model selection/hypothesis testing:

- it is sensitive to the assumed priors
- Bayesian inference via MCMC avoids estimating marginal likelihoods
- this requires estimation of the marginal likelihoods of candidate models

Model Selection: Bayesian Methods

Bayes factors

Recall Bayes theorem:

$$P(\theta_1, \theta_2, \ldots, \theta_k \mid \mathbf{X}, M_i) = \frac{P(\mathbf{X} \mid \theta_1, \theta_2, \ldots, \theta_k, M_i) P(\theta_1, \theta_2, \ldots, \theta_k \mid M_i)}{P(\mathbf{X} \mid M_i)}$$

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The *marginal likelihood* is the likelihood of the data averaged over the joint prior distribution of *all* model parameters:

$$P(\mathbf{X} \mid M_i) = \int_{\theta_1} \int_{\theta_2} \ldots \int_{\theta_k} P(\mathbf{X} \mid \theta_1, \theta_2, \ldots, \theta_k, M_i) P(\theta_1, \theta_2, \ldots, \theta_k \mid M_i) d\theta_1 \, d\theta_2 \, \ldots d\theta_k$$

Model Selection: Bayesian Methods

Bayes factors

The marginal likelihood is a *very* ugly multidimensional integral that cannot be calculated, which is what motivated the Metropolis–Hastings algorithm:

$$R = \min\left[1, \underbrace{\boxed{\frac{\Pr(X \mid \theta')}{\Pr(X \mid \theta)}}}_{\text{likelihood ratio}} \times \underbrace{\boxed{\frac{\Pr(\theta')}{\Pr(\theta)}}}_{\text{prior ratio}} \times \underbrace{\boxed{\frac{\Pr(\theta' \to \theta)}{\Pr(\theta \to \theta')}}}_{\text{proposal ratio}}\right]$$

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This allows us to estimate the posterior probability density while avoiding computation of the marginal likelihood:

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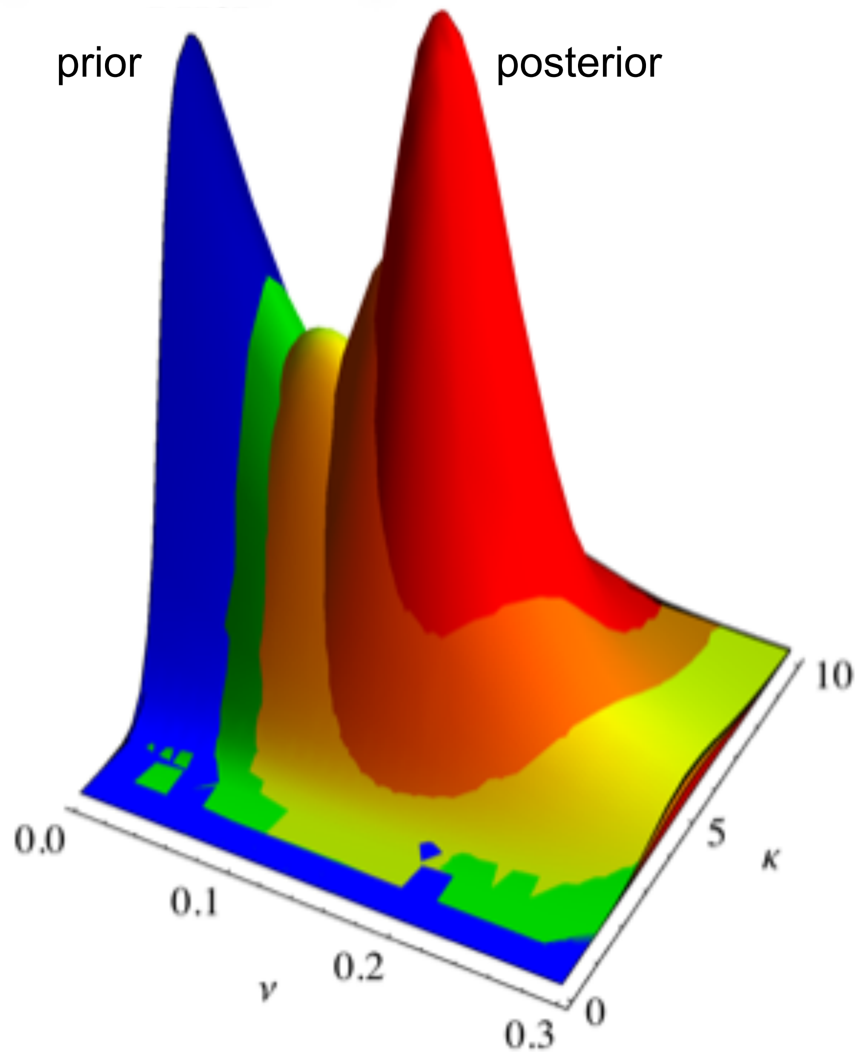
But, to compare models (test hypotheses), we need the marginal likelihoods!

Model Selection: Bayesian Methods

Estimating marginal likelihoods: power-posterior simulation

A reliable (but computationally) marginal-likelihood estimator



Xie *et al.* 2010

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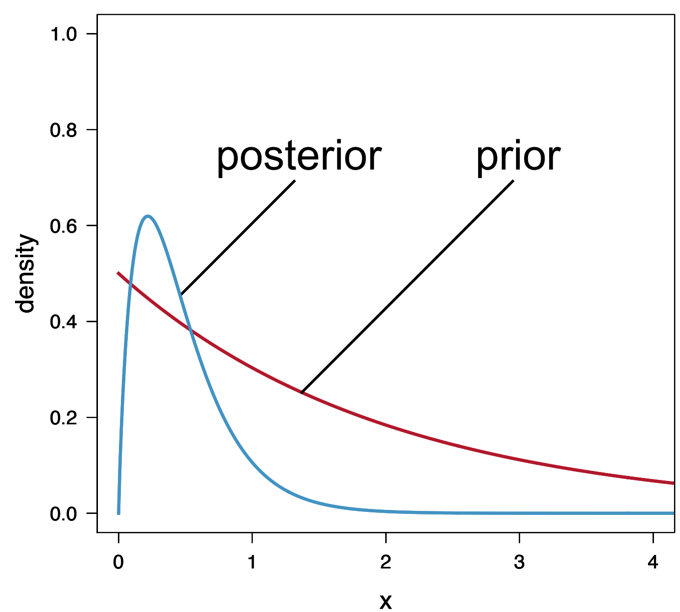

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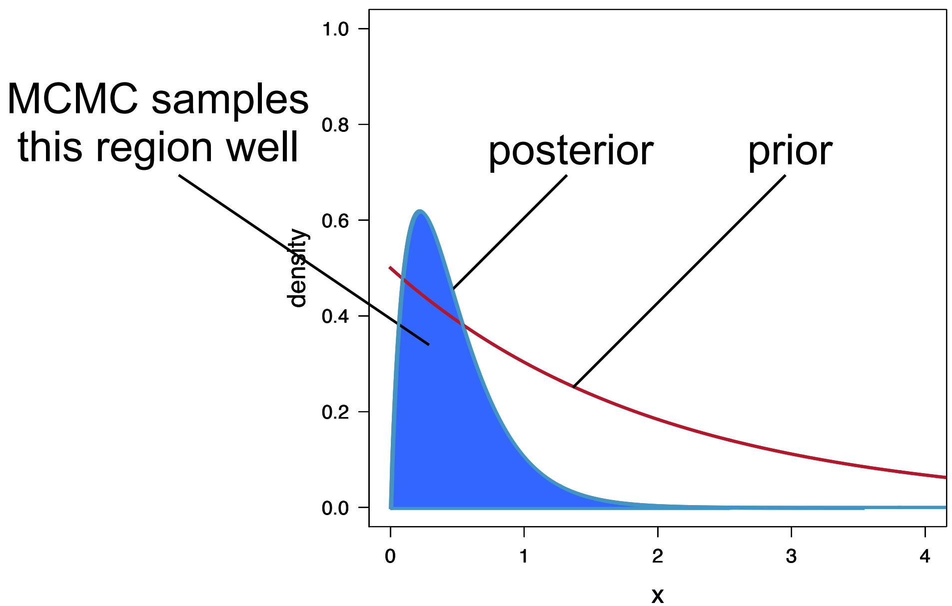

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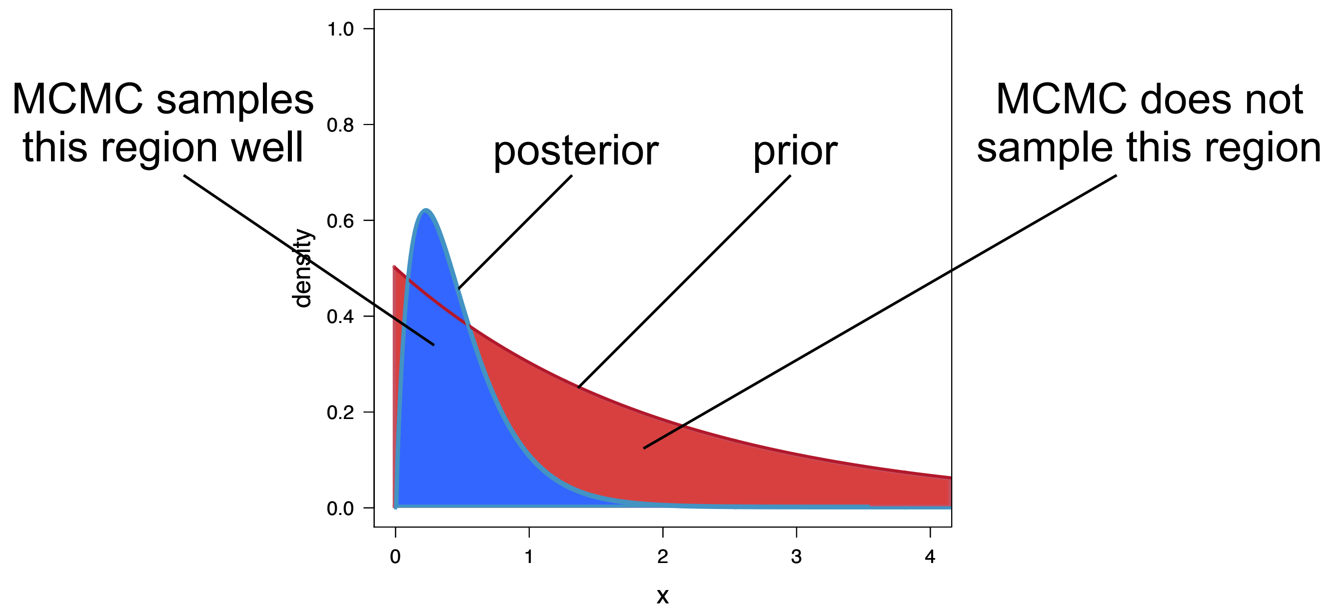

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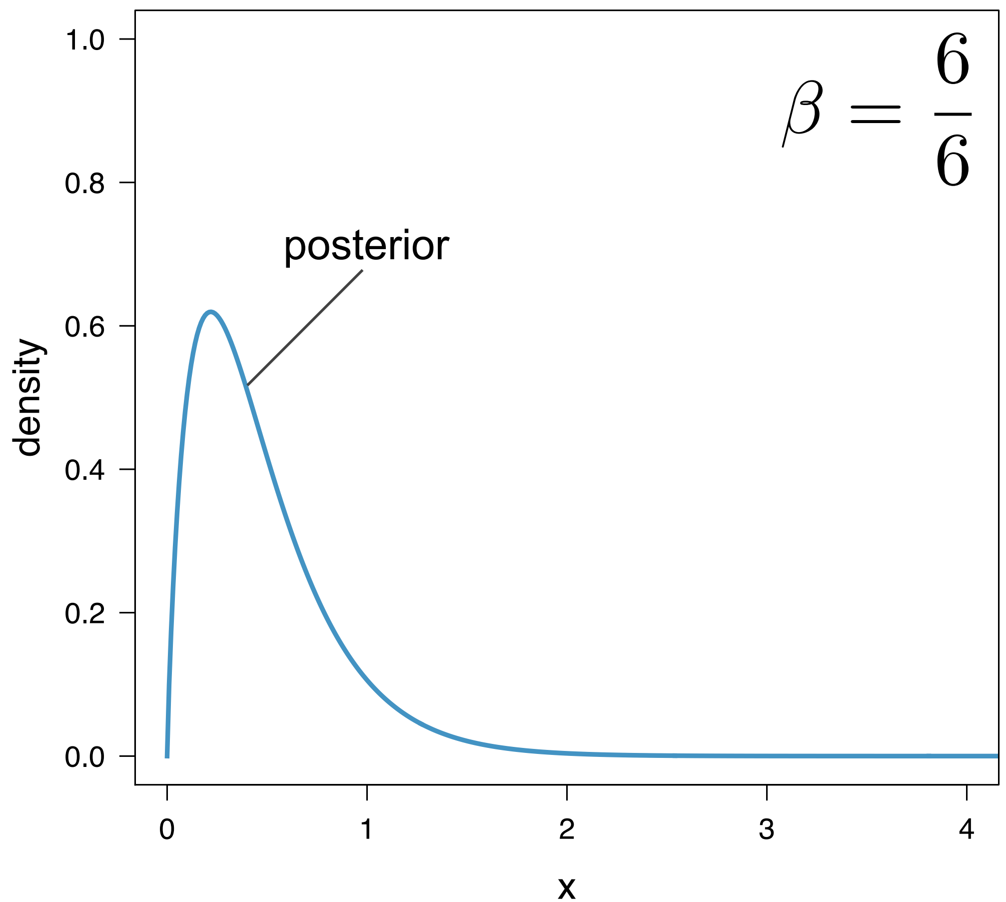
When $\beta = 0$, the MCMC targets the joint prior probability.

We run an MCMC simulation across many power posteriors from $\beta = 0$ to $\beta = 1$ to more accurately characterize the marginal likelihood.

Model Selection: Bayesian Methods

Estimating marginal likelihoods: power-posterior simulation

We simulate a Markov chain across a series of steps from the posterior to the prior, where each step corresponds to a power posterior, β.



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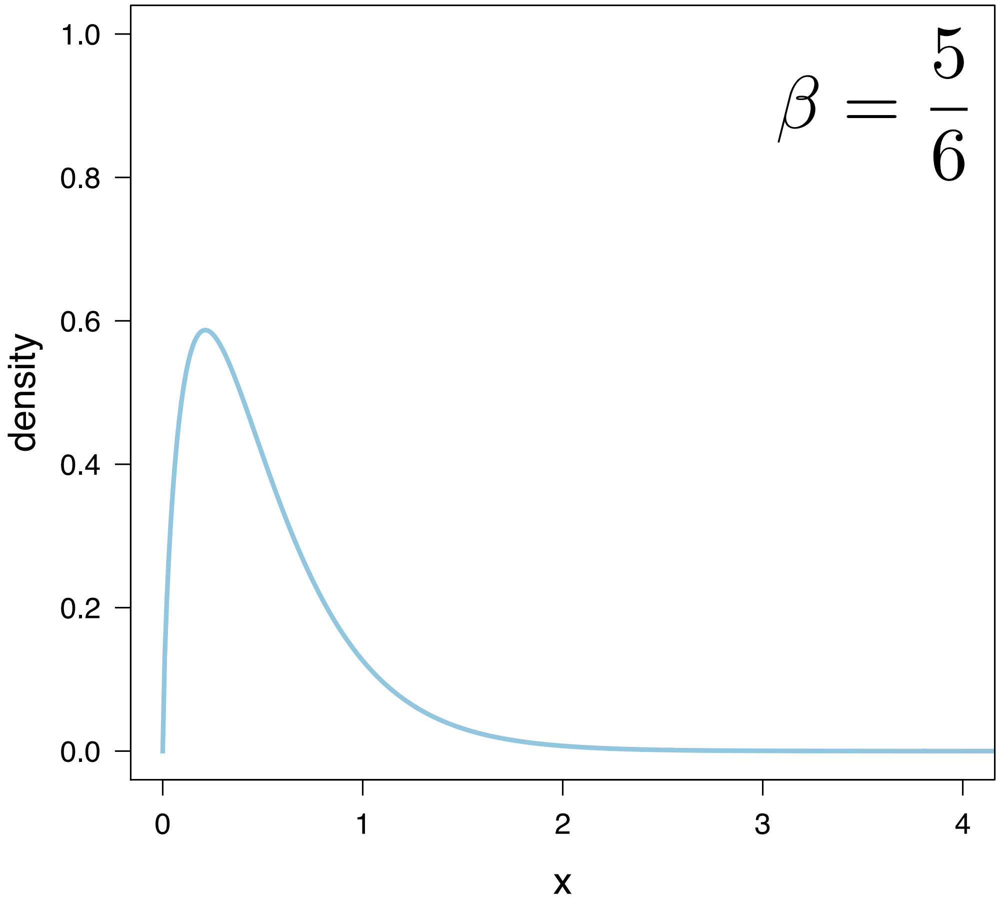

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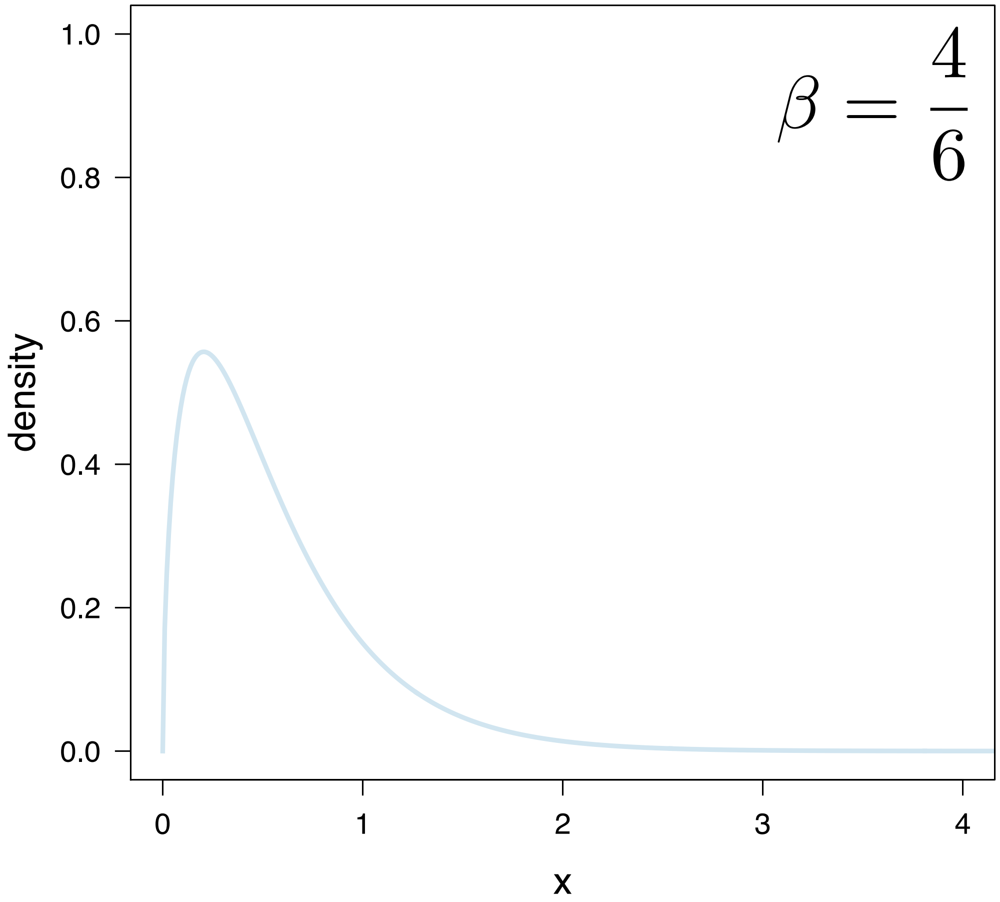

