A Brief Introduction to Bayesian Model Selection and Validation

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Outline

I. Model selection

What is the <u>relative</u> 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

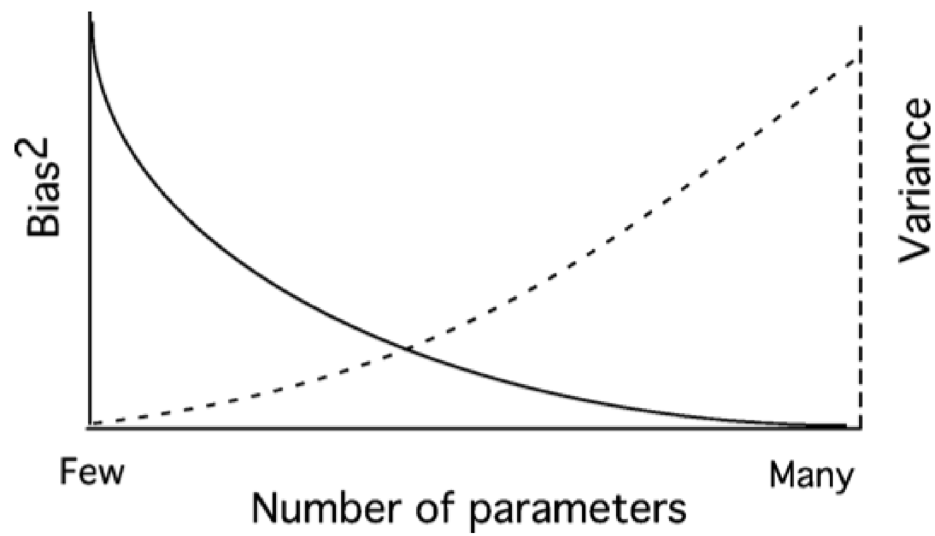
How do we accommodate uncertainty in the choice among candidate models?

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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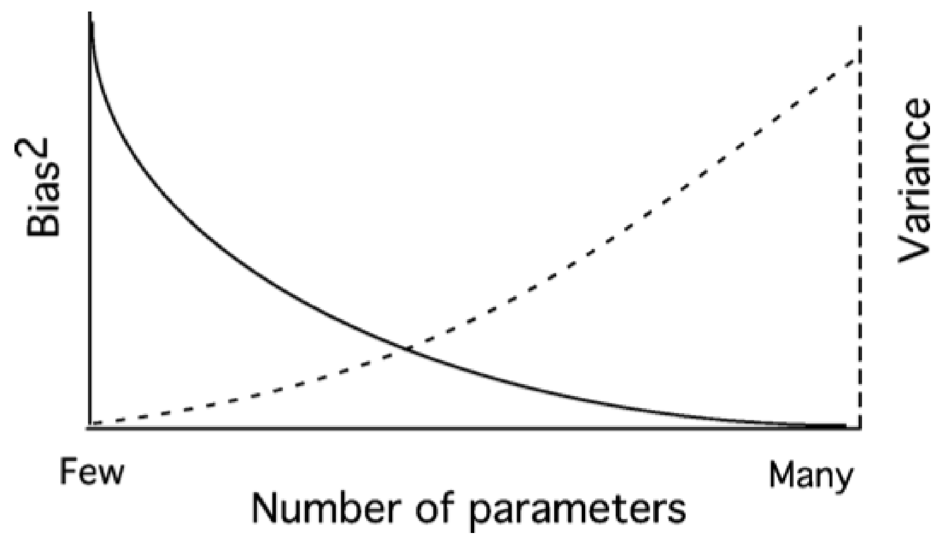

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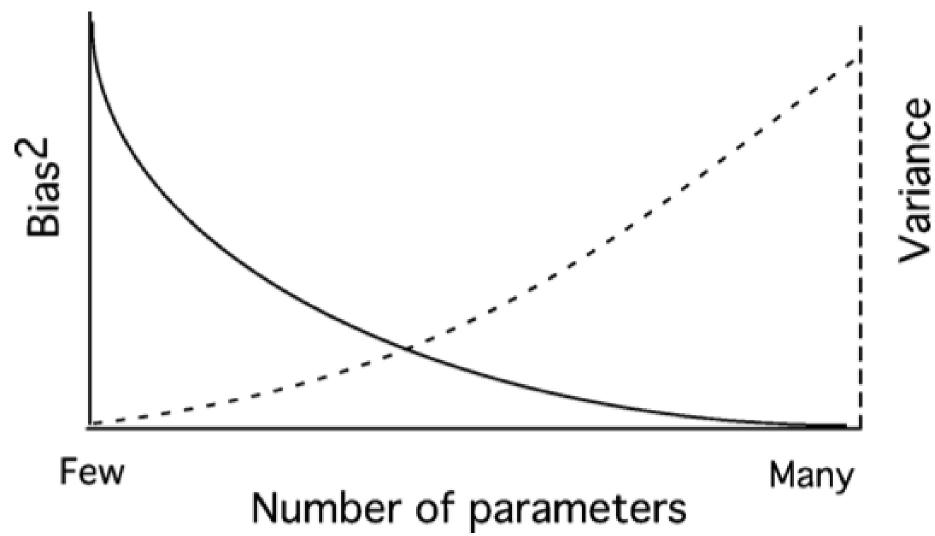

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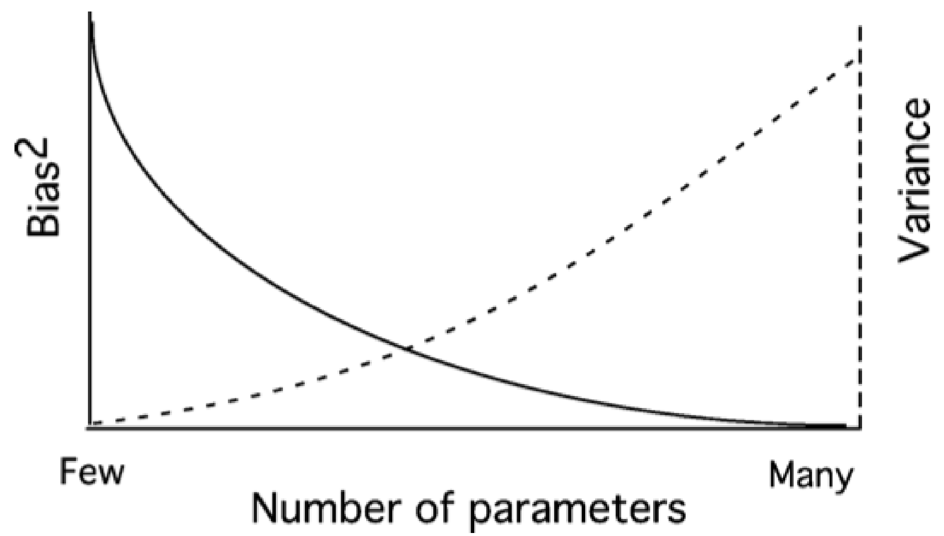
- an over-specified model will inflate the error variance of parameter estimates



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

Inference Method

Data

sequence alignment

Model

tree with branch lengths

substitution model

Model 1

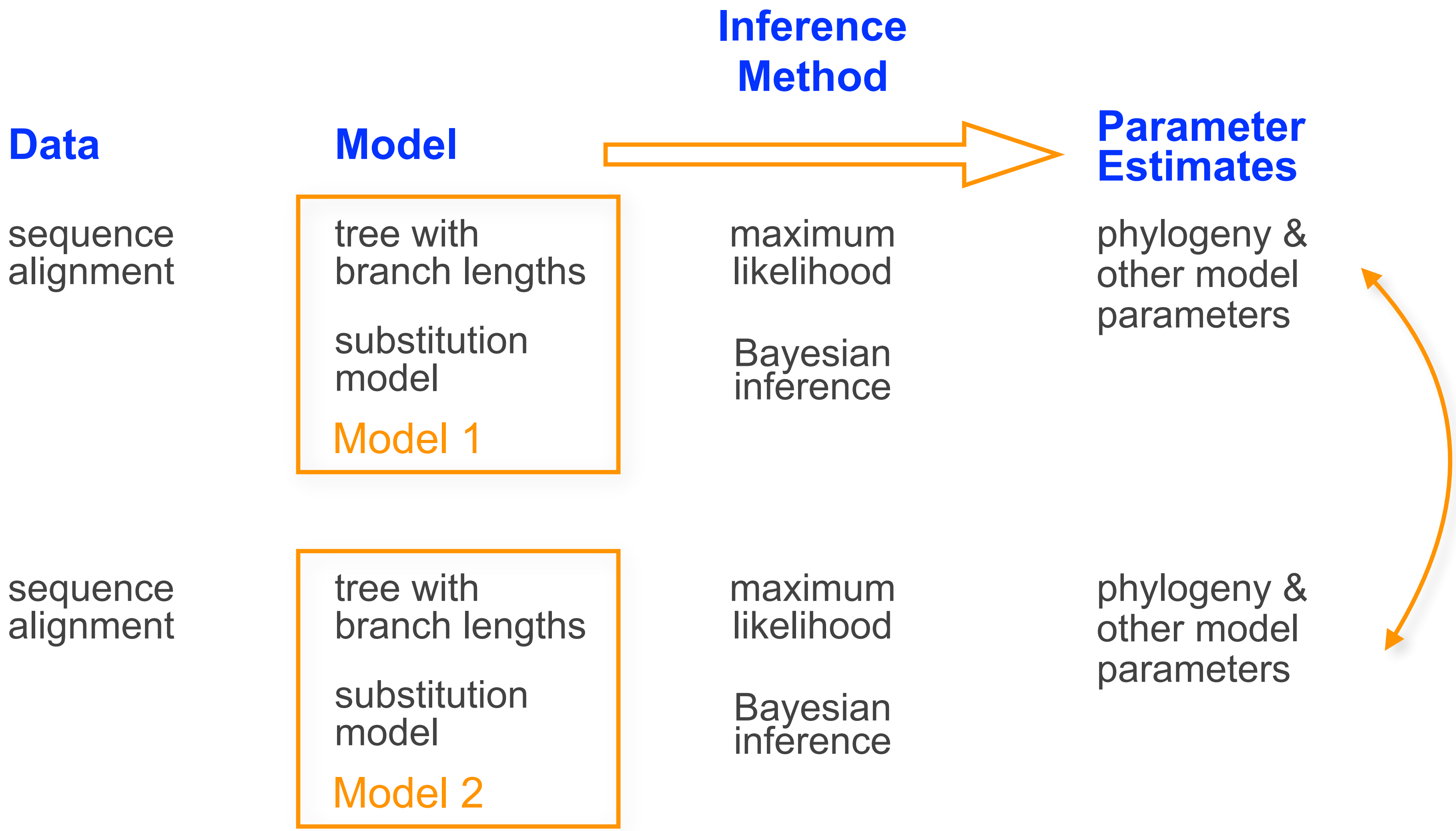
maximum likelihood

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 unbiassed parameter estimates

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Model comparison is critical for obtaining unbiassed 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:

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

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

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:

$$\mathrm{BF}_{01} = \frac{P(\mathbf{X} \mid M_0)}{P(\mathbf{X} \mid M_1)}$$

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$$2\ln \mathrm{BF}_{01} = 2\left[\ln P(\mathbf{X} \mid M_0) - \ln P(\mathbf{X} \mid M_1)\right]$$

- models are preferred by virtue of their relative ability to predict the data

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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

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

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- it is (intentionally) 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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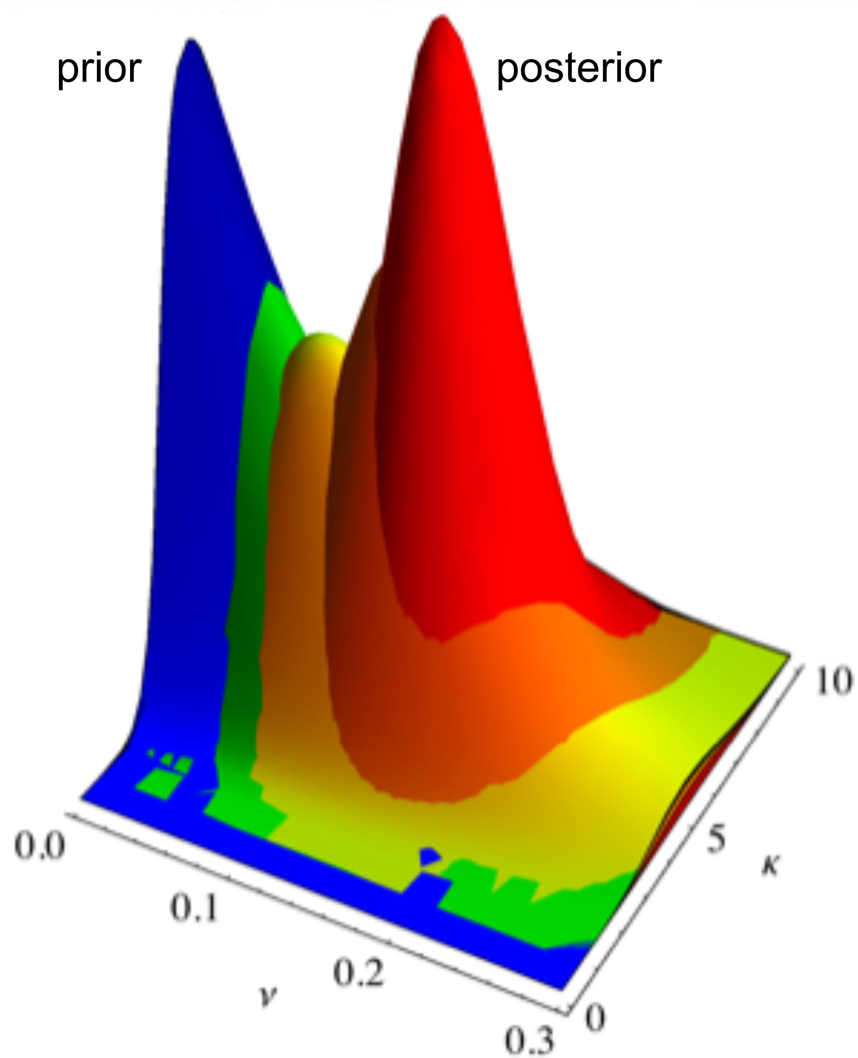
But, to compare models (test hypotheses), we need the marginal likelihoods!