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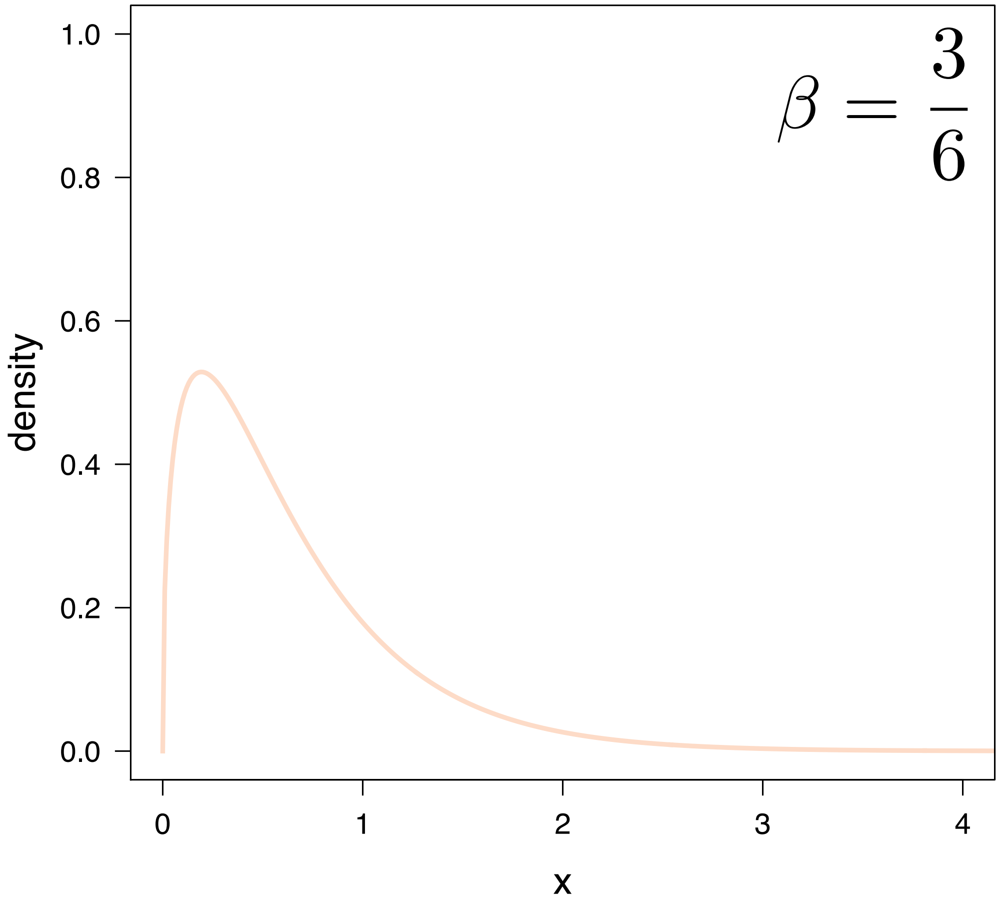

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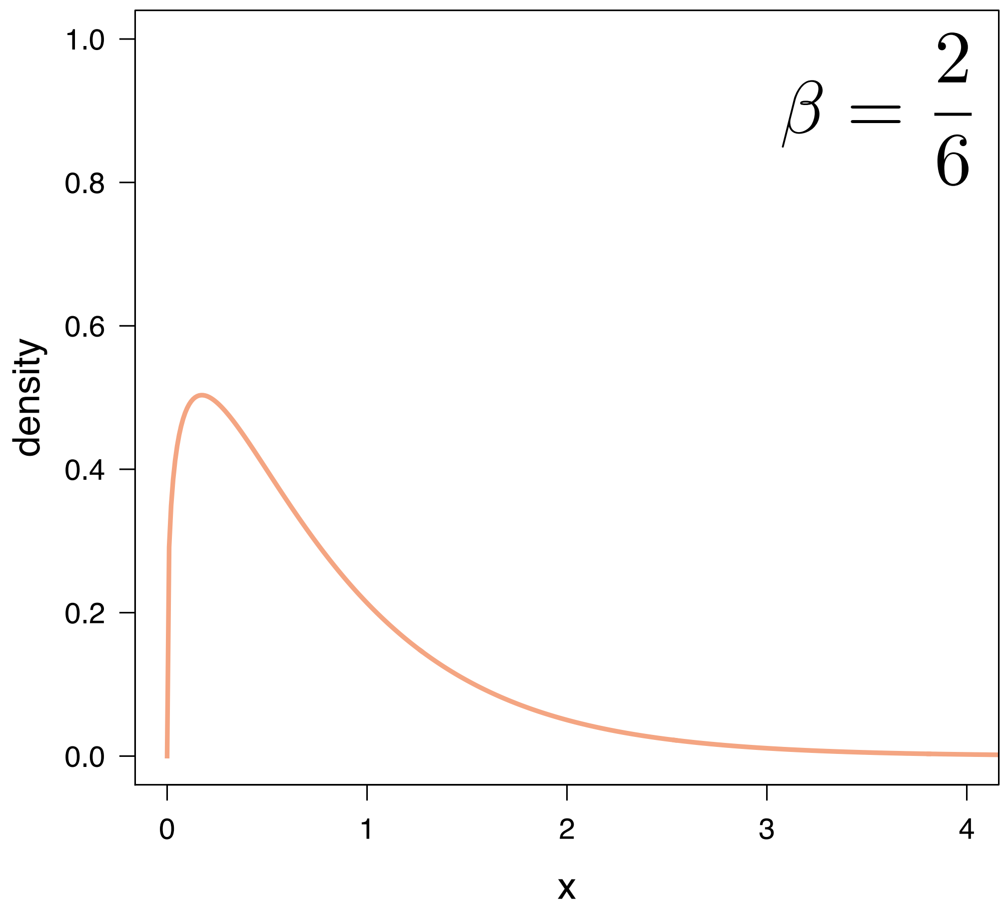

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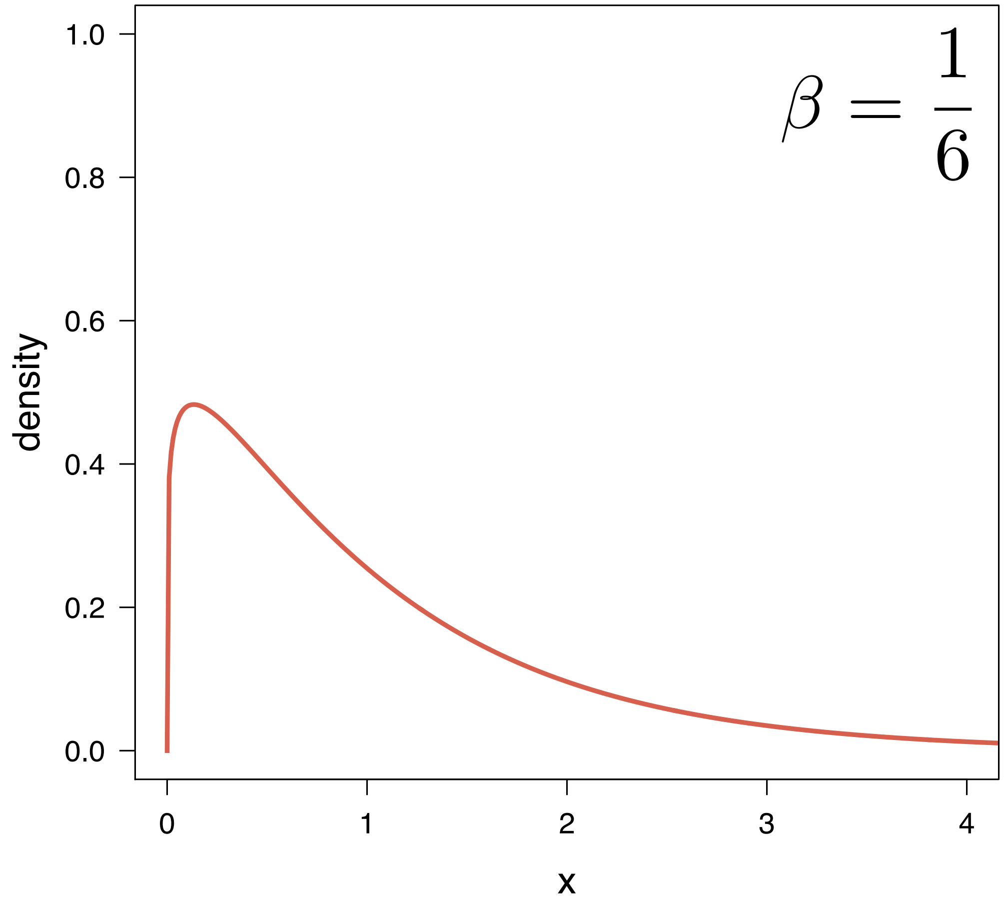

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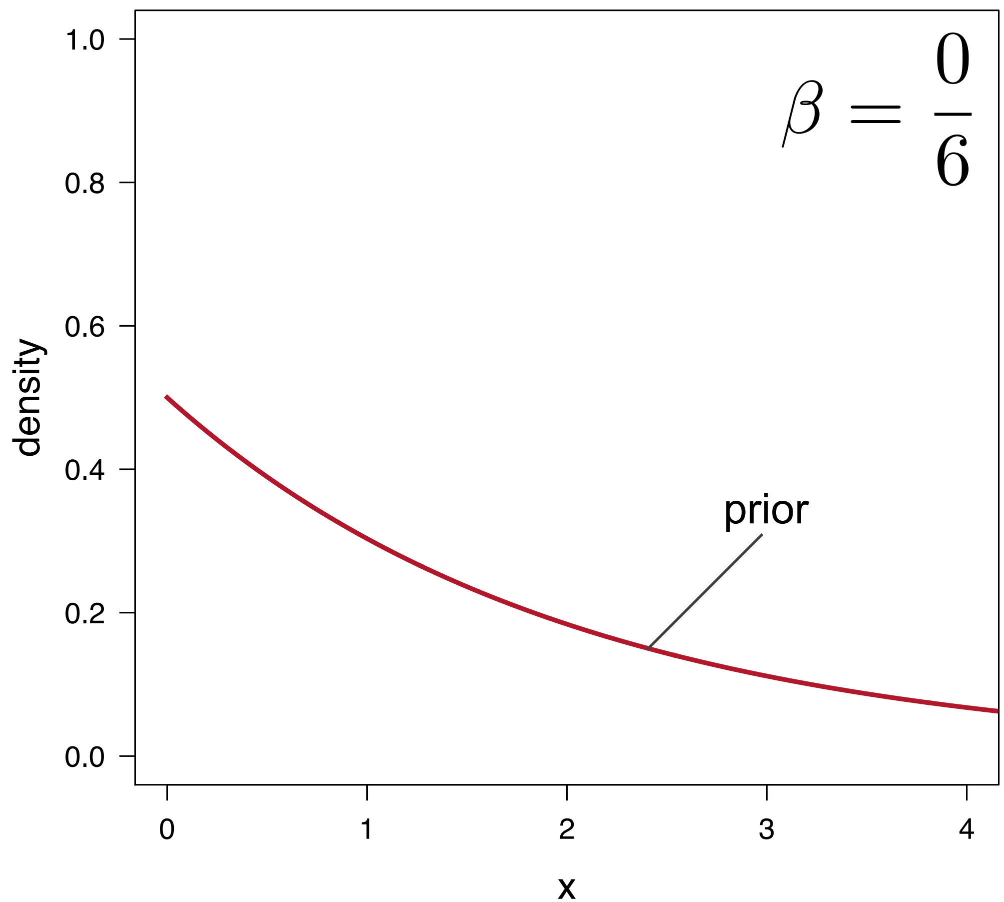

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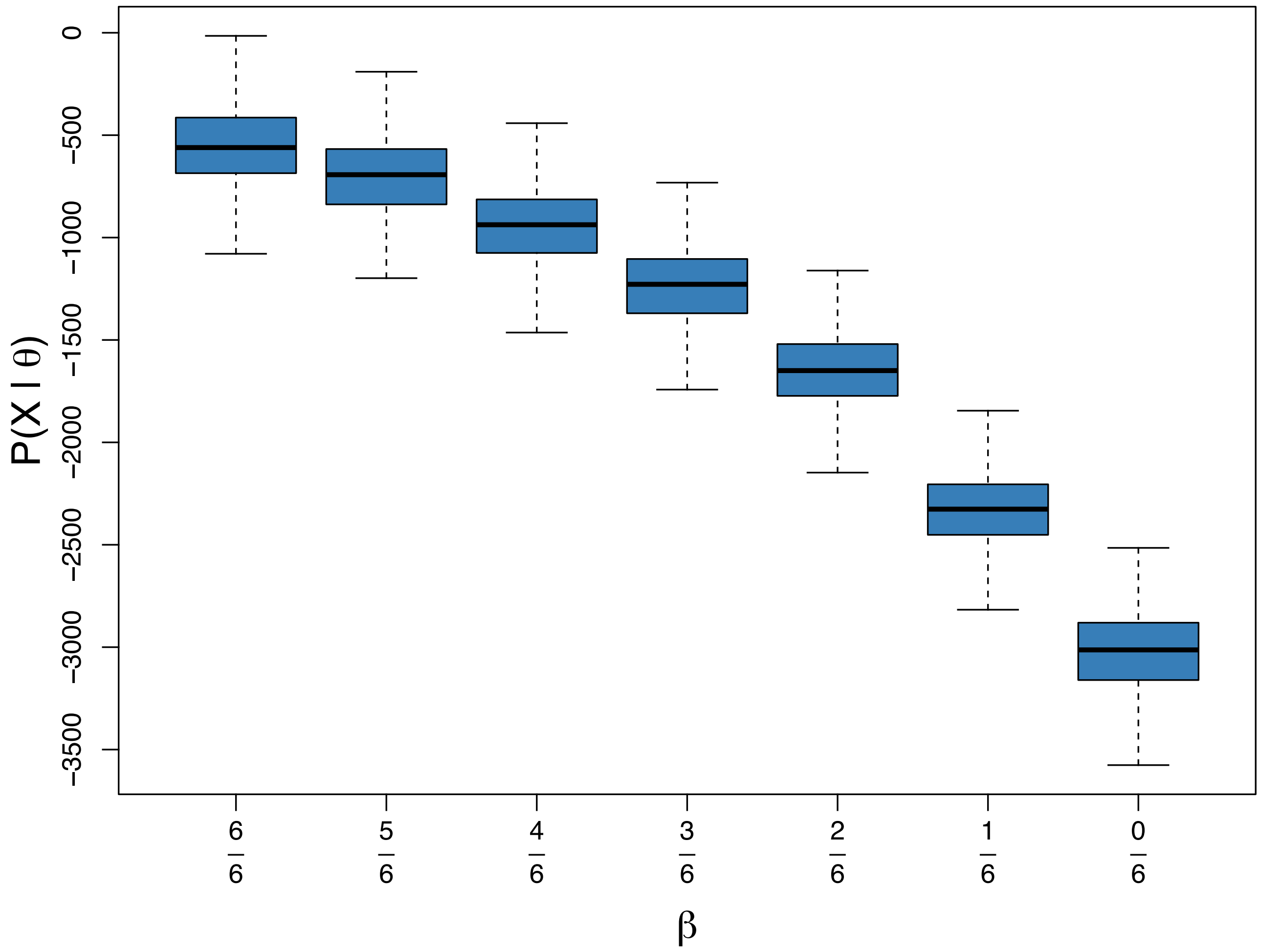
The sampled likelihoods at each stone can be used to estimate the marginal likelihood: path samplers[1] and stepping-stone samplers[2].



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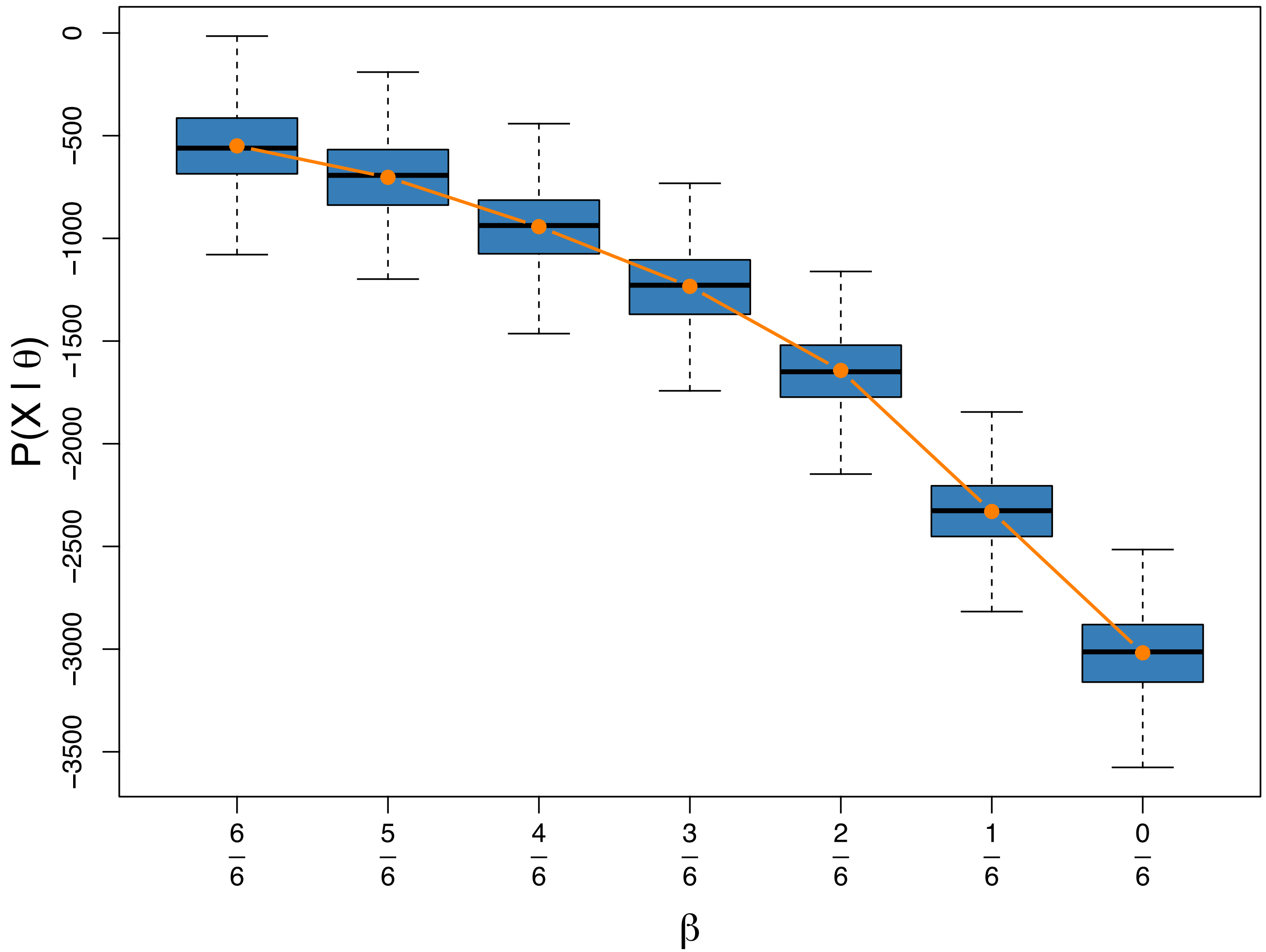

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Estimating marginal likelihoods: power-posterior simulation

How should the stones be distributed between the posterior and the prior to efficiently estimate the marginal likelihood?