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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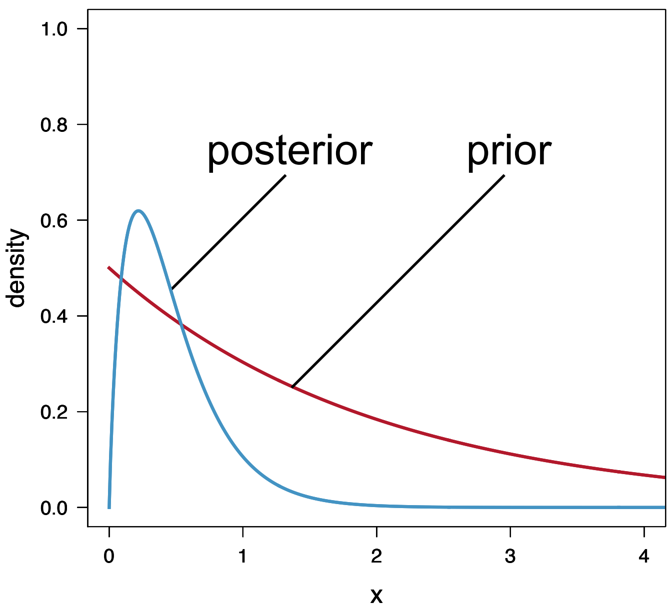
It is difficult to estimate the marginal likelihood from MCMC because the posterior is (hopefully) very focused compared to the prior (so we cannot accurately estimate the likelihood in large regions of parameter space).



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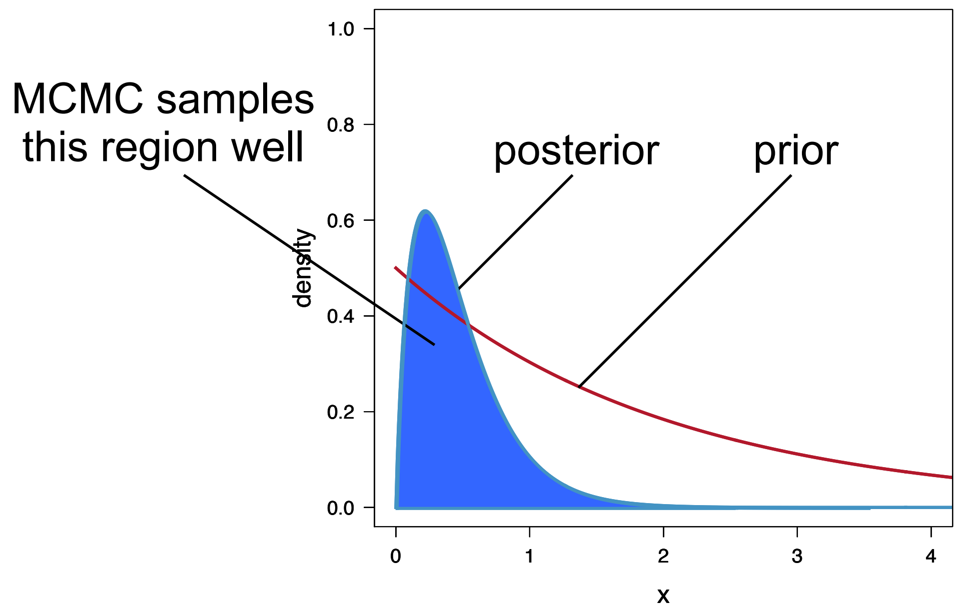

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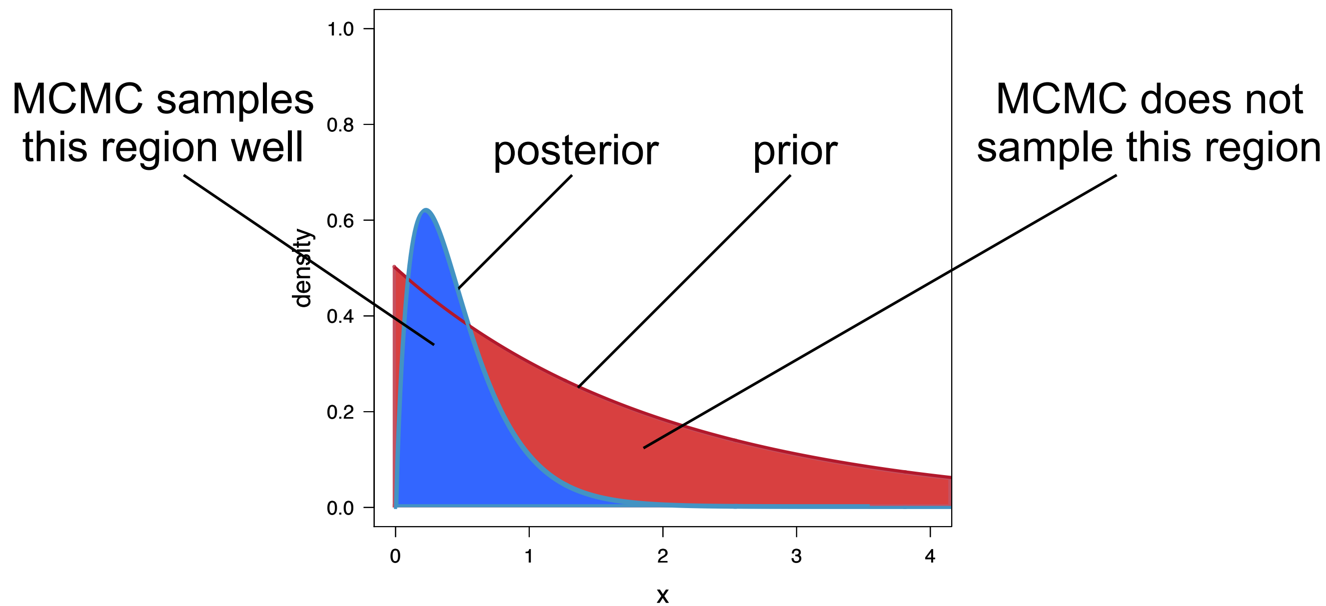

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Stepping-stone sampling forces the MCMC to sample from power posterior densities ranging from the prior to the posterior.

$$P(\theta \mid \mathbf{X})_{\beta_i} = \frac{P(\mathbf{X} \mid \theta)^{\beta_i} P(\theta)}{P(\mathbf{X})_{\beta_i}}$$

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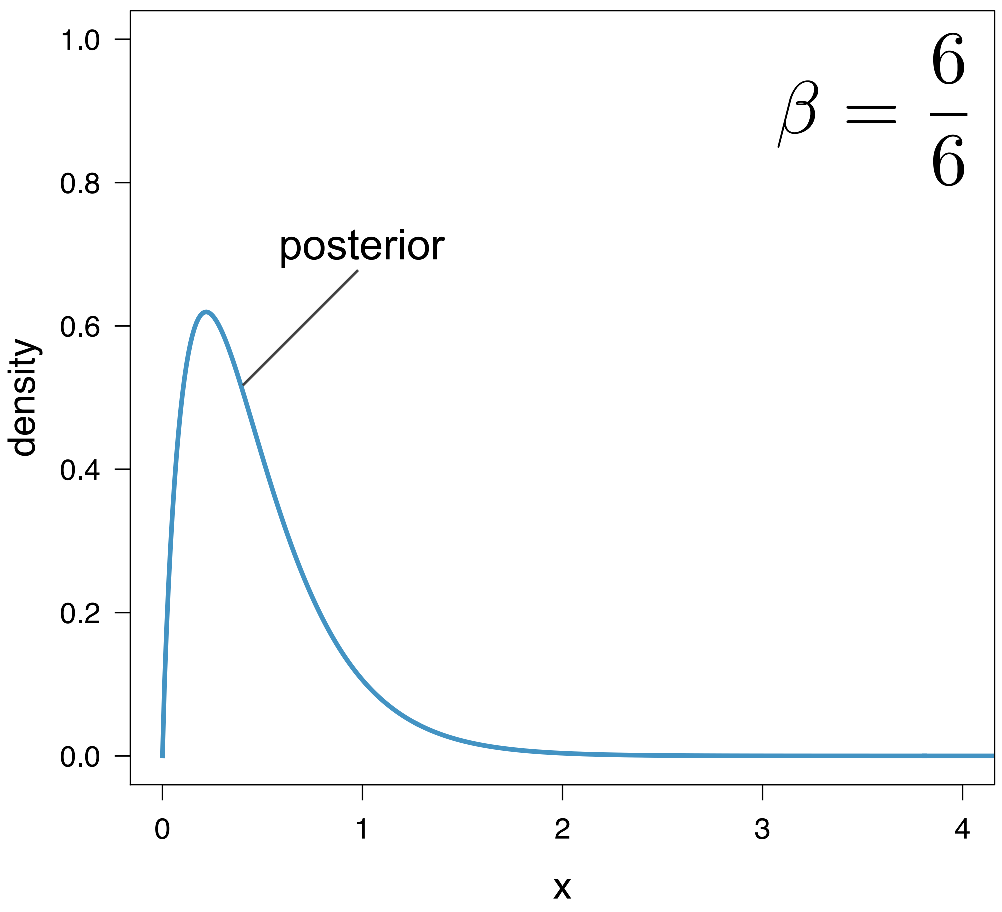
When $\beta = 0$, the MCMC targets the joint prior probability.

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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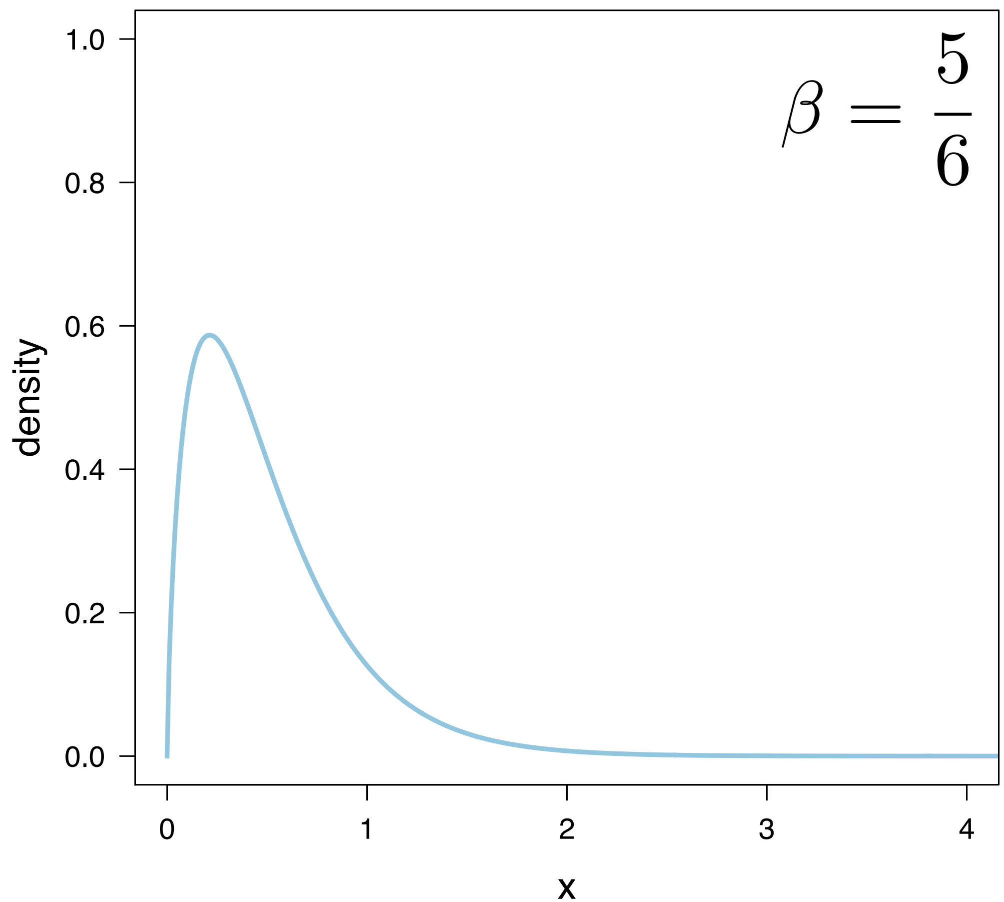