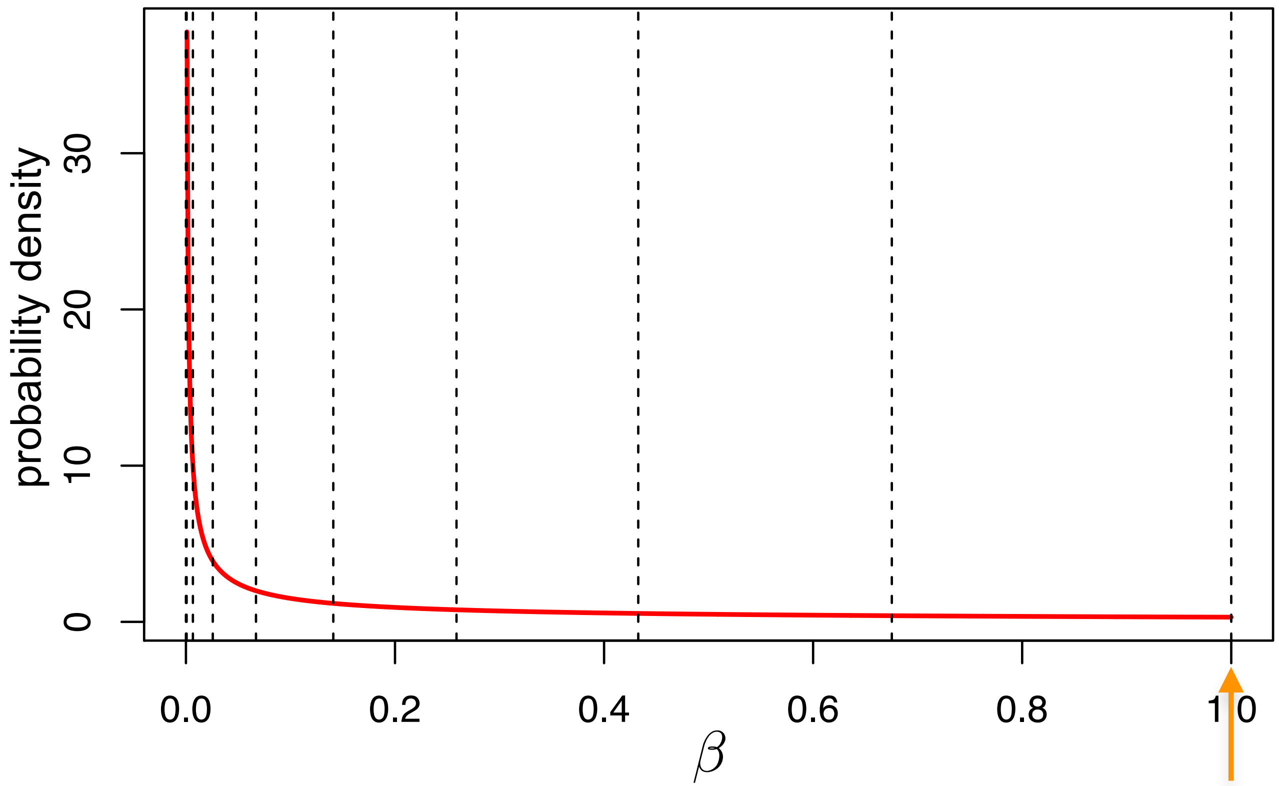
It is more difficult to sample adequately from the relatively diffuse prior compared to the more concentrated posterior distribution.

In order to improve the efficiency of the stepping-stone simulation, the stones are therefore spaced so that they are concentrated near the prior.

Model Selection: Bayesian Methods

Estimating marginal likelihoods: power-posterior simulation

Experience suggests that spacing the stones as evenly distributed quantiles of a beta distribution works well, where by convention $\mathrm{Beta}(0.3, 1.0)$.



1st stone
(posterior)

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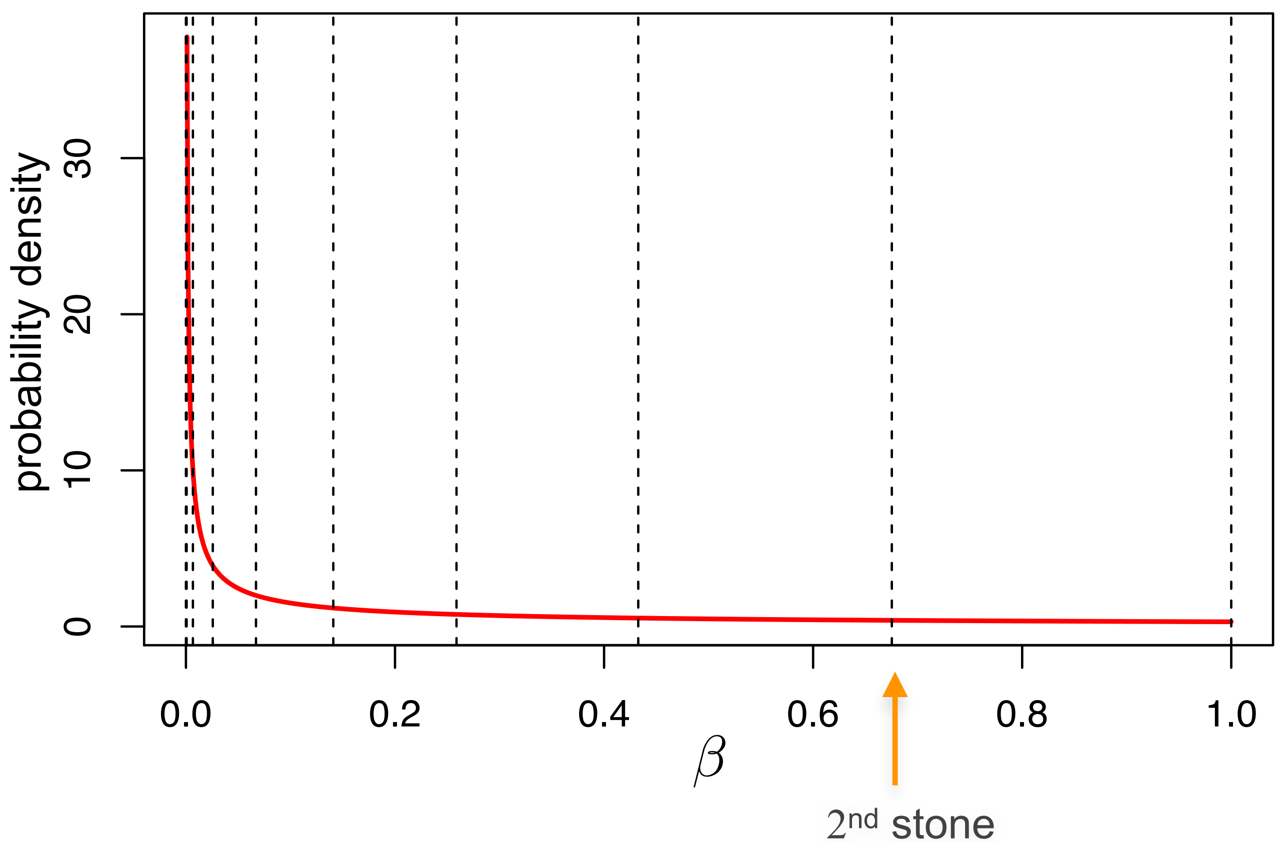

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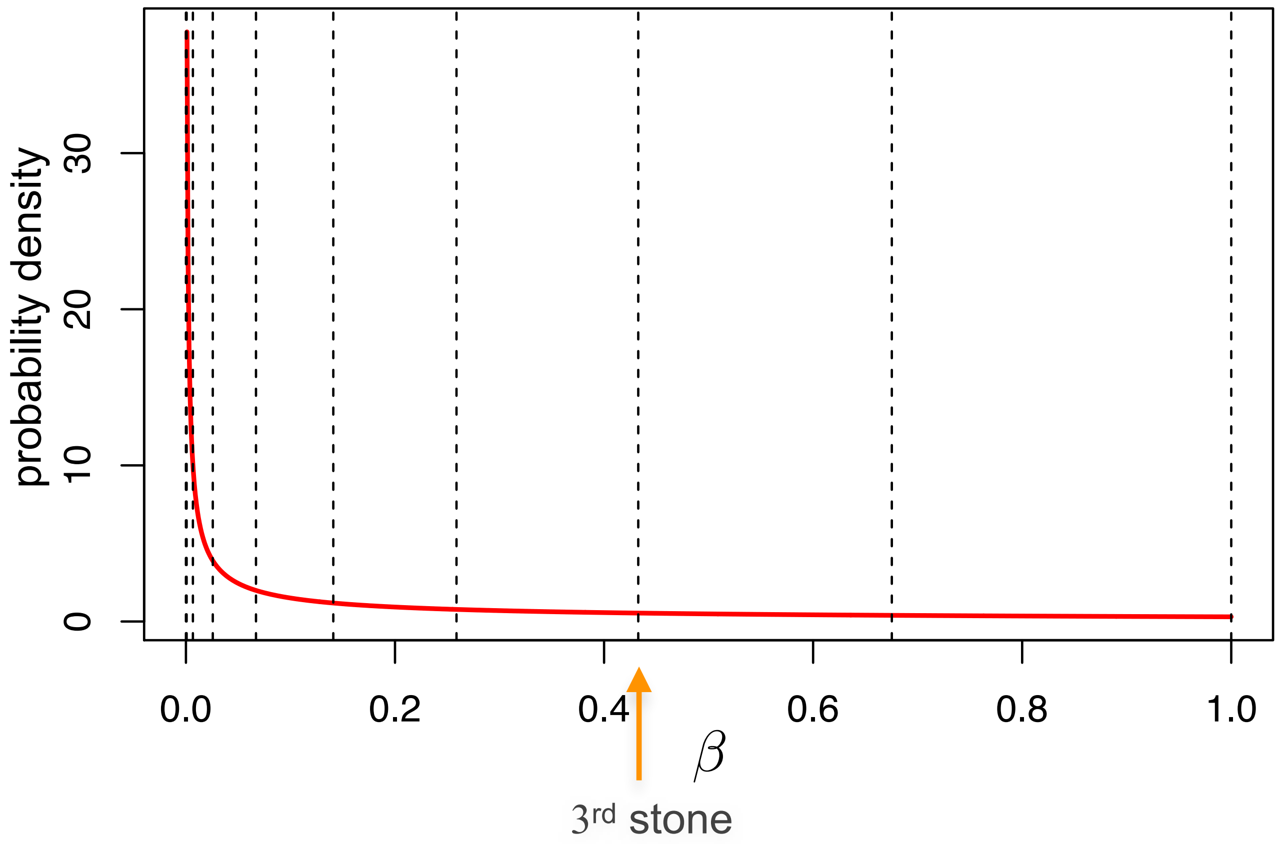

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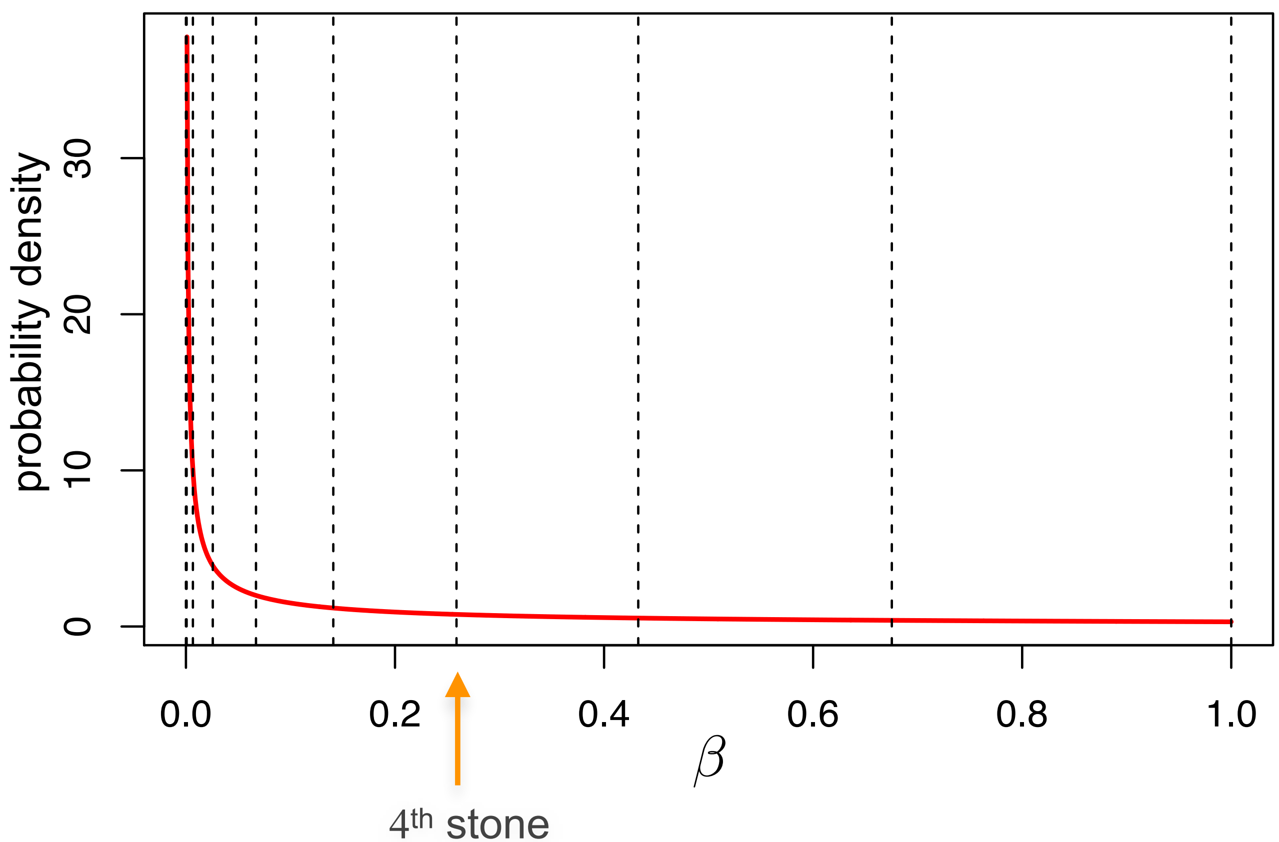

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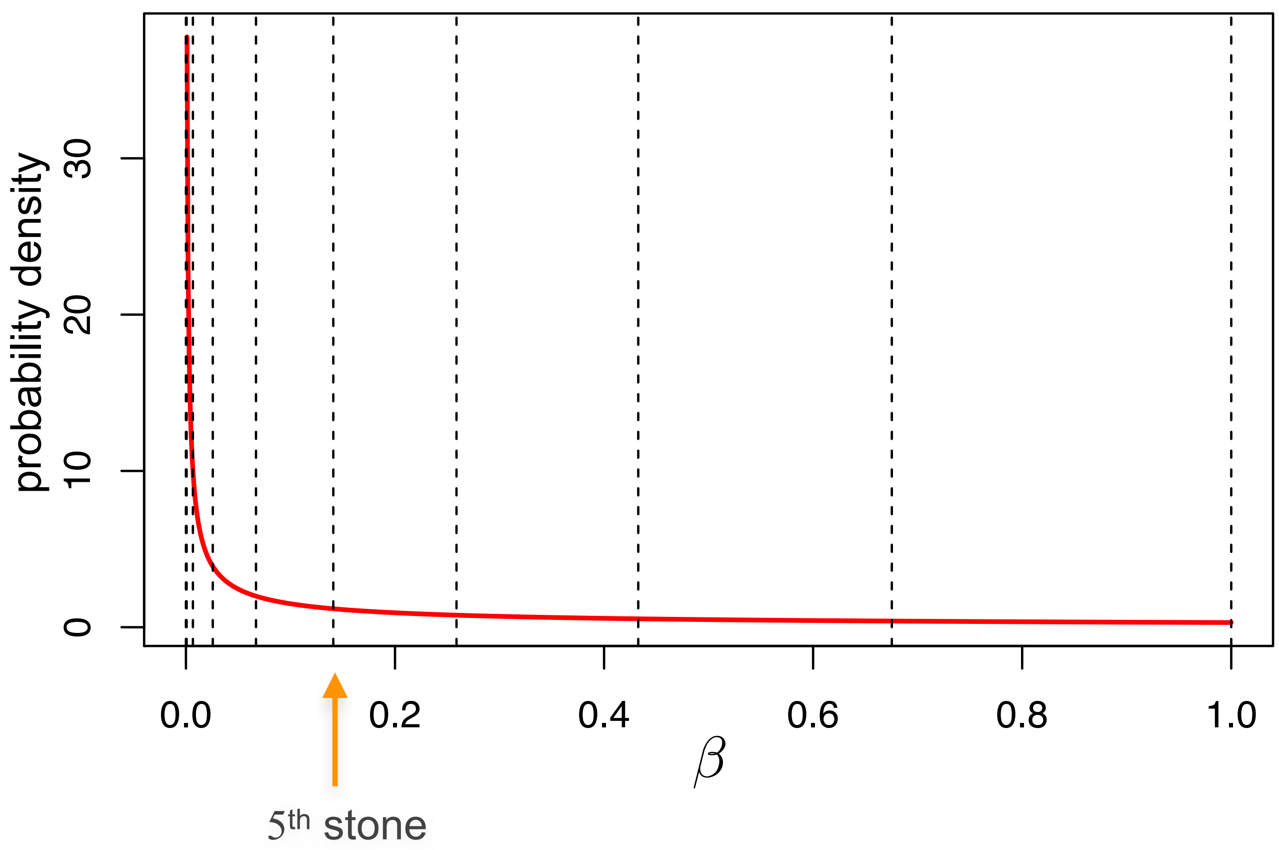

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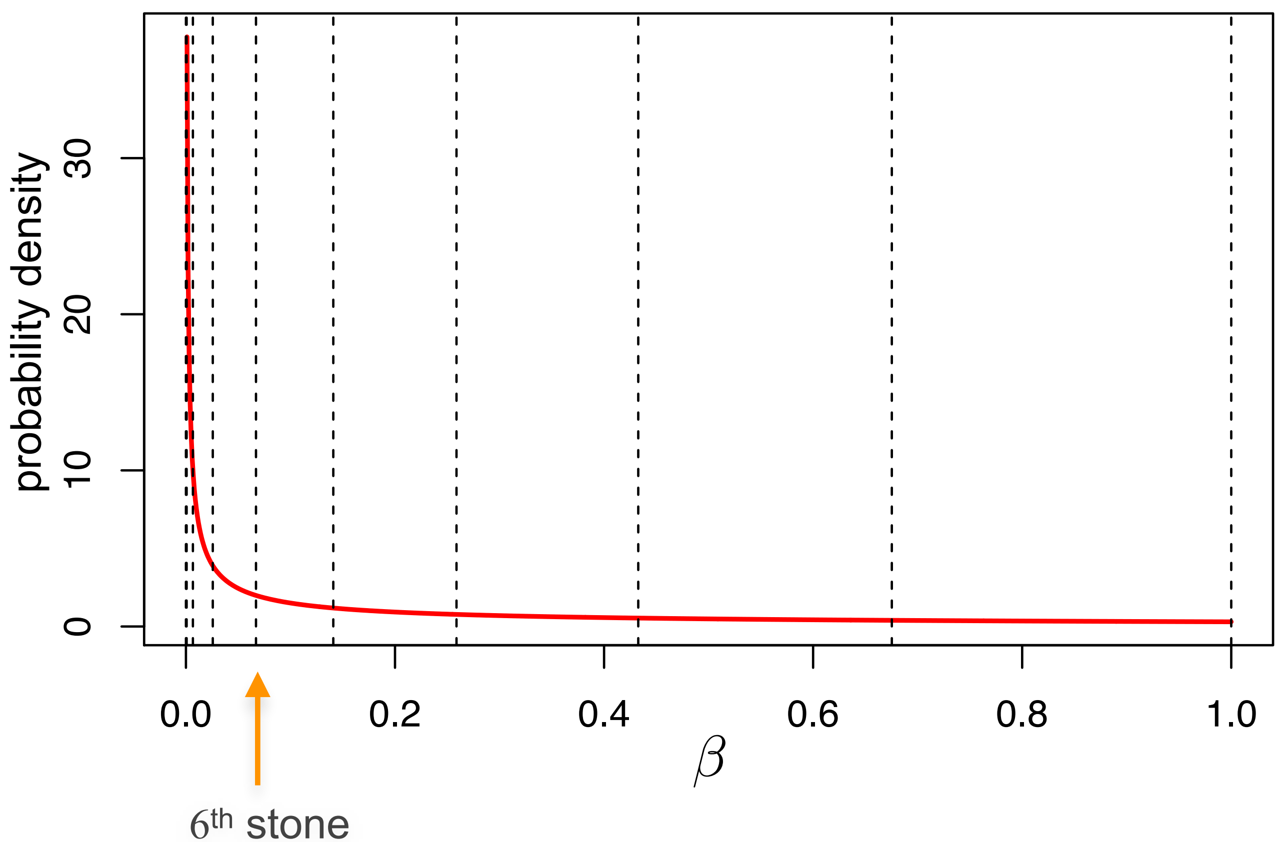