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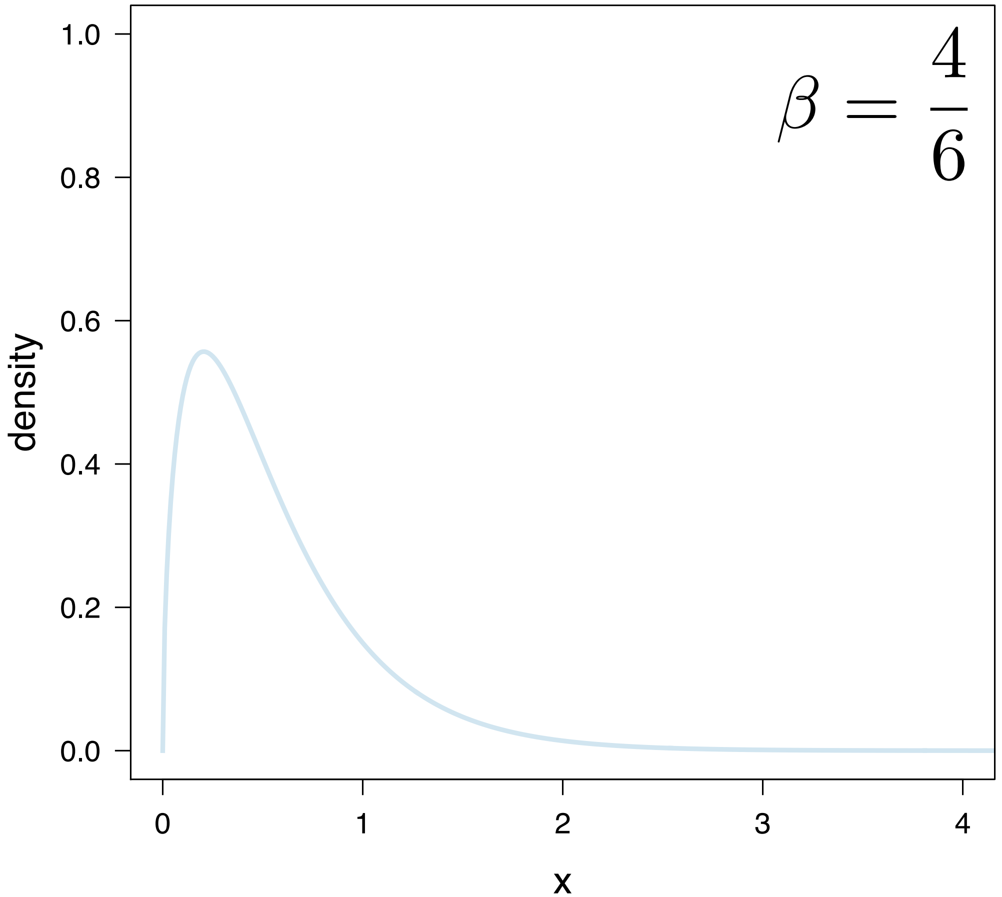

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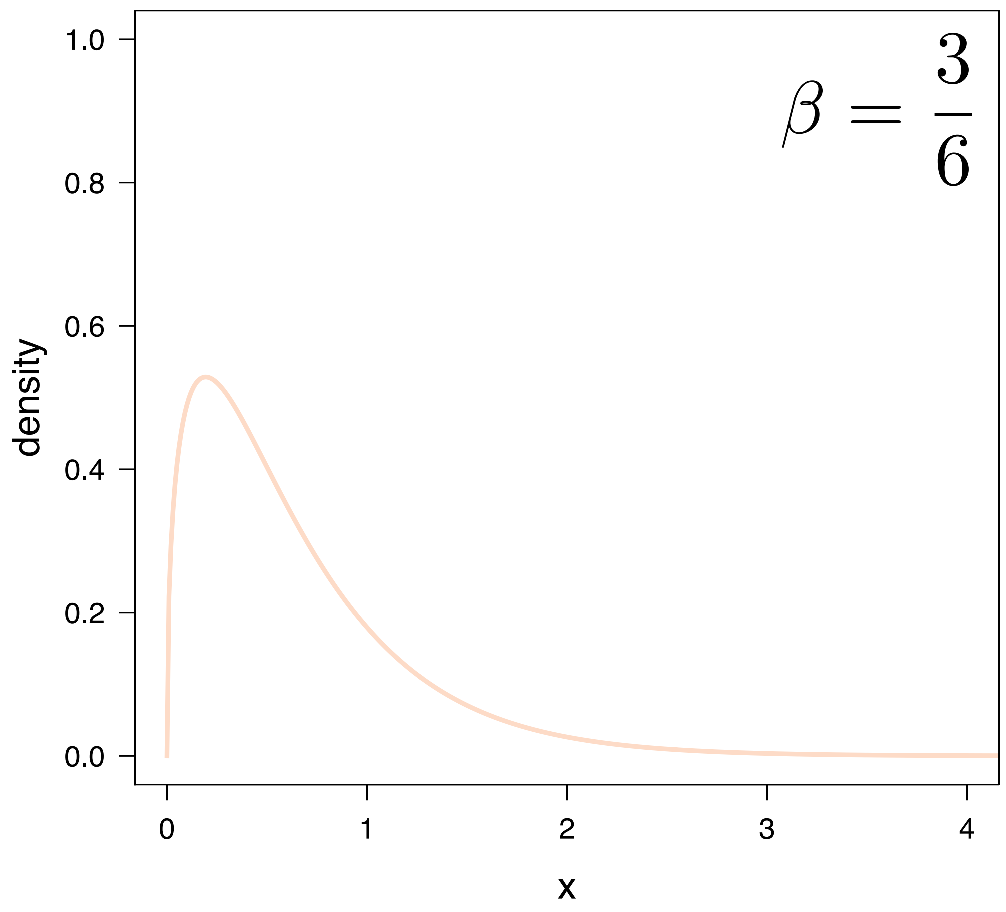

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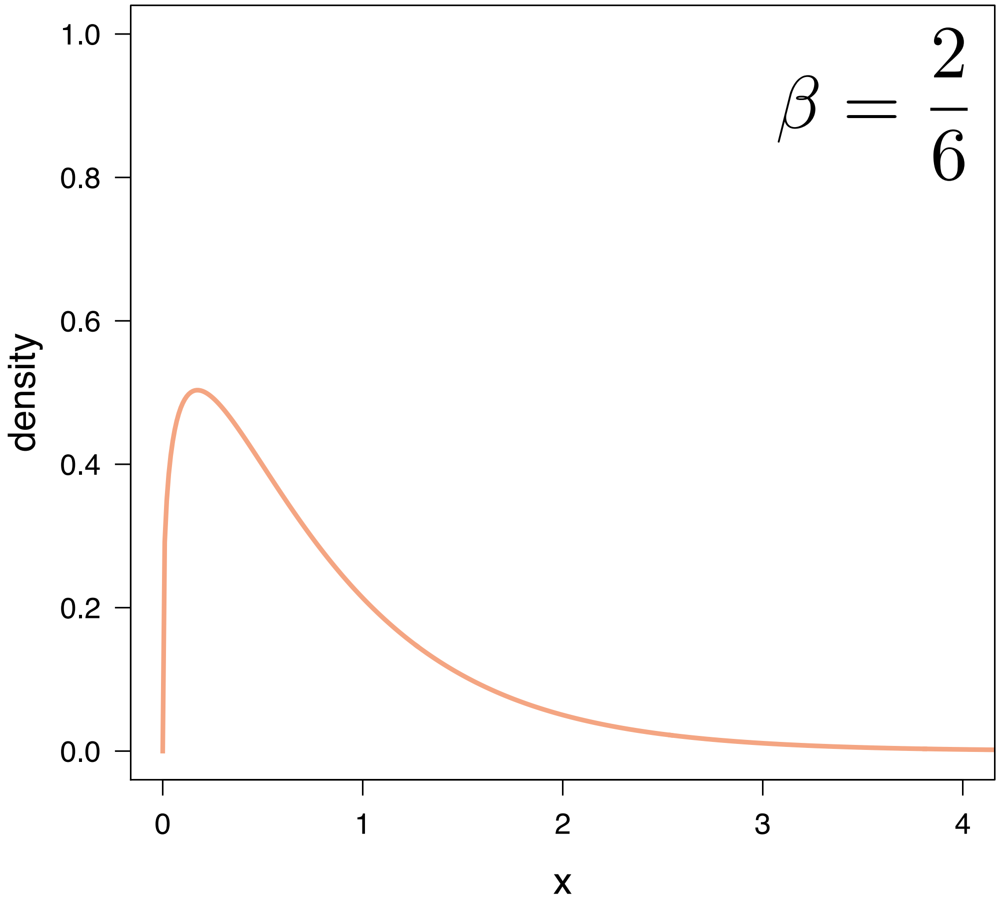