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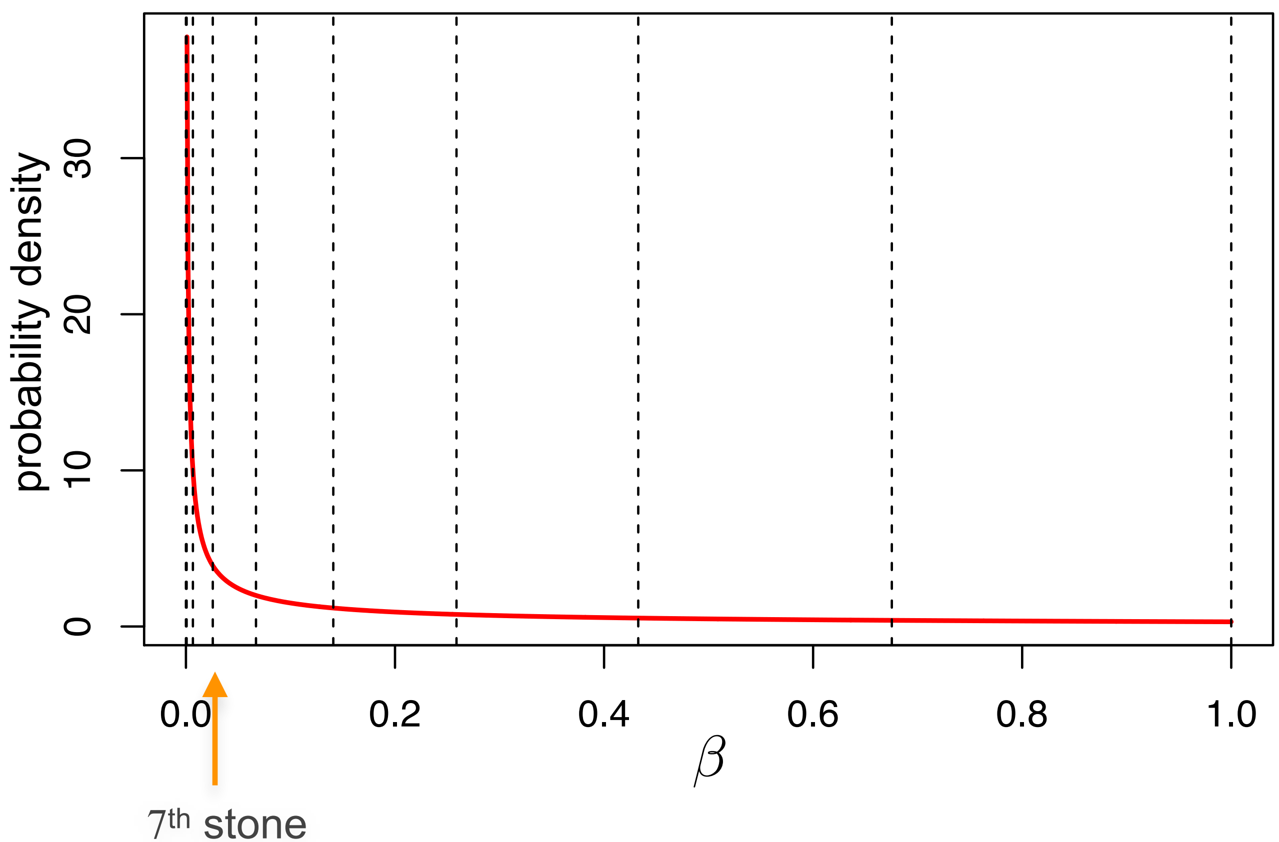

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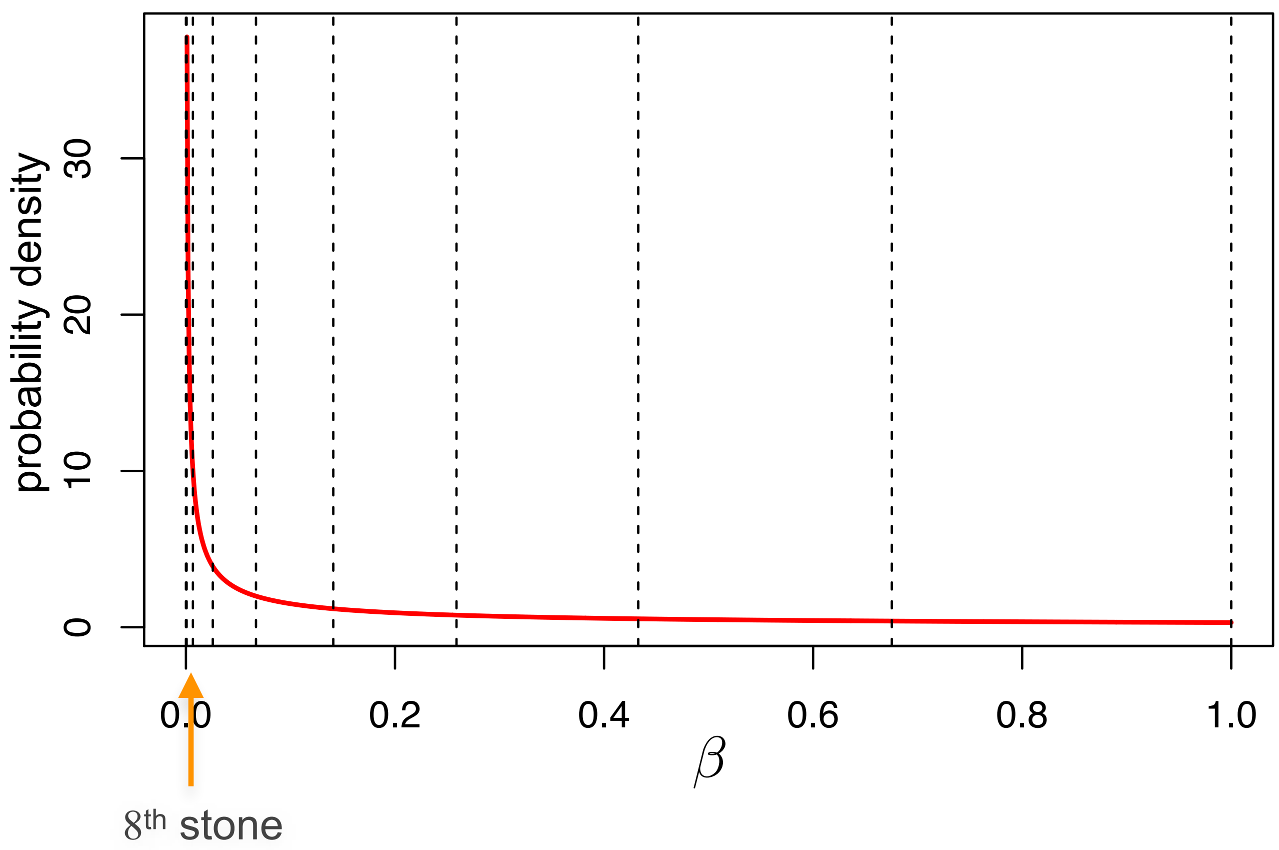

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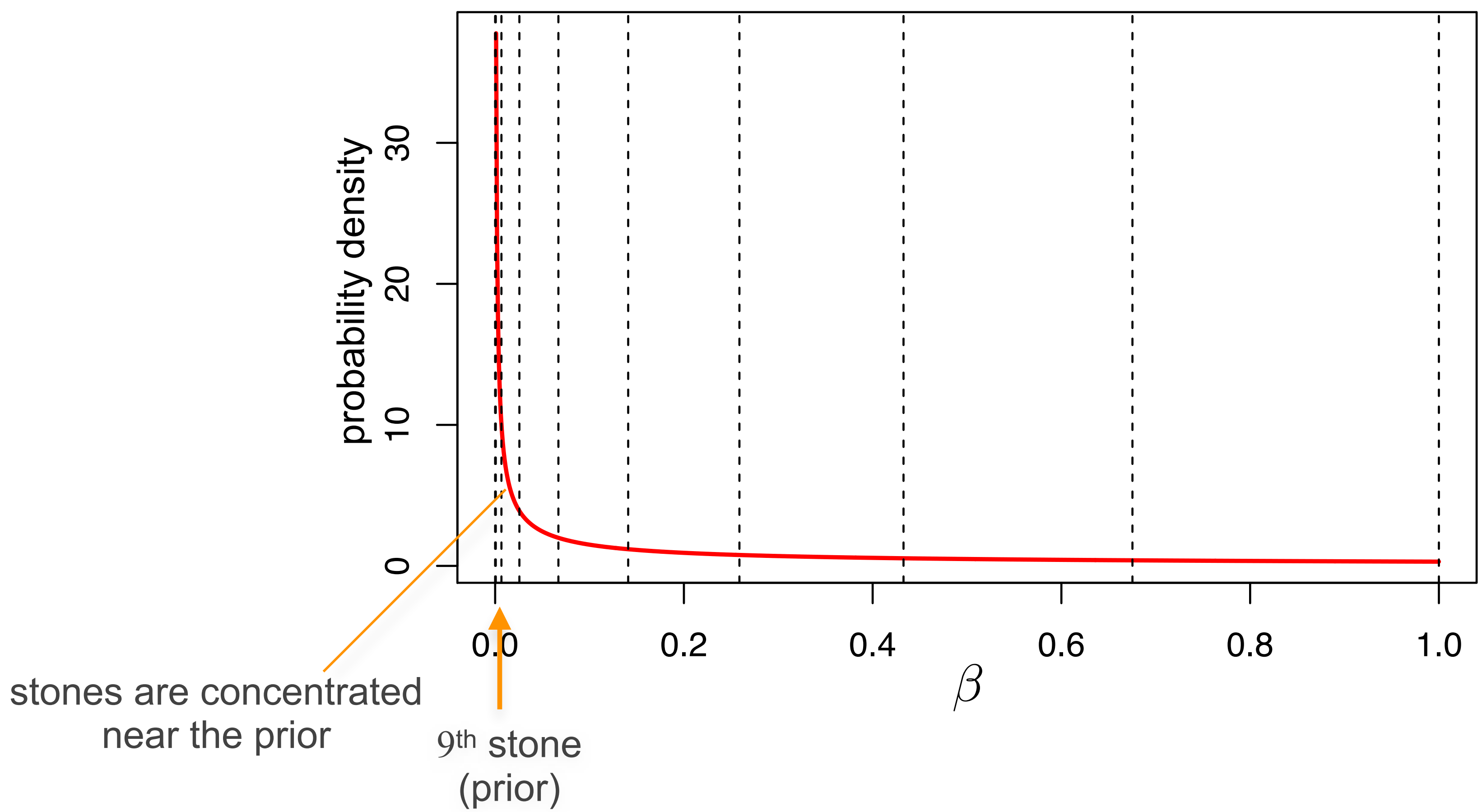

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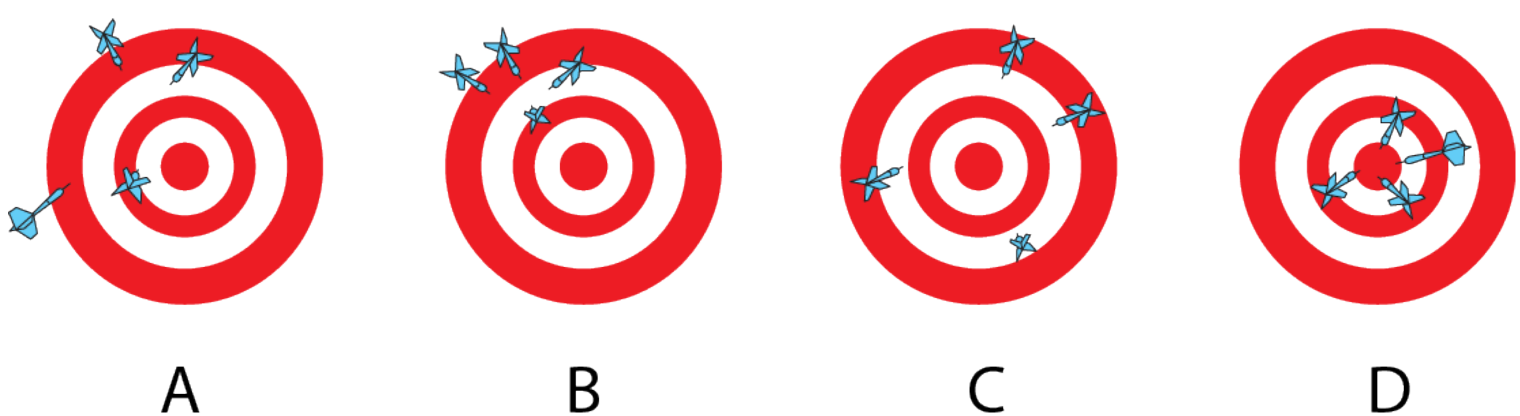

Outline

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What is the <u>relative</u> fit of the candidate models (hypotheses) to our data?

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We therefore need to assess the *absolute* fit of a given model to our data.

To assess adequacy, we adopt the premise that if a given model provides an adequate description of the process that gave rise to our data, then we should be able to use that model to simulate datasets that look like our data.

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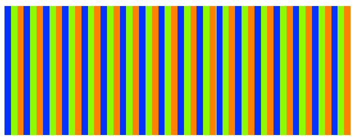
8. Compare T_{obs} to the distribution predicted from the posterior distribution.

Bayesian Evaluation of Model Adequacy

Posterior-predictive simulation

Original data
matrix



compute the summary
statistic for the observed
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Bayesian Evaluation of Model Adequacy

Posterior-predictive simulation

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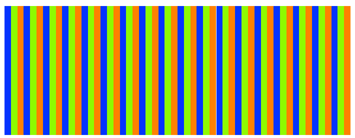
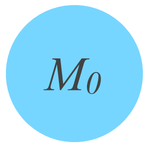


Candidate model



estimate the joint posterior probability distribution using MCMC

Bayesian Evaluation of Model Adequacy

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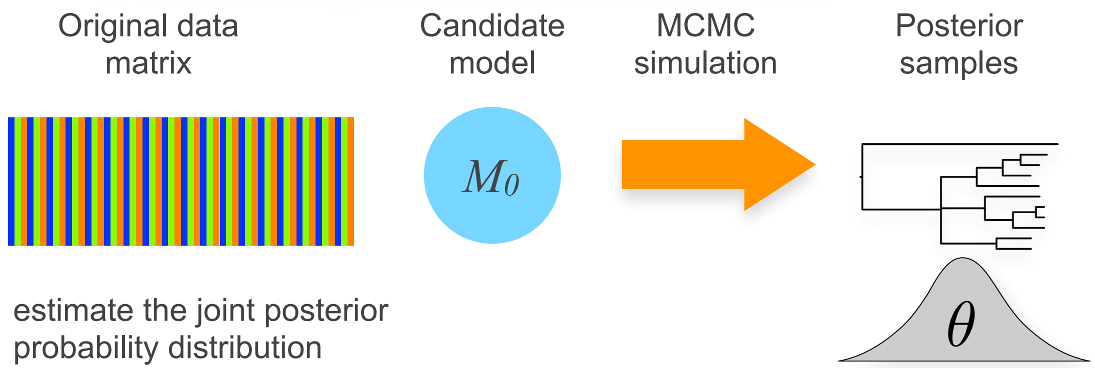

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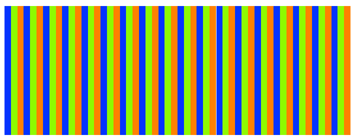

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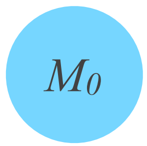
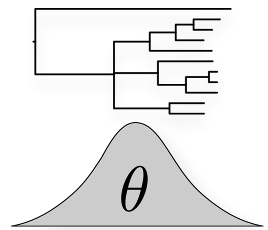


MCMC simulation

Posterior samples



Simulate

sample a marginal vector
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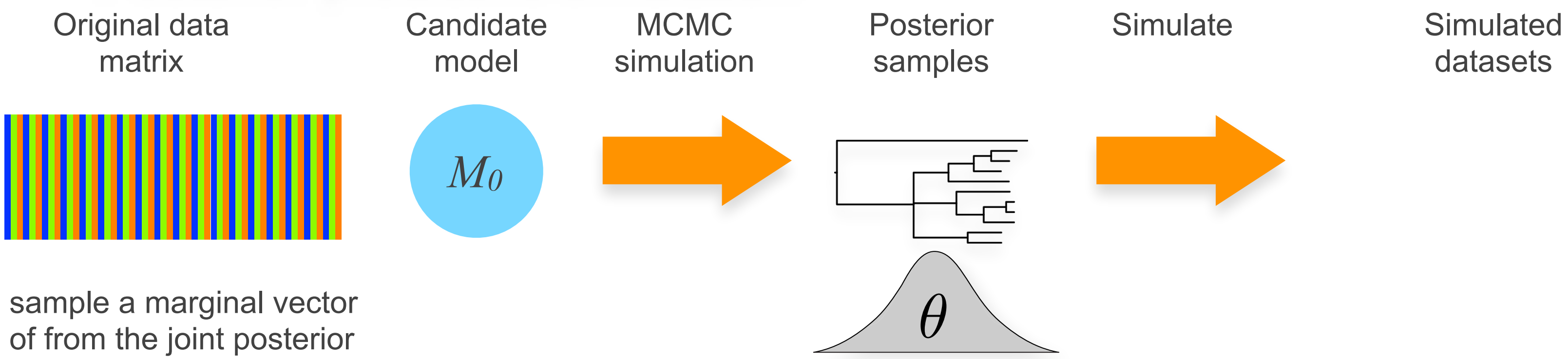
Bayesian Evaluation of Model Adequacy

Posterior-predictive simulation



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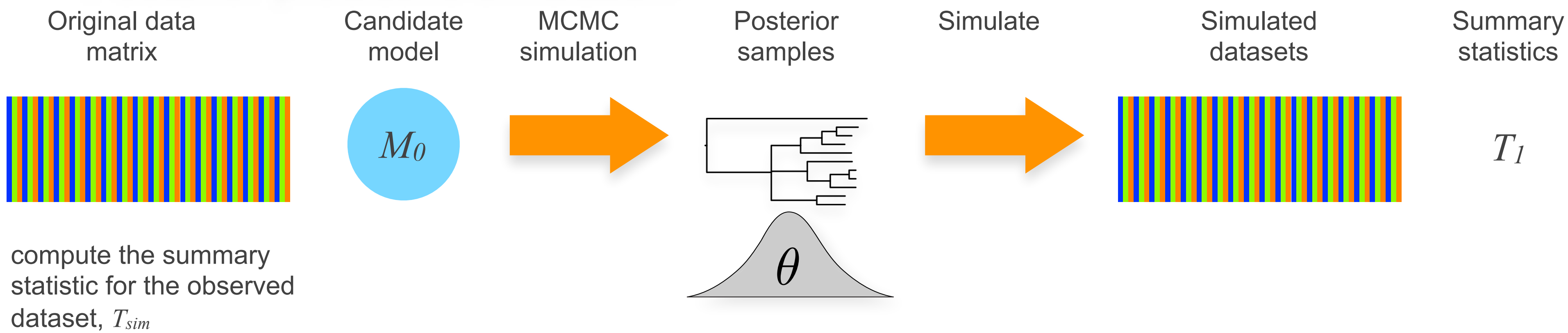

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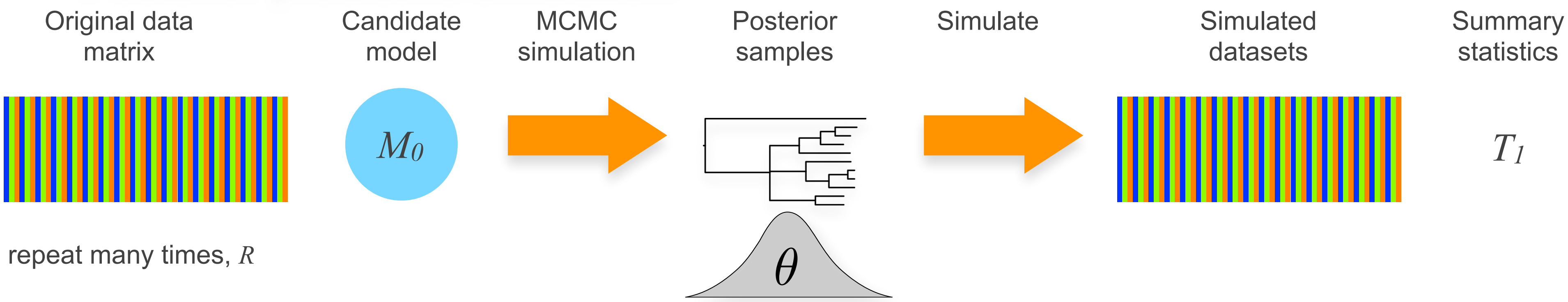

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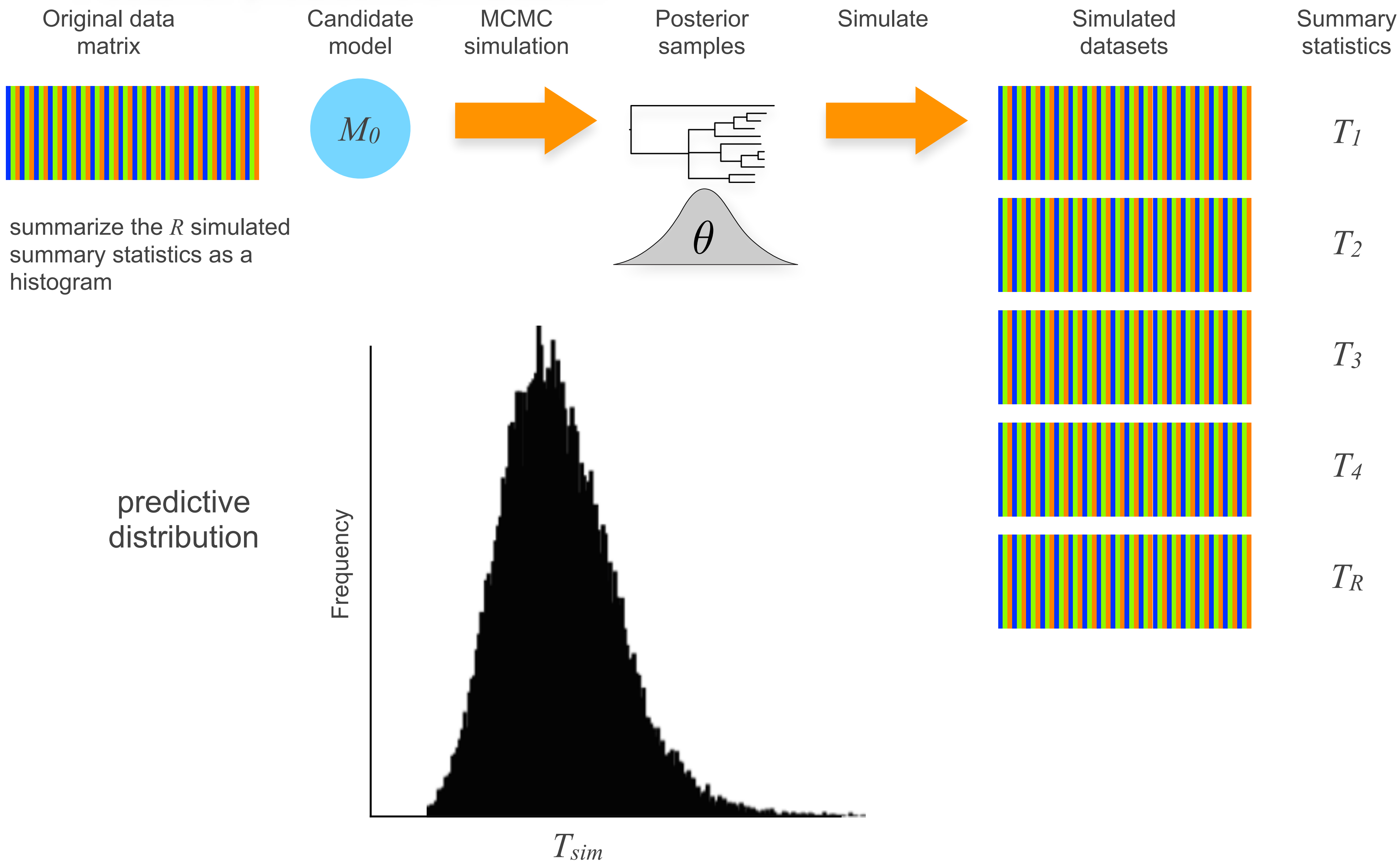

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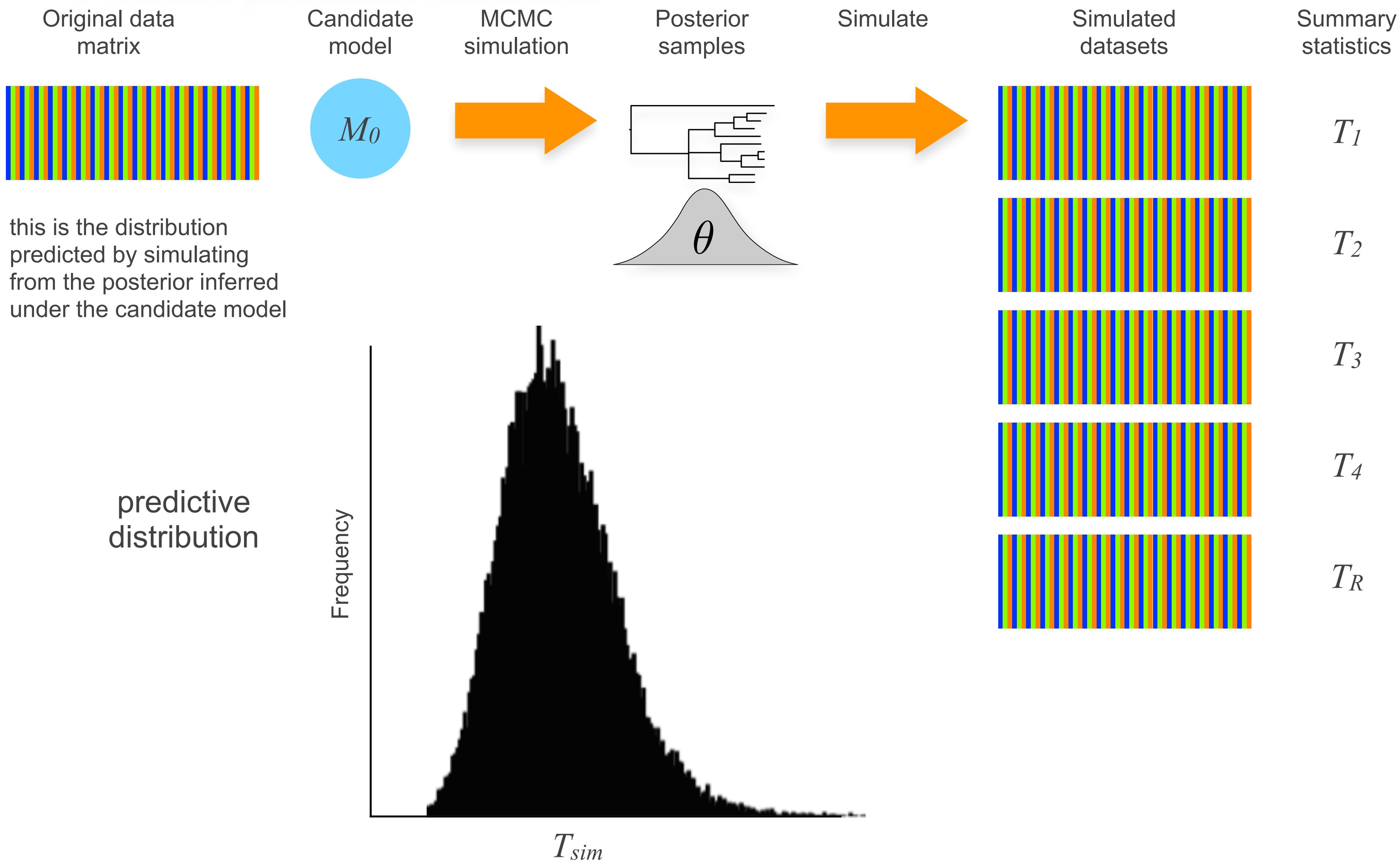

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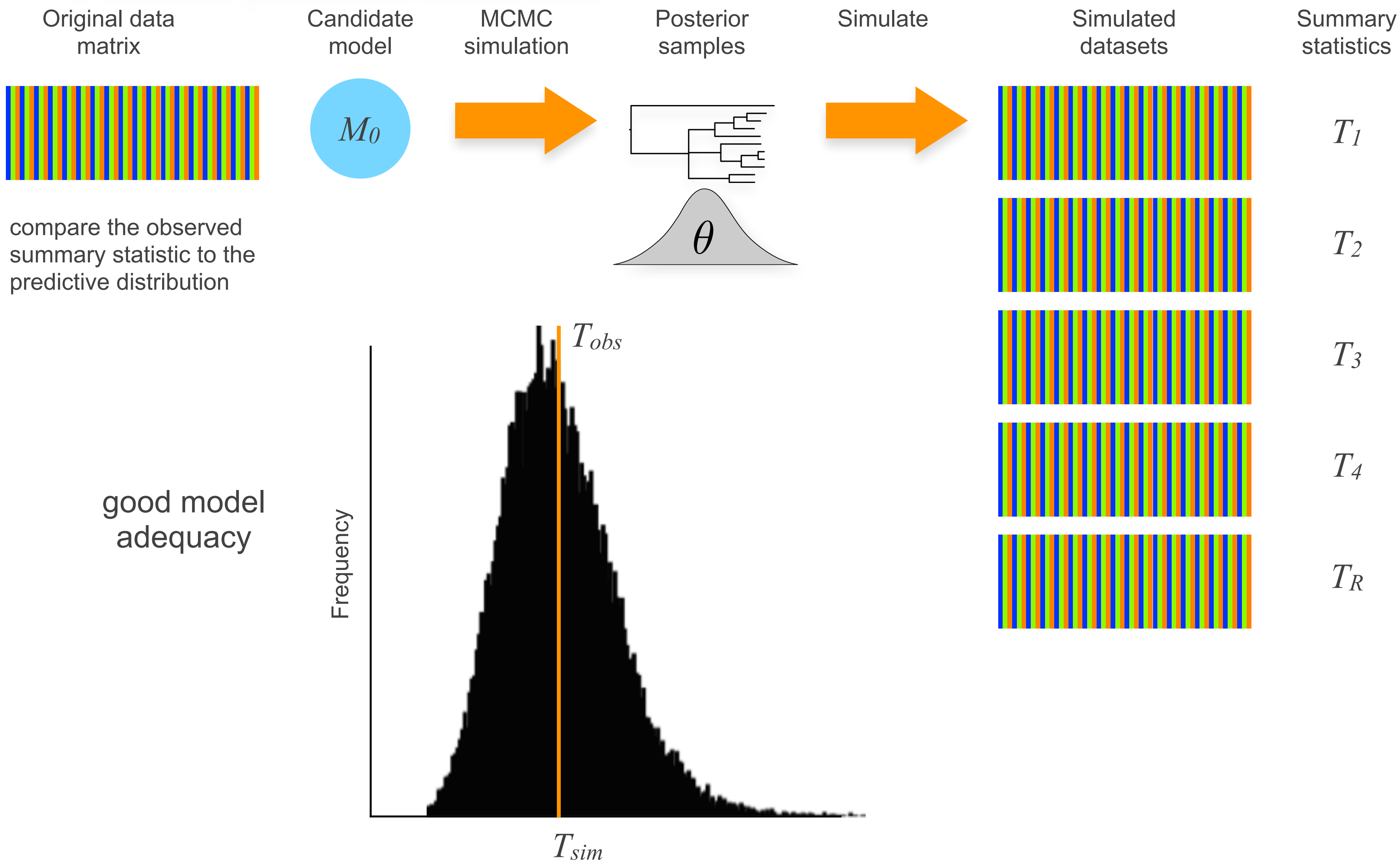

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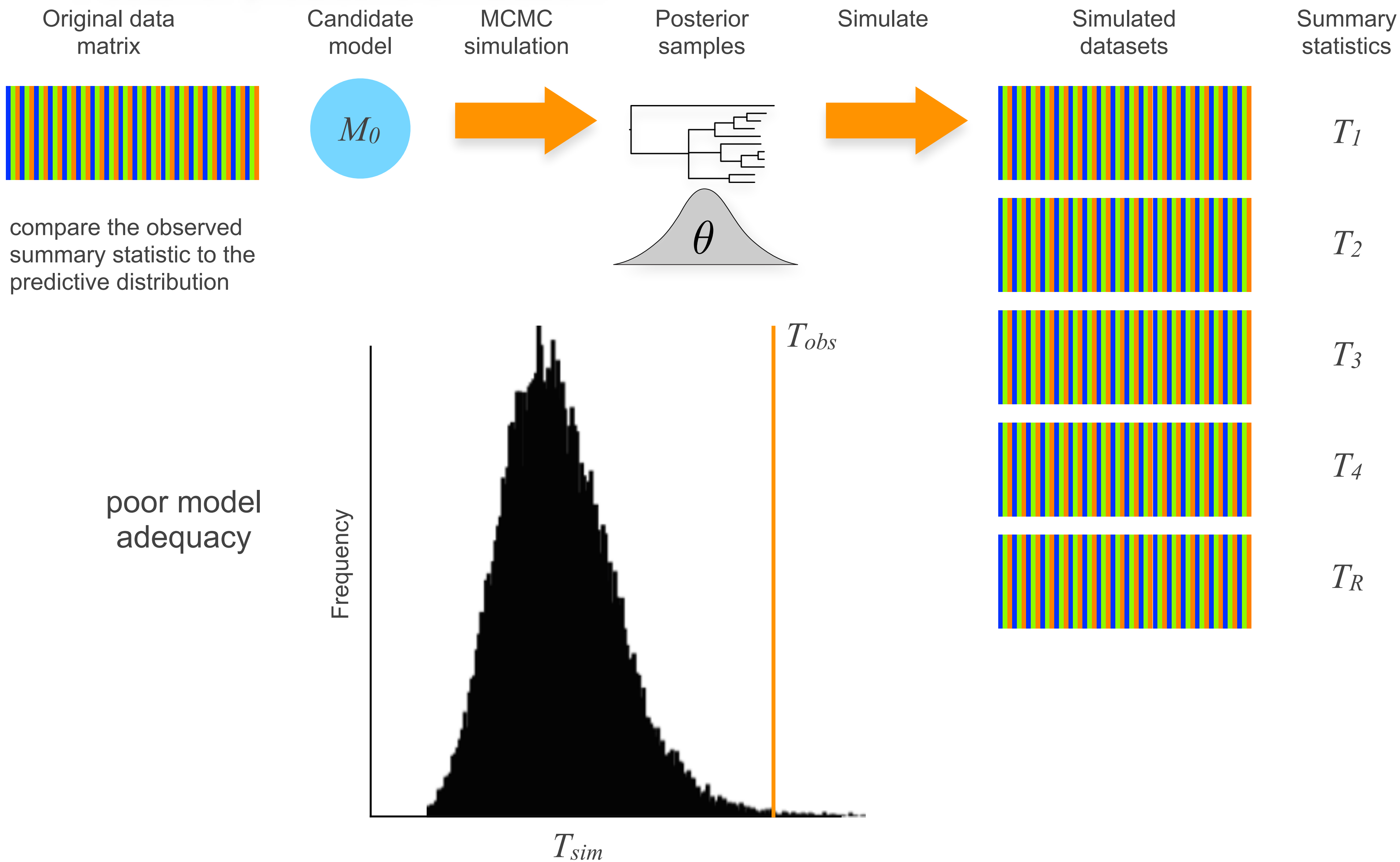

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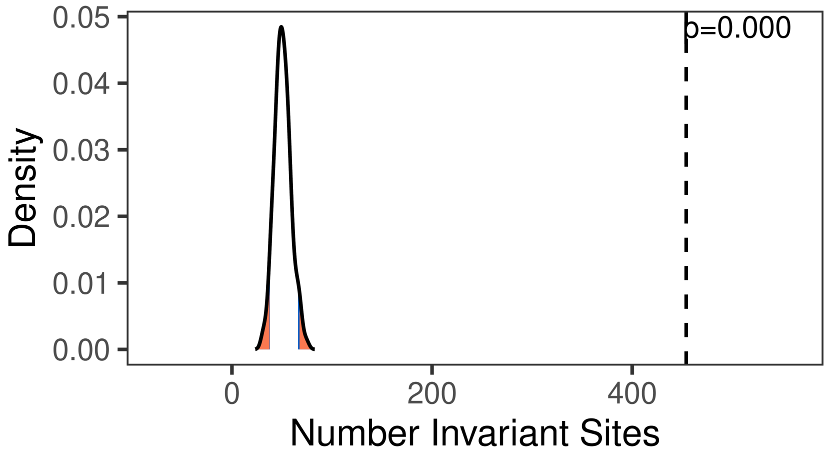

Höhna *et al.* (2018)

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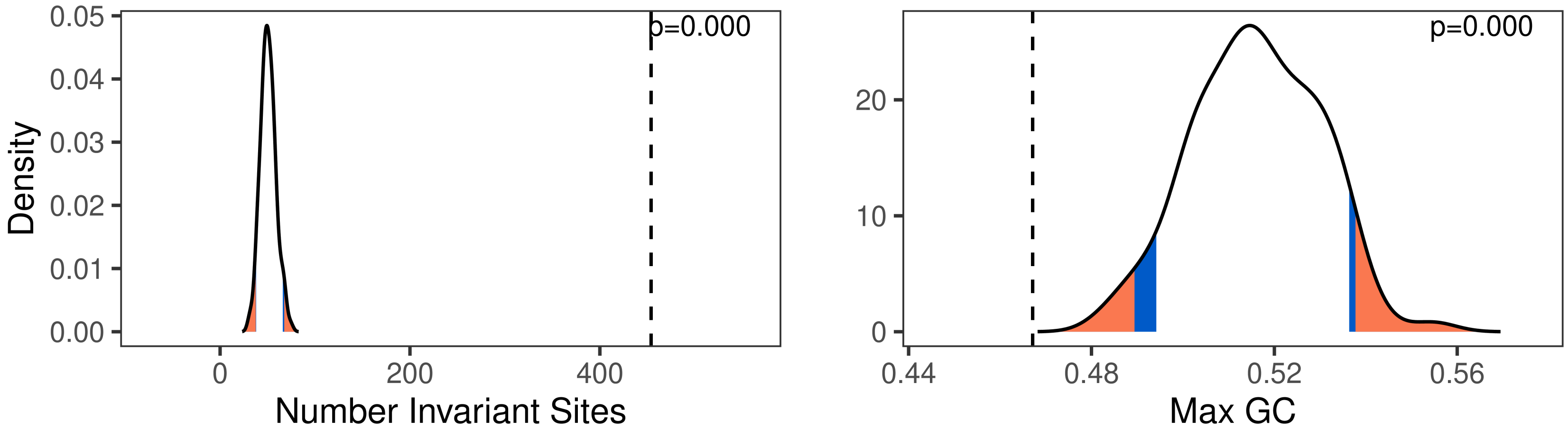