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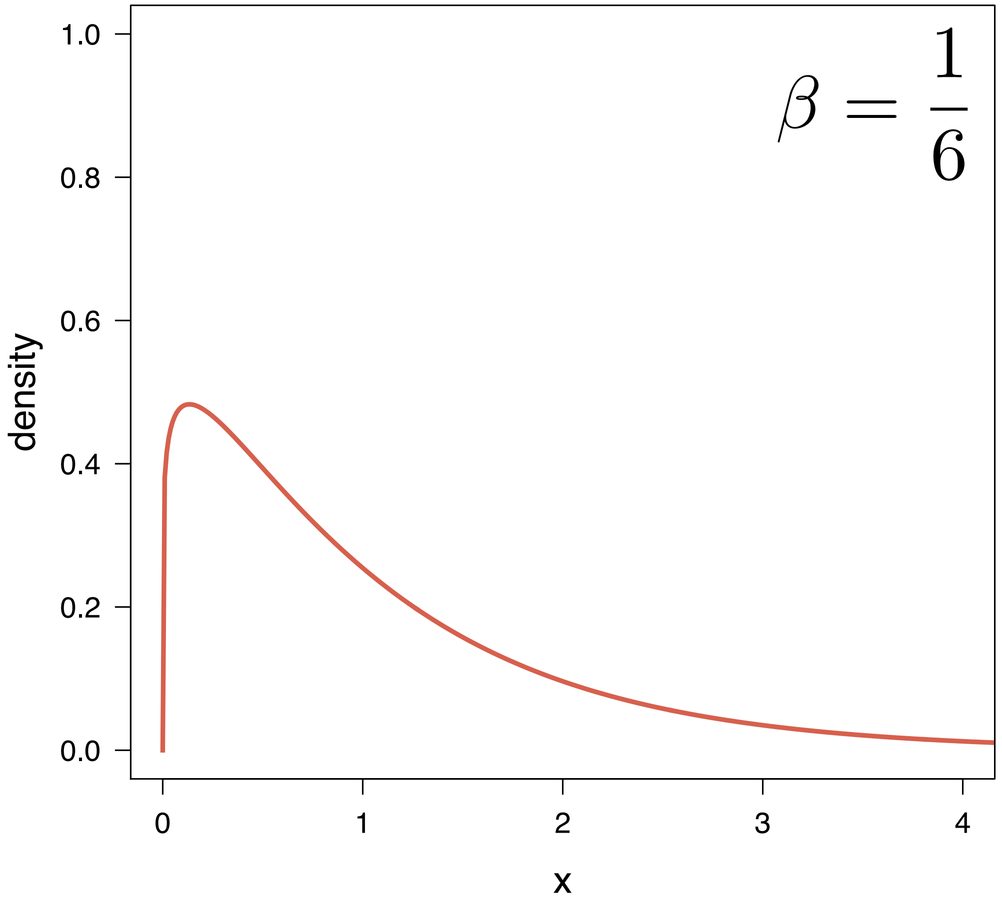

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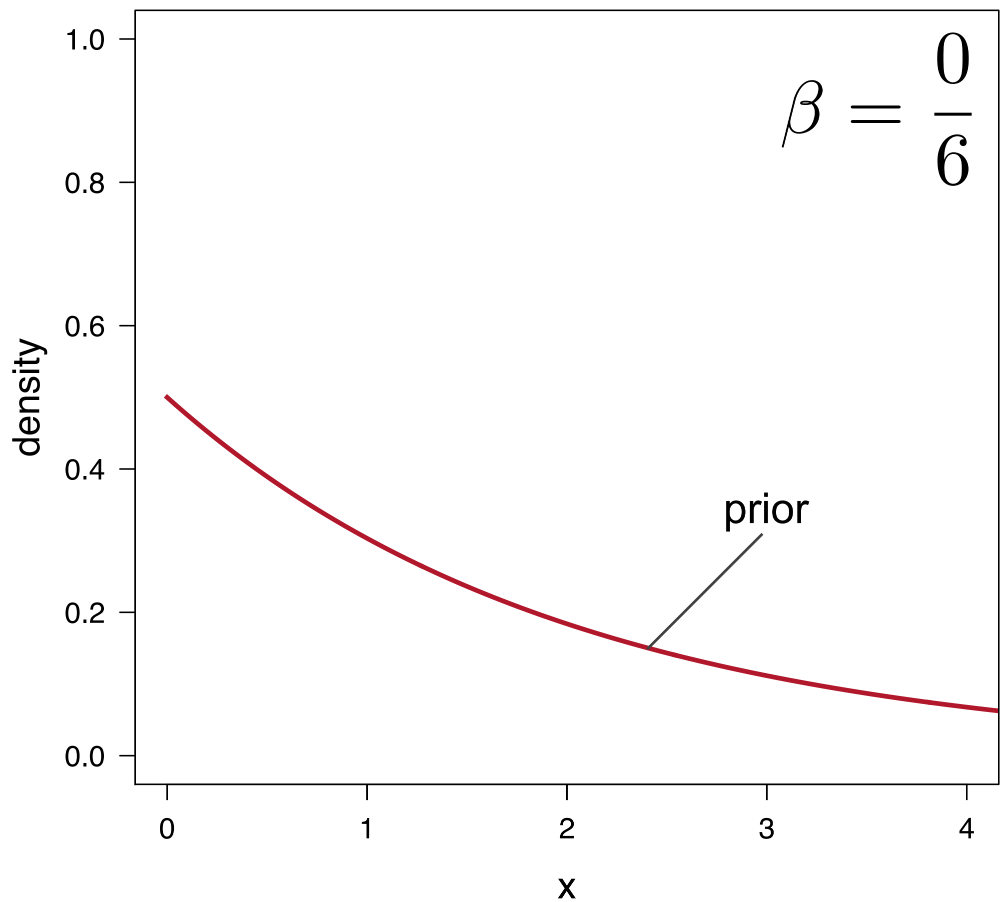