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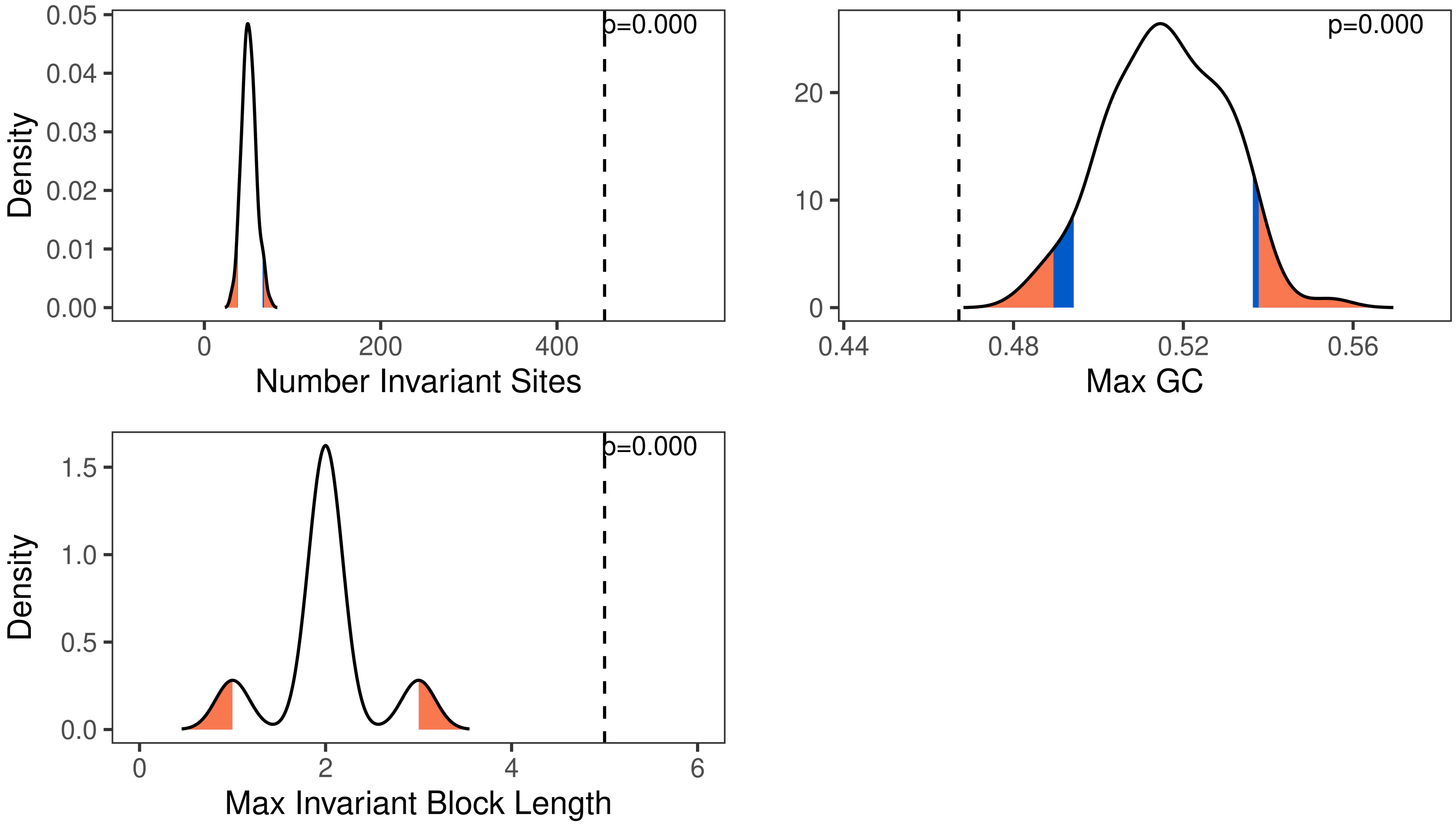

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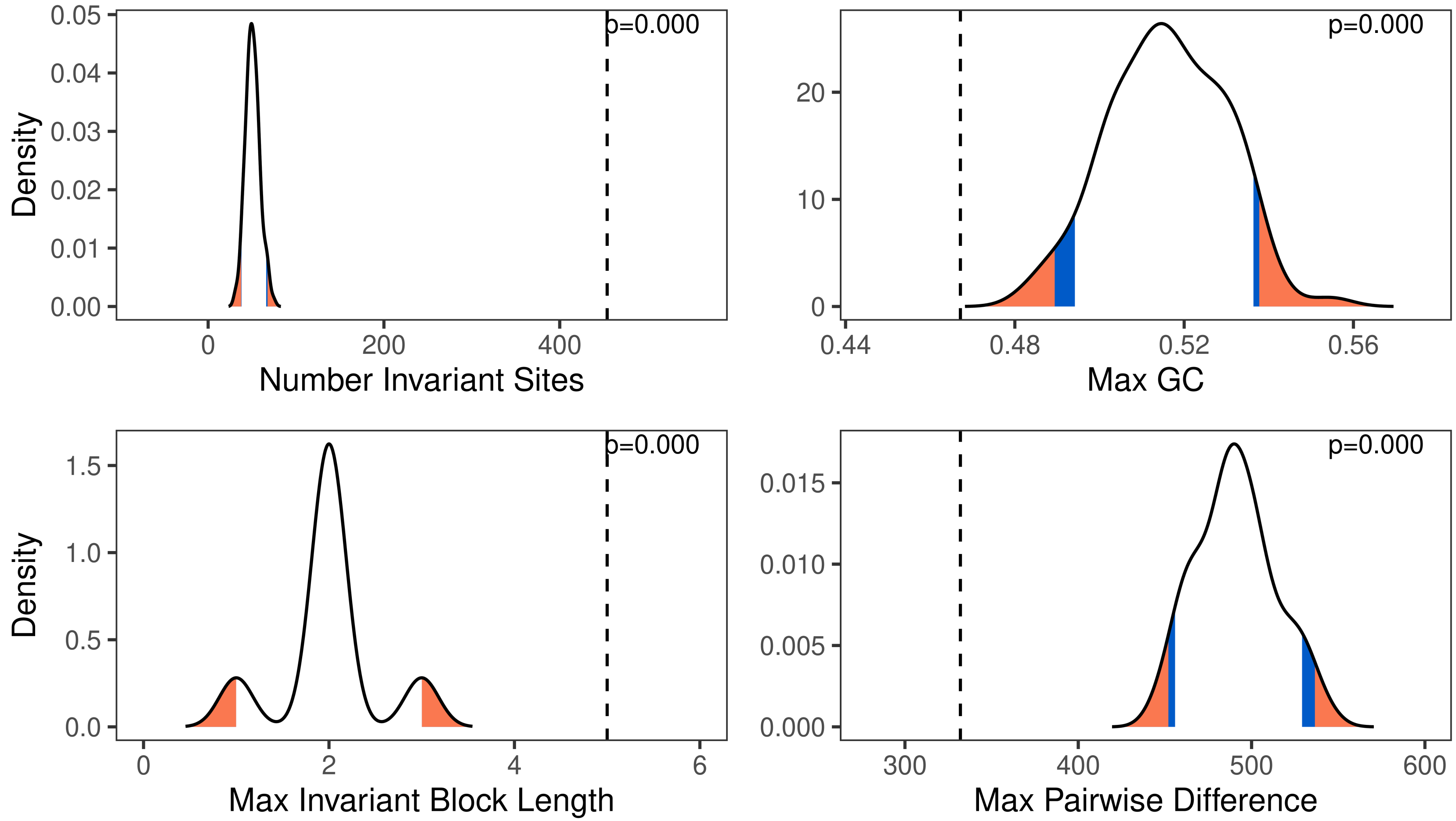

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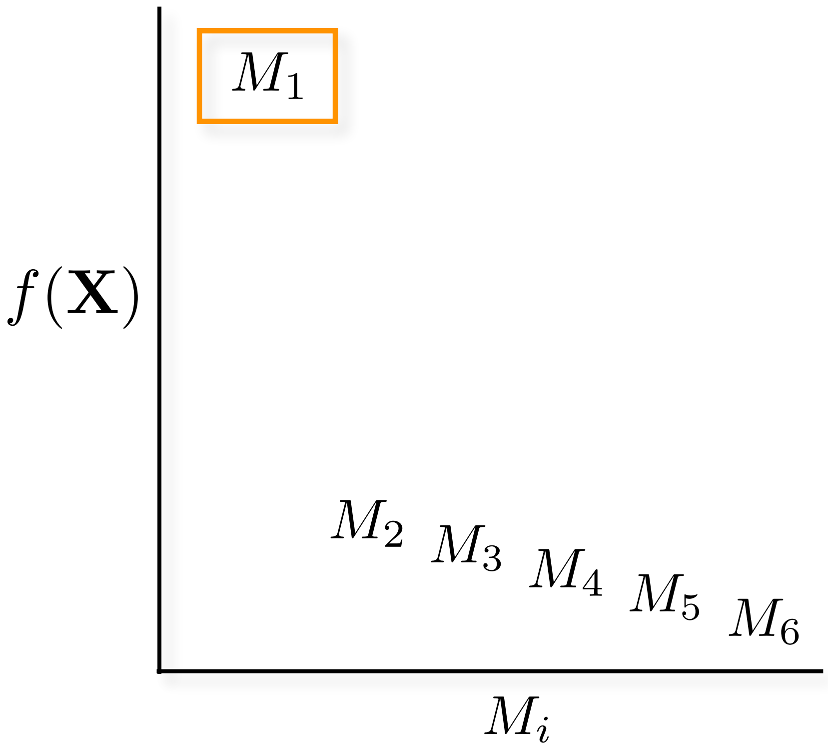

If the fit of the data to the selected mixed model is vastly better than other candidate models, conditioning on the best model may be justified.

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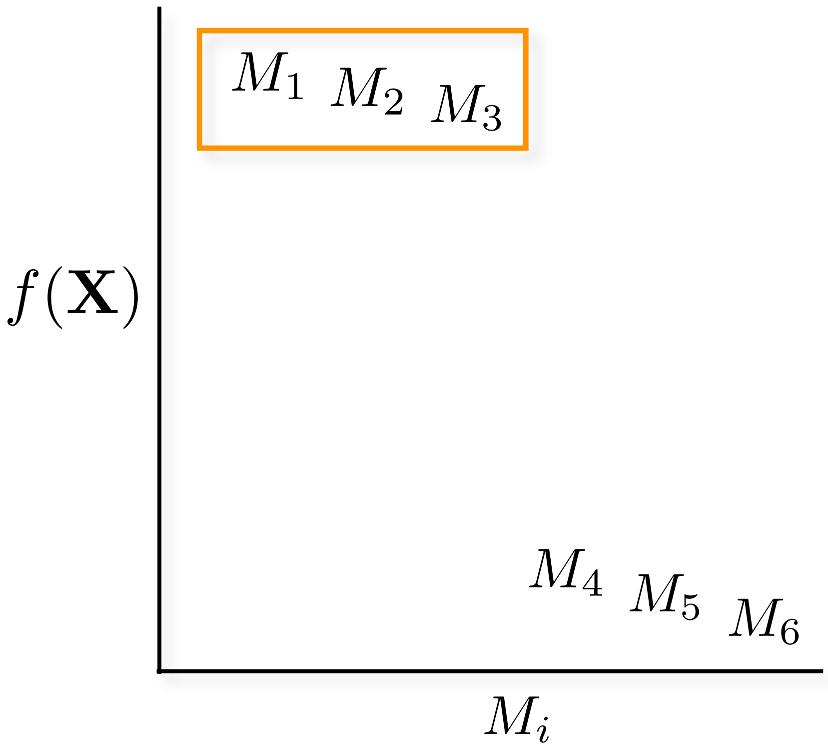

Conversely, if the fit of the data to the selected model is only marginally better than other candidate models, it would be unwise to condition on the best model.

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Bayesian model averaging: reversible-jump MCMC (rjMCMC)

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likelihood ratio   prior ratio   proposal ratio

The parameter estimates are averaged over all possible models

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- the models may differ in dimensionality, which must be accommodated:

$$R = \min\left[1, \boxed{\frac{f(\mathbf{X}|\theta')}{f(\mathbf{X}|\theta)}} \cdot \boxed{\frac{f(\theta')}{f(\theta)}} \cdot \boxed{\frac{f(\theta|\theta')}{f(\theta'|\theta)}}\right]$$

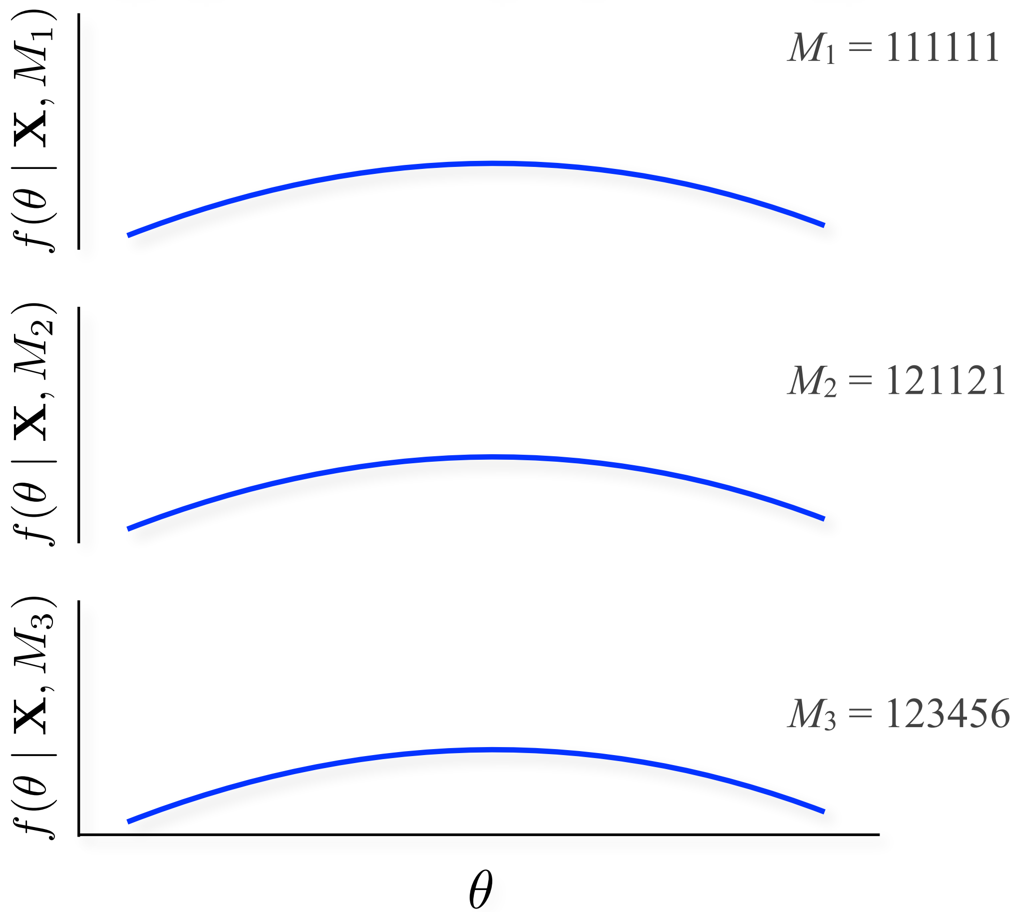
likelihood ratio prior ratio proposal ratio

The parameter estimates are averaged over all possible models

The proportion of time spent on each model is an estimate of its posterior probability

Bayesian Model Selection

Bayesian model averaging: reversible-jump MCMC (rjMCMC)



We infer the joint posterior probability distribution by averaging over a set of models, M_i.

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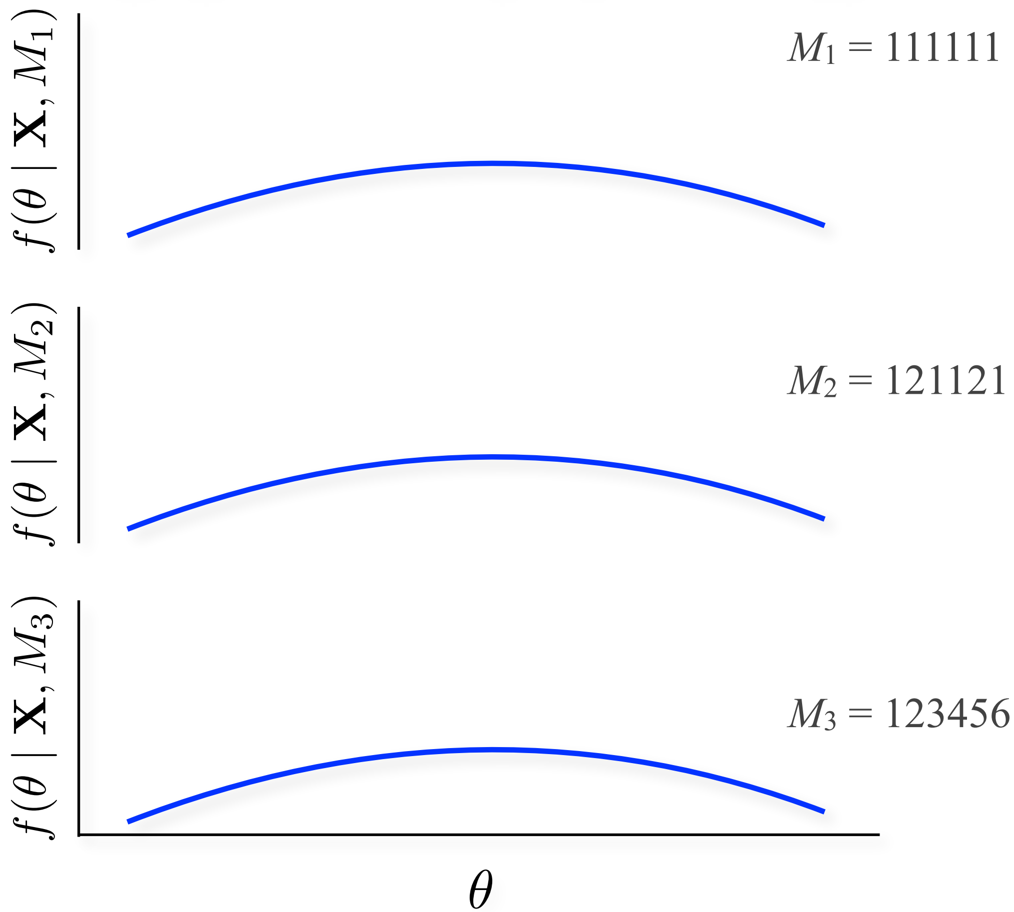

Like other variables, we specify the prior probability distribution for the models.

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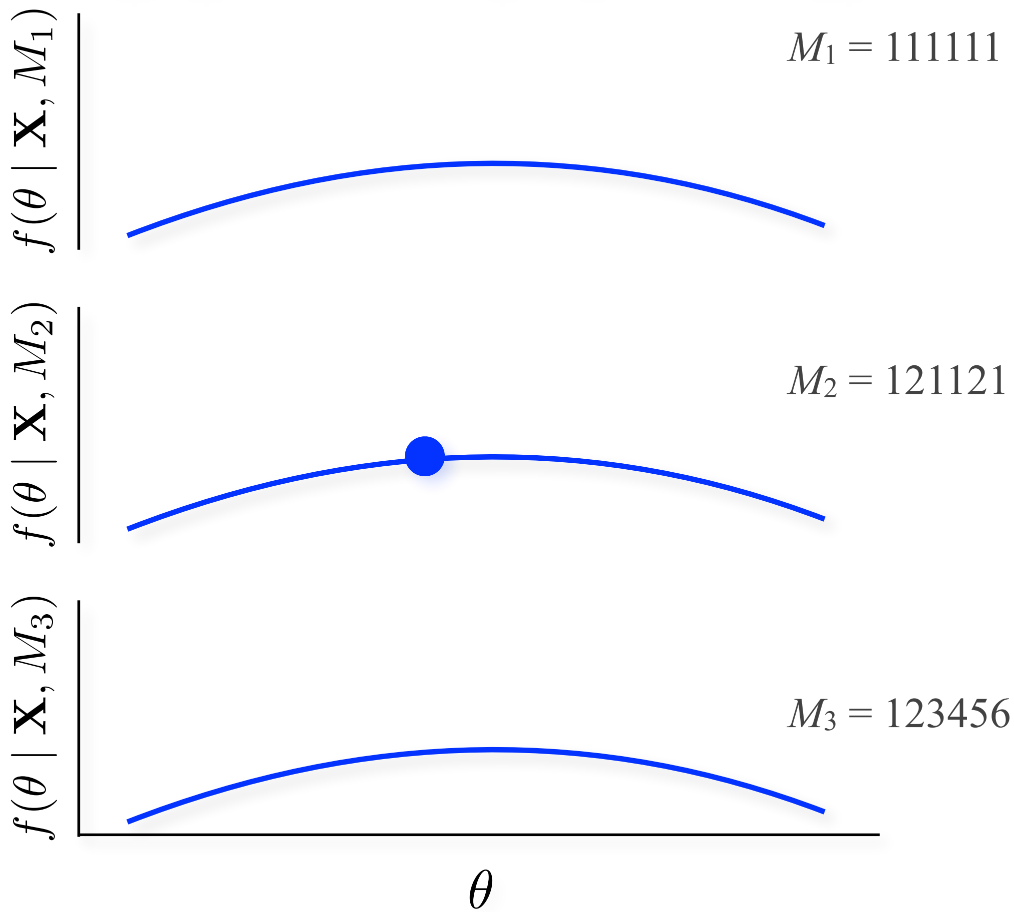

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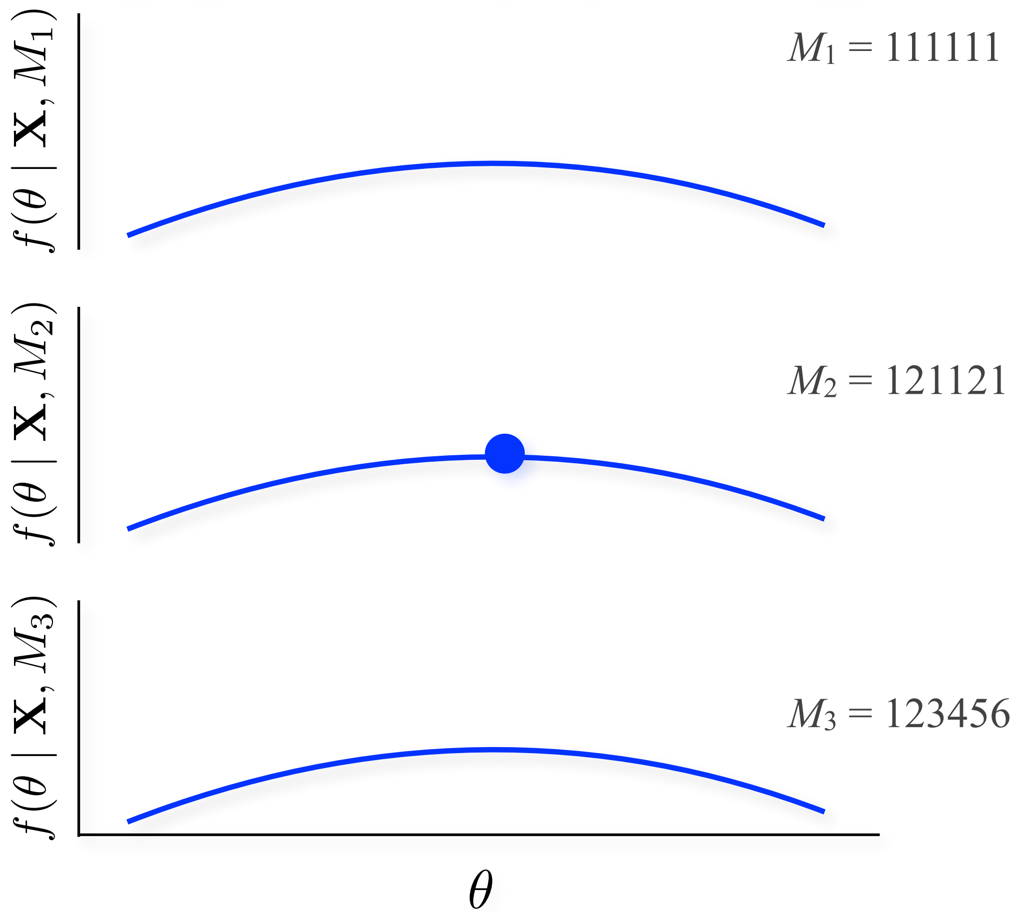

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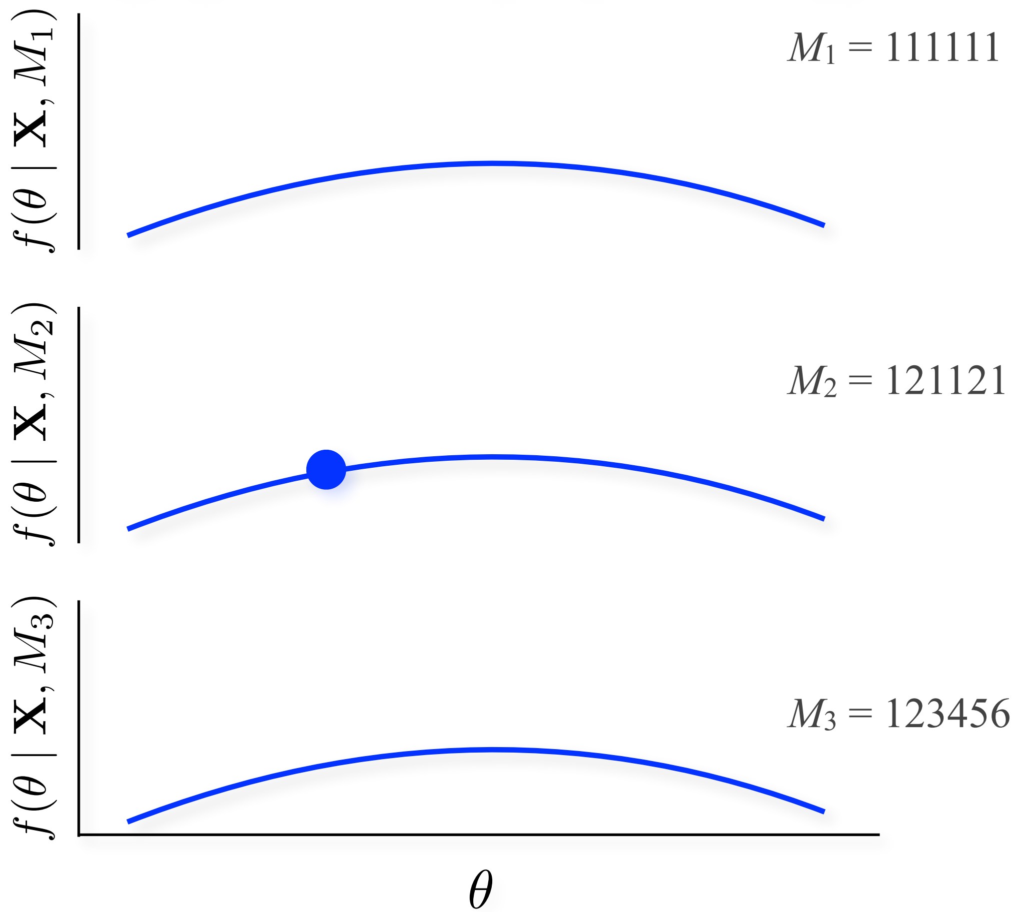

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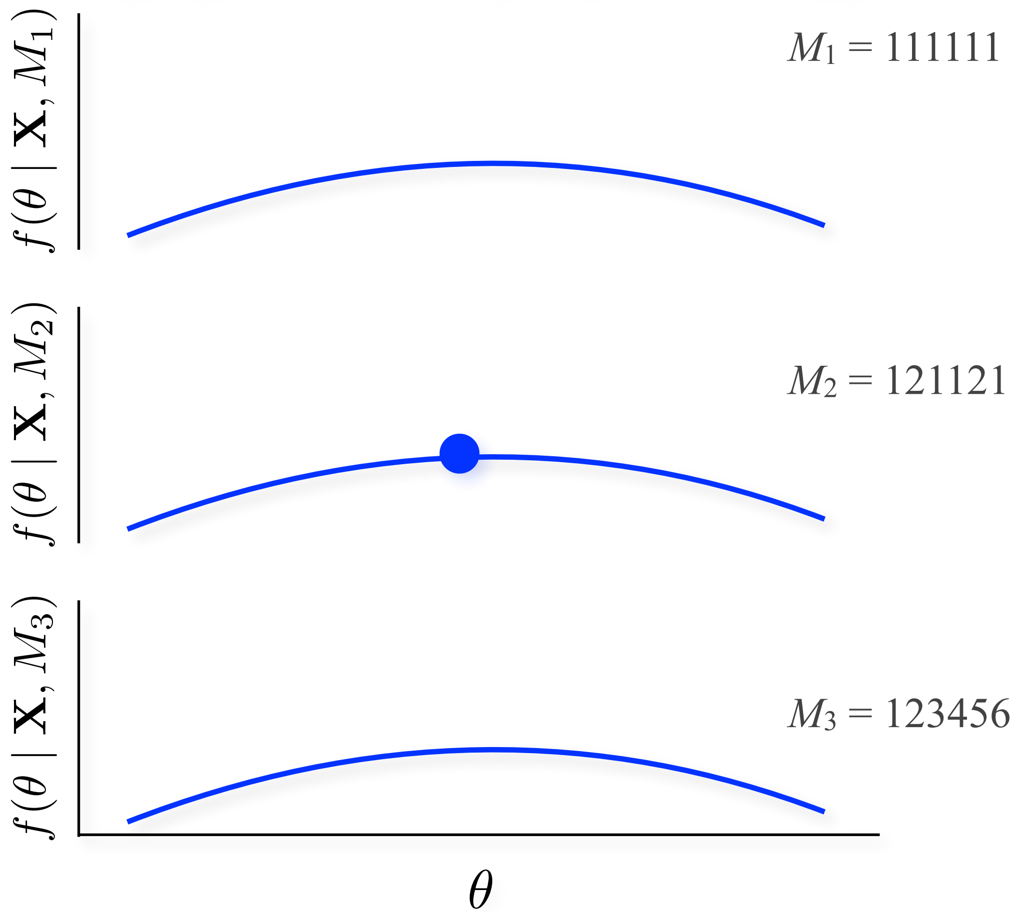

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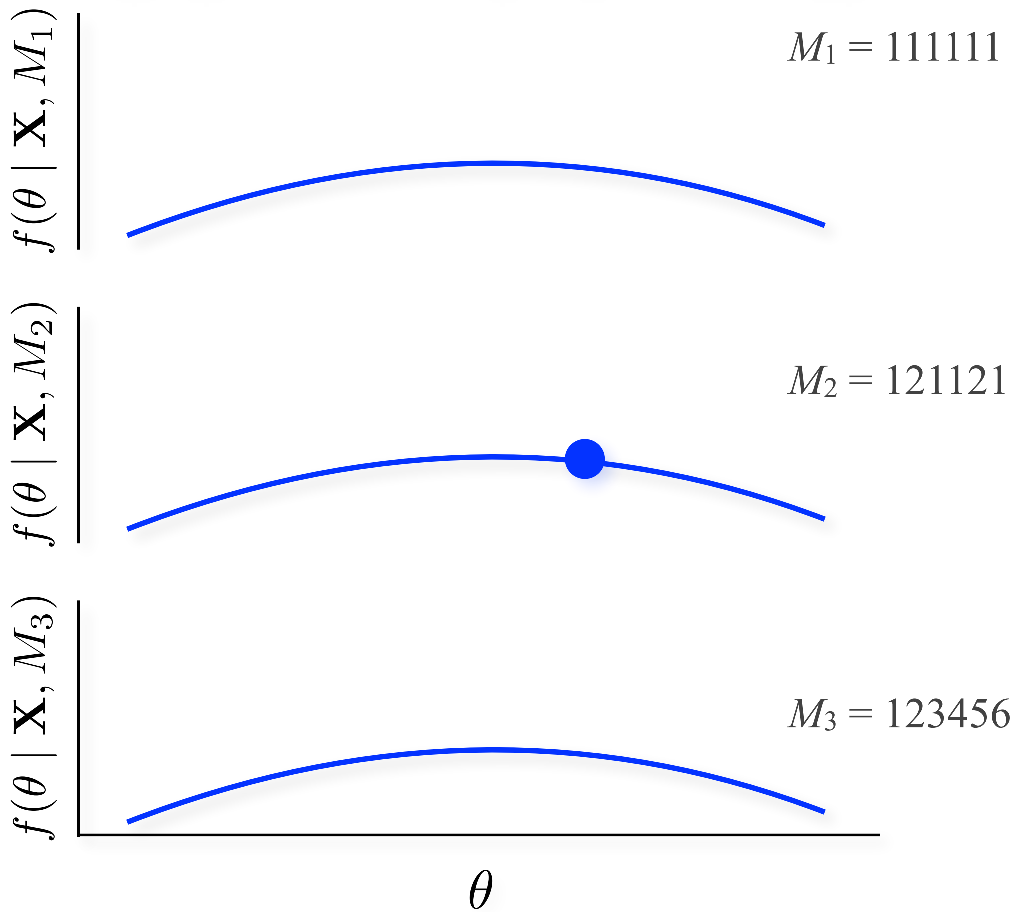

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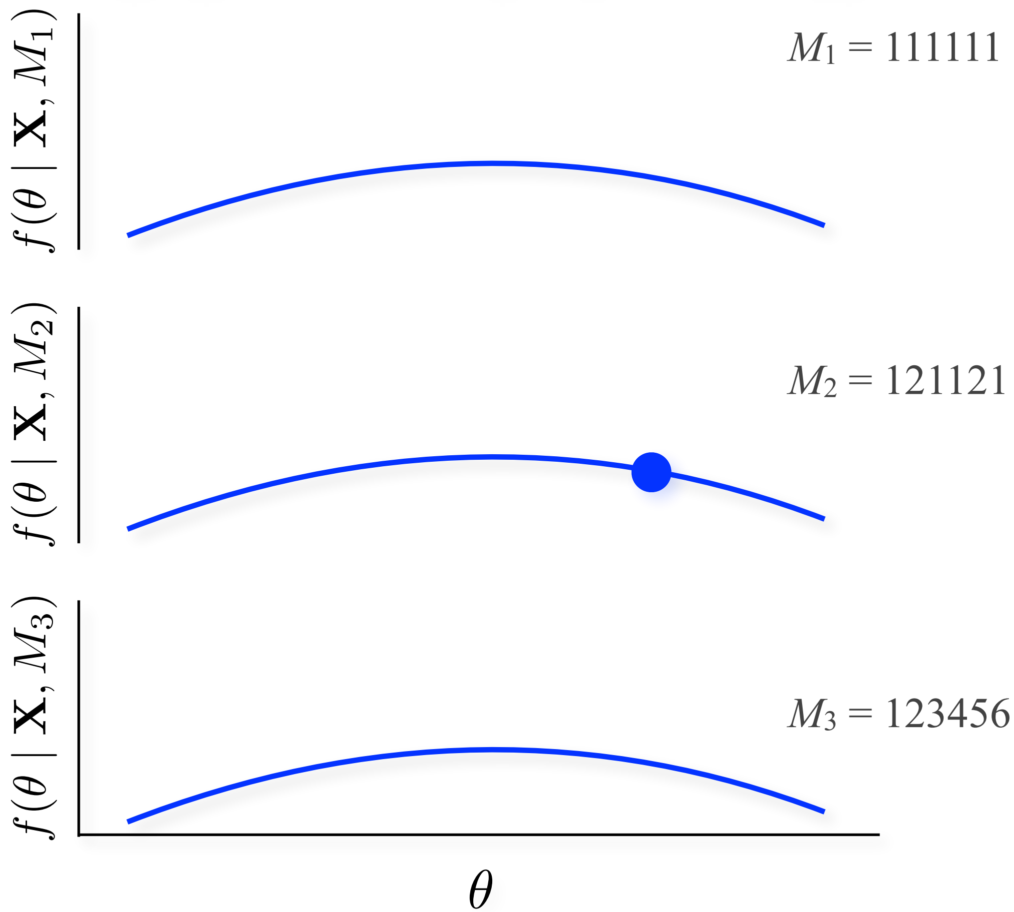

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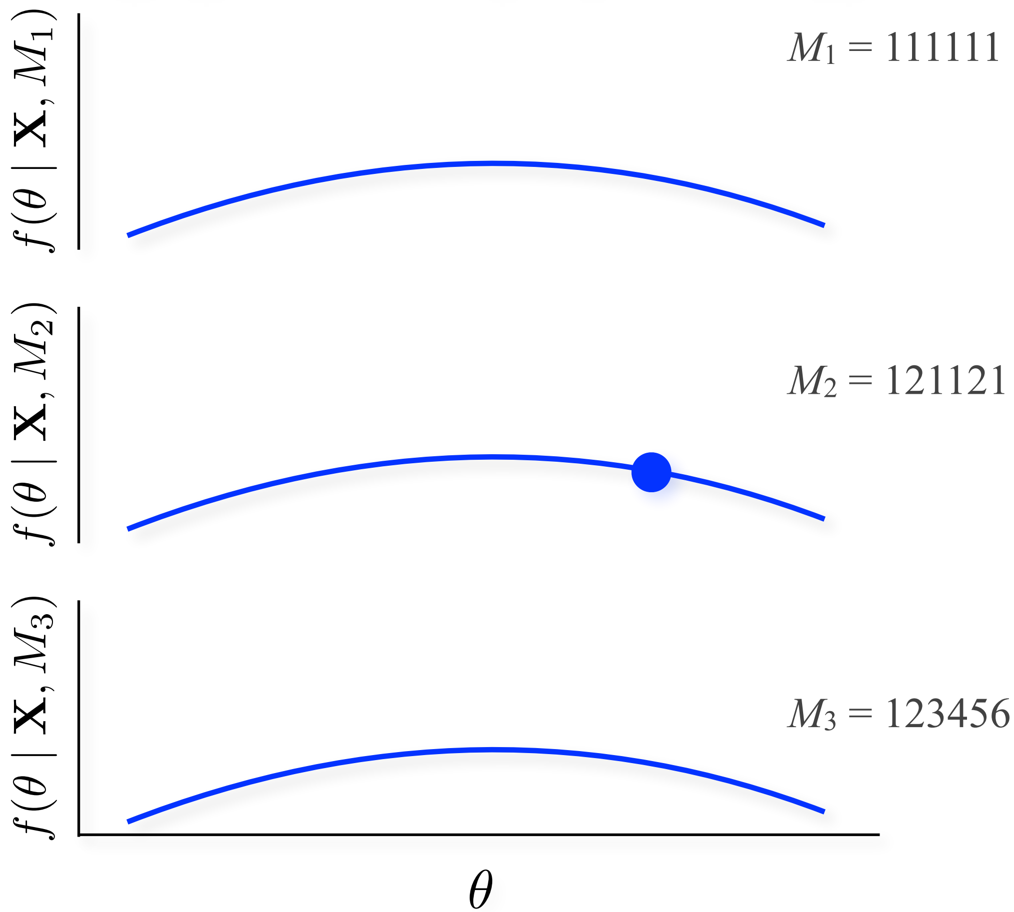

Occasionally, we propose a move to a new model

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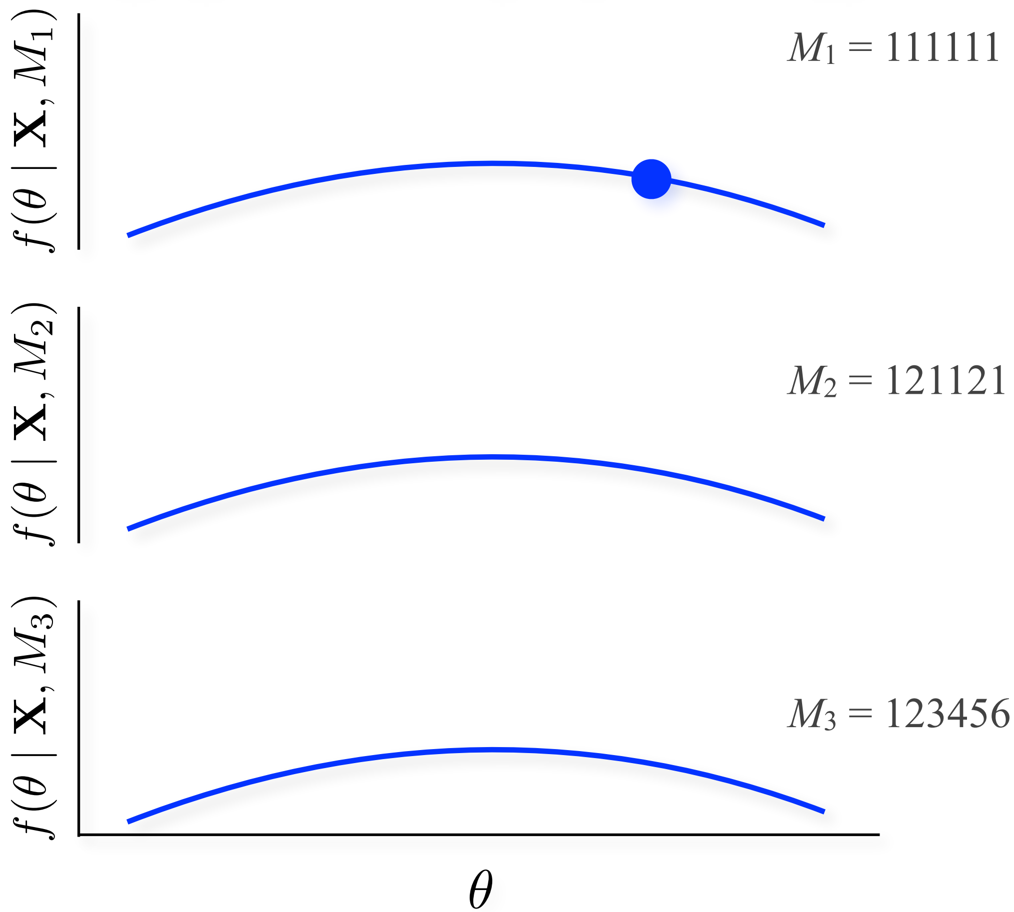

Occasionally, we propose a move to a new model, and accept/reject in the usual way.