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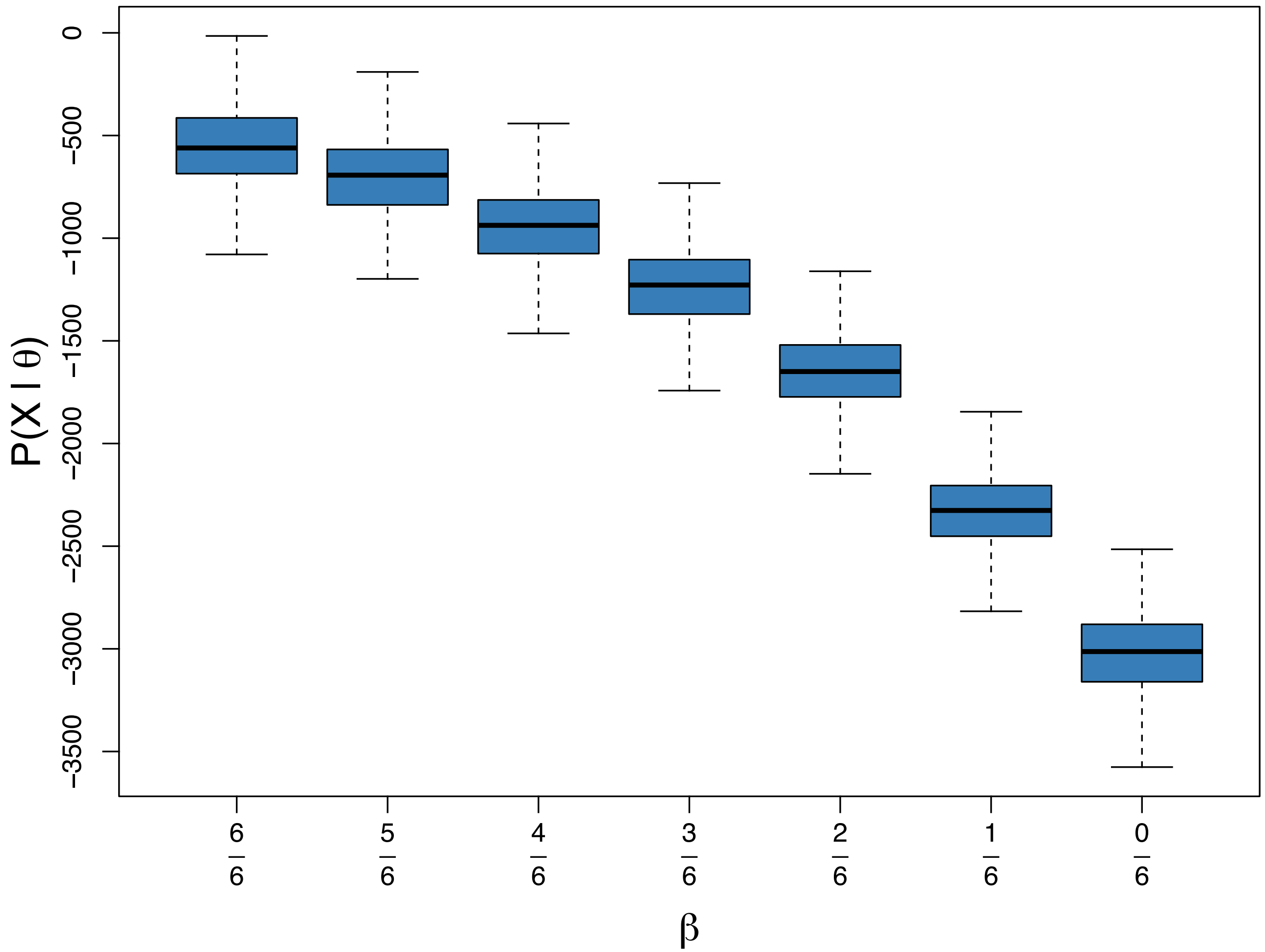
The sampled likelihoods at each stone can be used to estimate the marginal likelihood: path samplers[1] and stepping-stone samplers[2].



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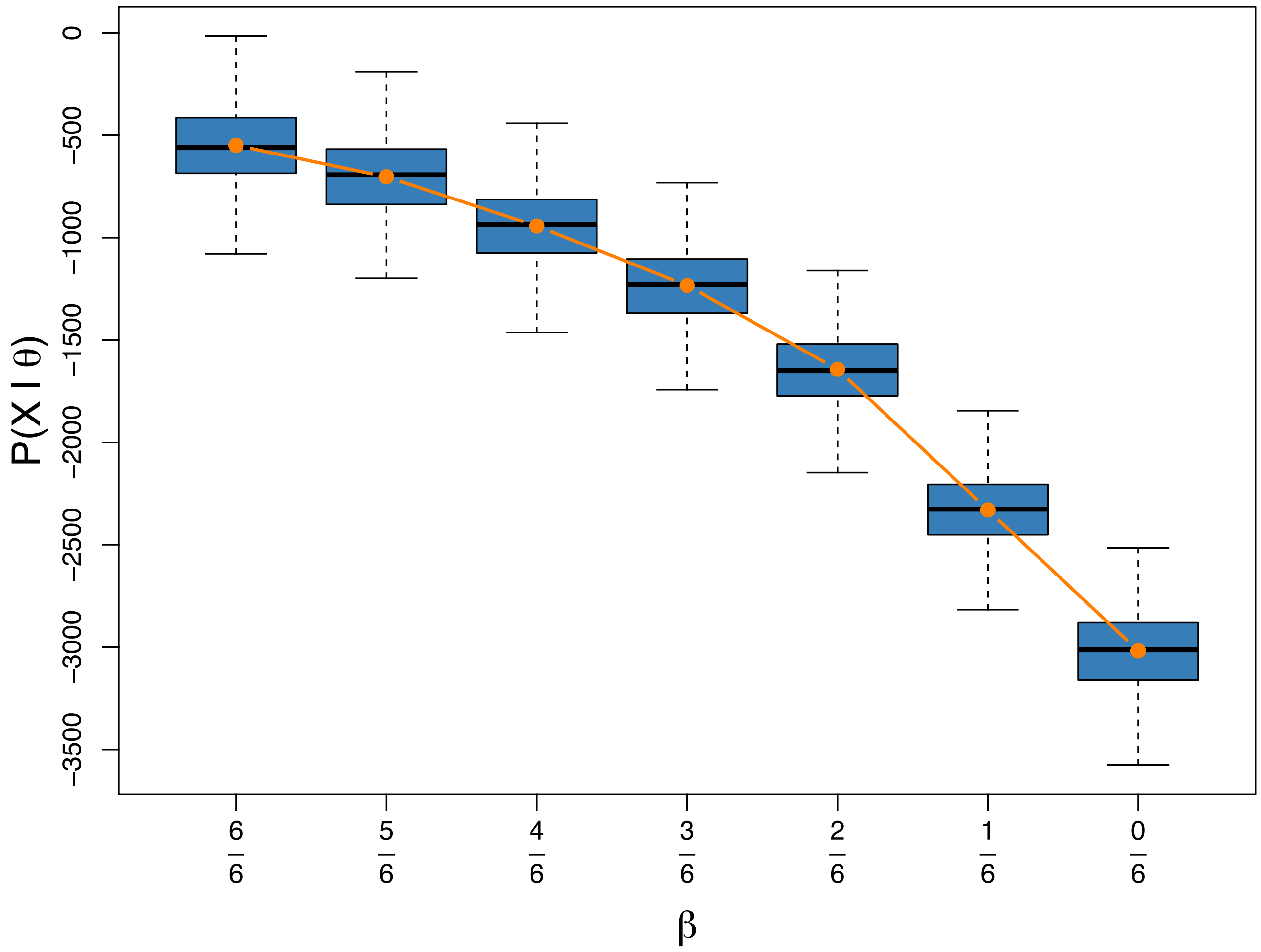

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How should the stones be distributed between the posterior and the prior to efficiently estimate the marginal likelihood?