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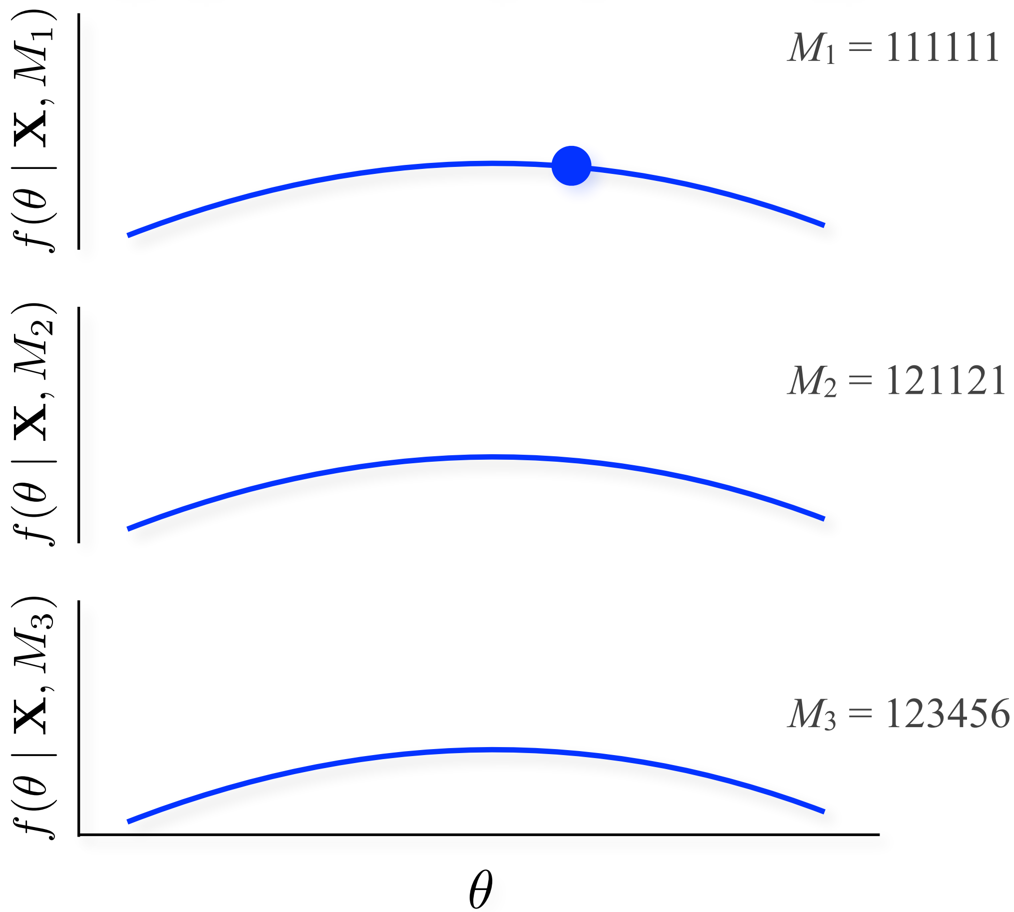

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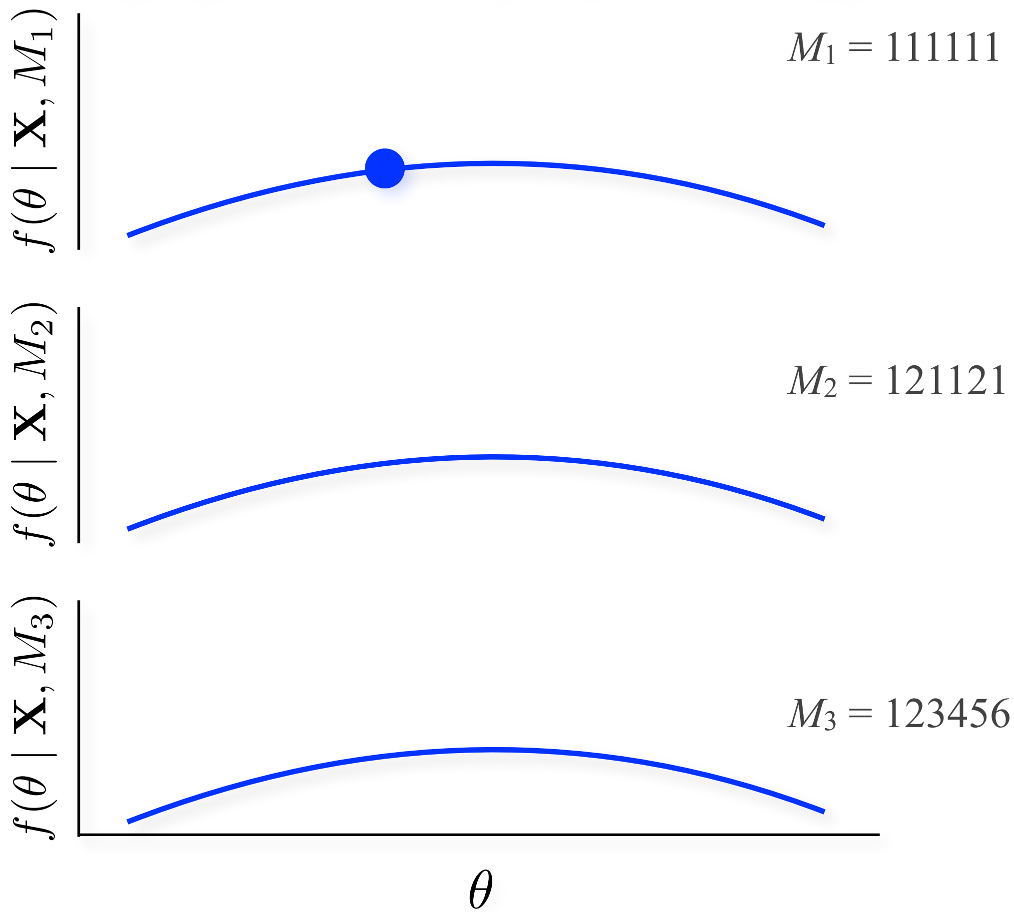

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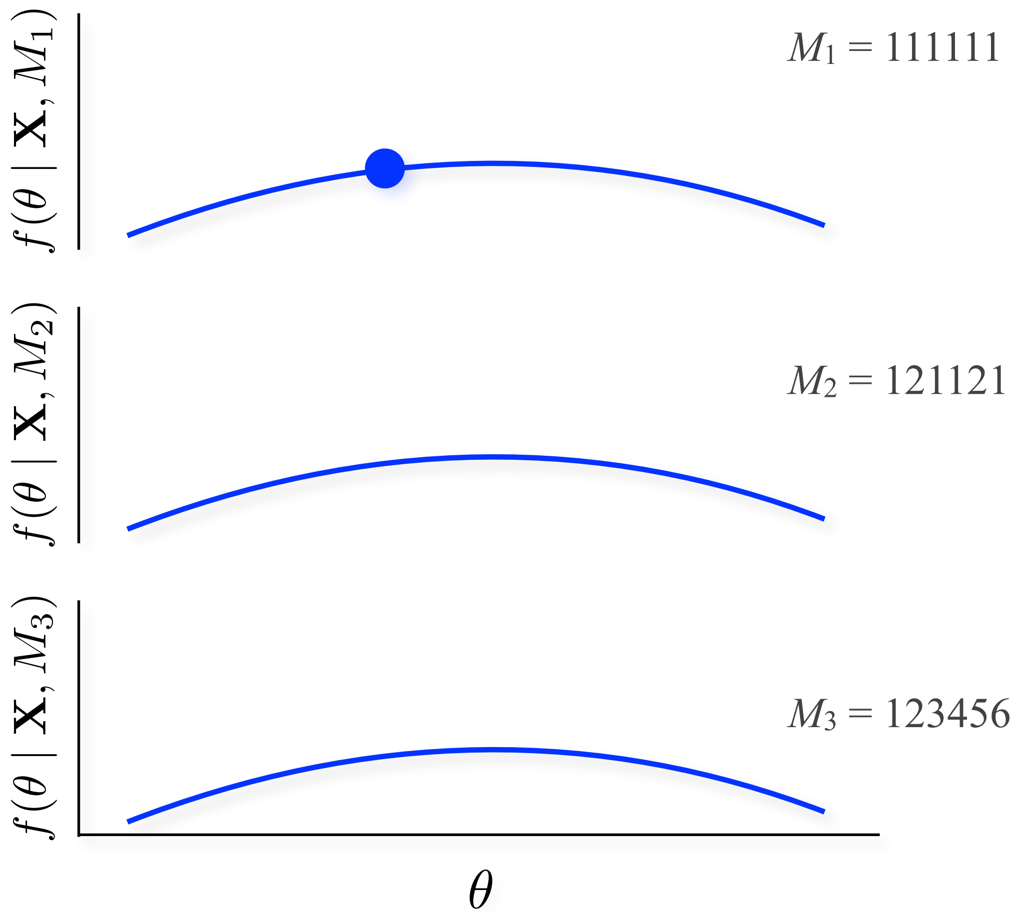
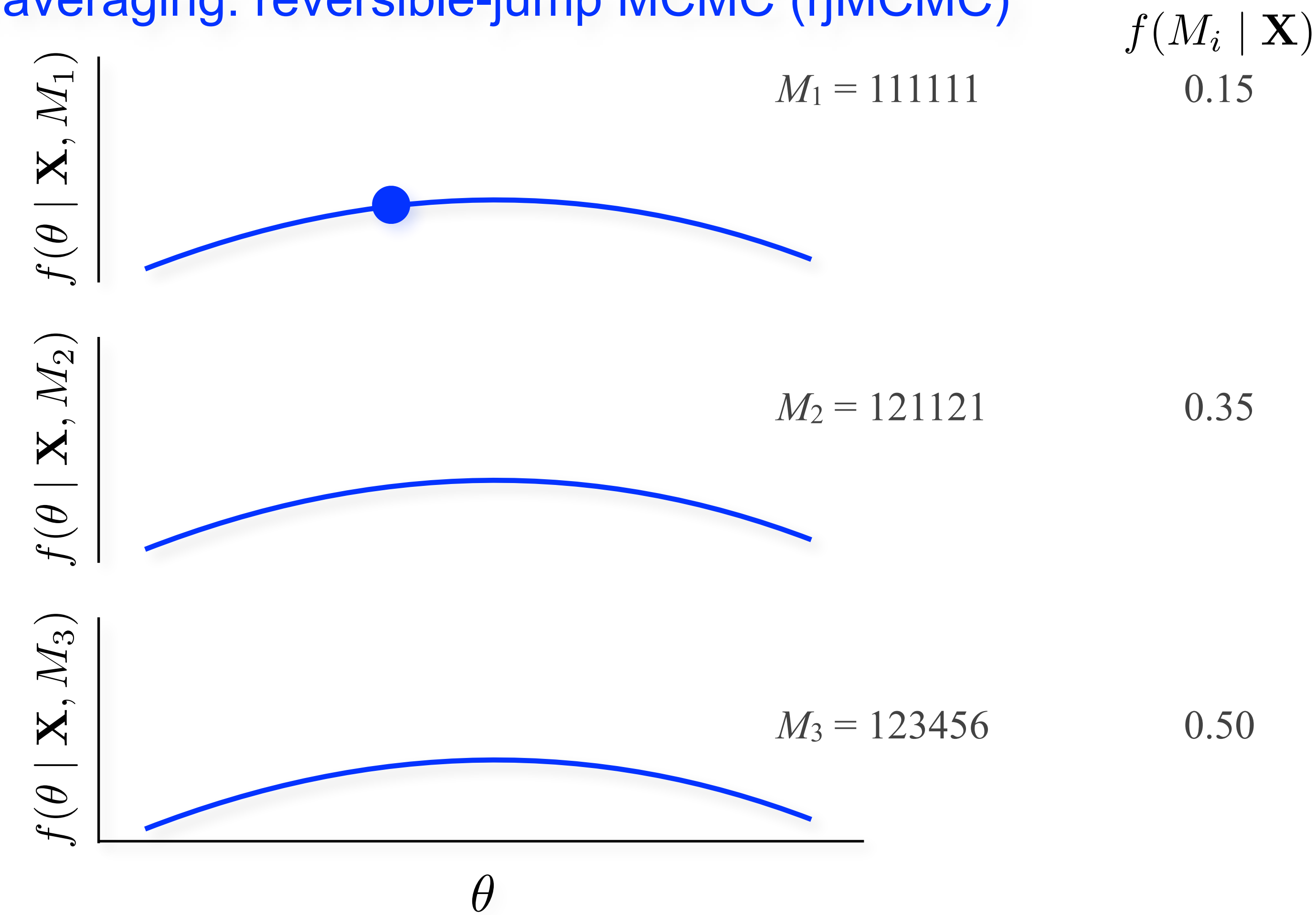


Parameter estimates for all parameters are therefore averaged over all models.

Bayesian Model Selection

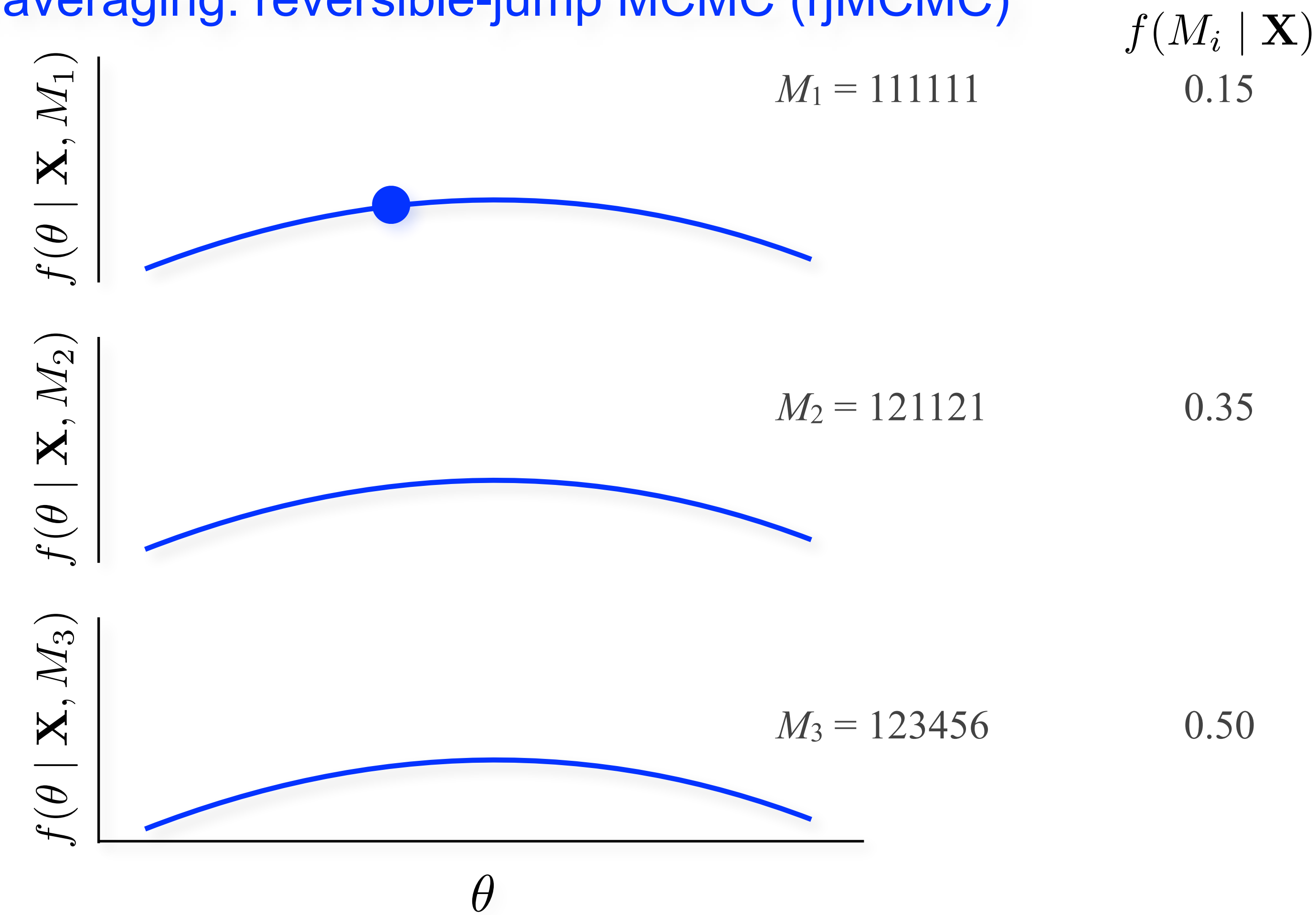
Bayesian model averaging: reversible-jump MCMC (rjMCMC)



The proportion of time the jMCMC spends visiting each model is an estimate of its marginal posterior probability.

Bayesian Model Selection

Bayesian model averaging: reversible-jump MCMC (rjMCMC)



The proportion of time the jMCMC spends visiting each model is an estimate of its marginal posterior probability, so we get model selection for free!

Model-Based Inference of Phylogeny

Model-based inference is based on the model

We have to assess our ability to estimate parameters of a given model:

- likelihood optimization: have we found the global MLE?
- MCMC simulation: have we found accurately approximated the posterior?

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We have to be careful about our choice of model:

- model selection: what is the <u>relative</u> fit of candidate models to my dataset?
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Comparing the (relative or absolute) fit of alternative models is how we learn

- we can test competing hypotheses by comparing the fit of competing models to our data
- we can learn what parameters are important to describe the process that gave rise to our data
- we can simultaneously improve our estimates of phylogenies and also our understanding of the factors impacting molecular evolution