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

Model Selection: Bayesian Methods

Estimating marginal likelihoods: power-posterior simulation

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

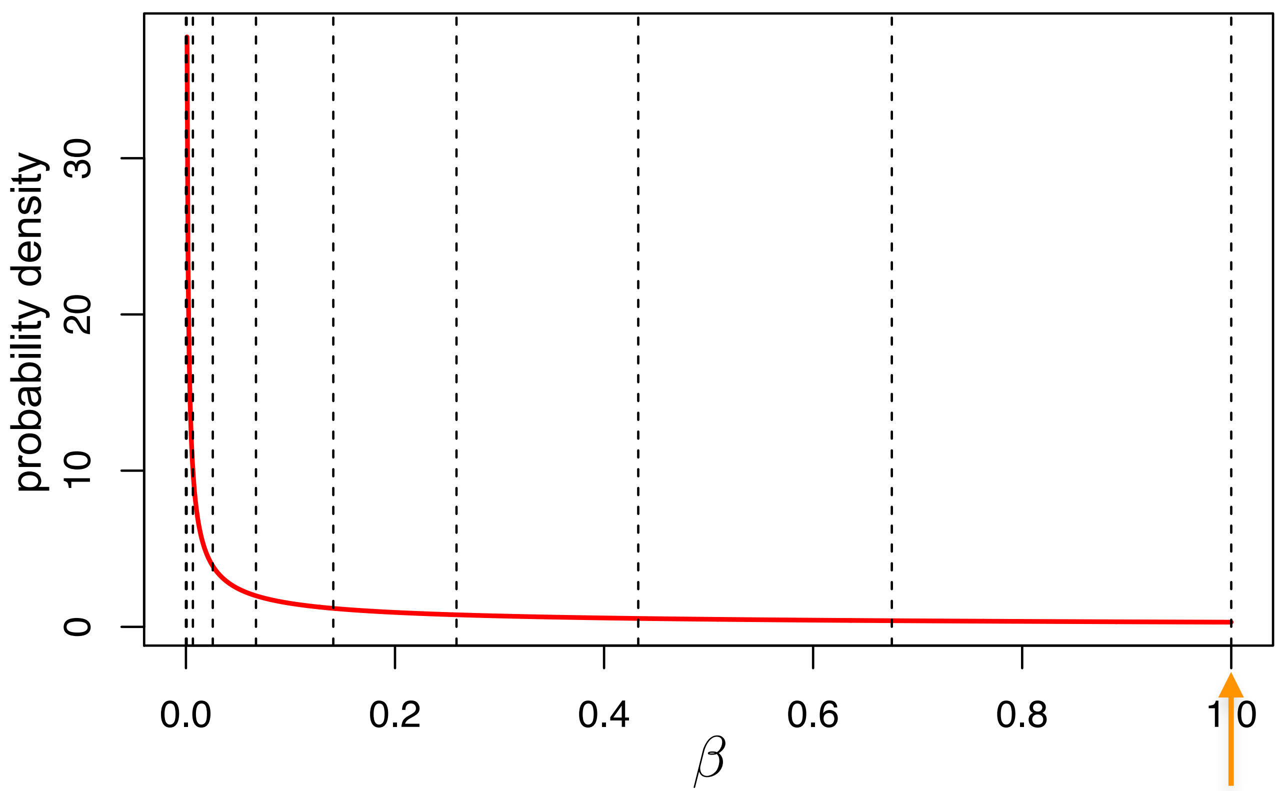
It is more difficult to sample adequately from the relatively diffuse prior compared to the more concentrated posterior distribution.

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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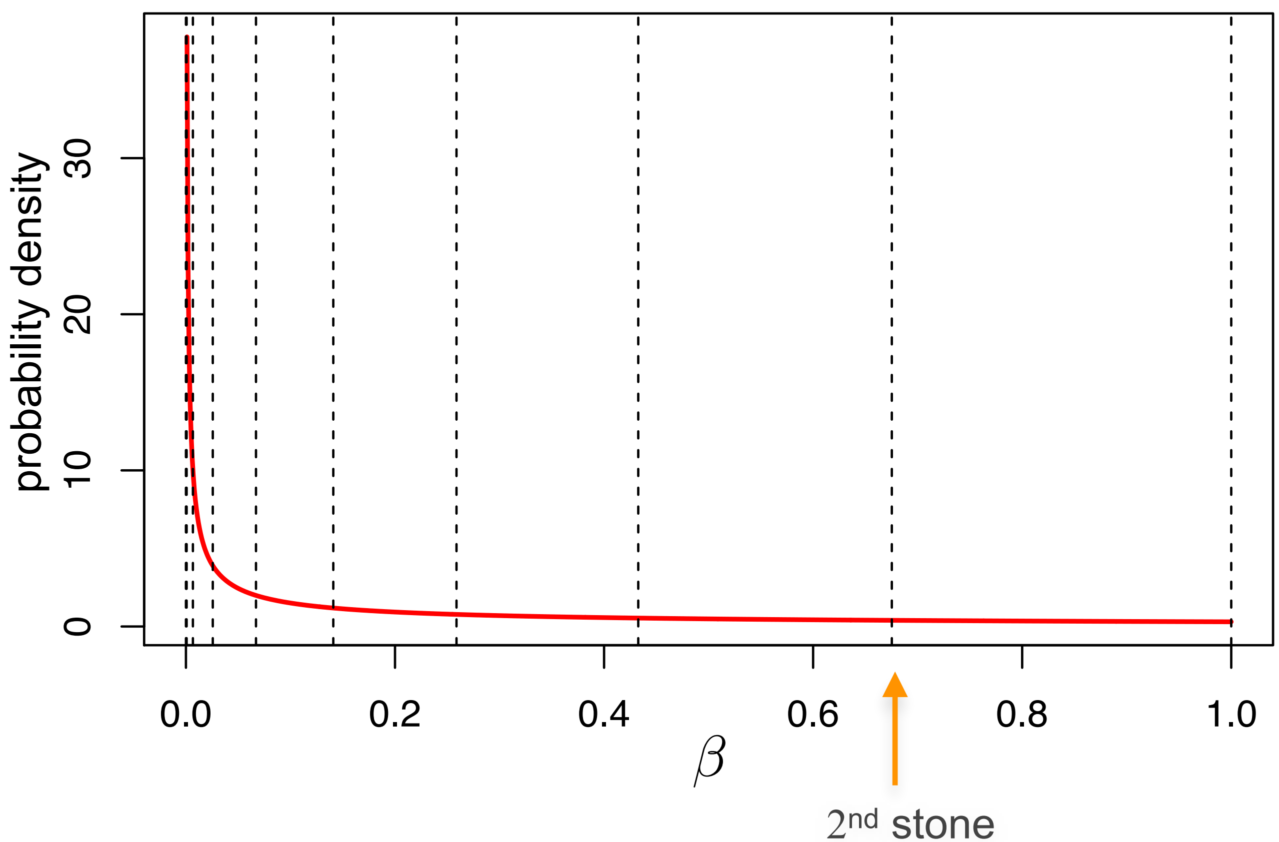

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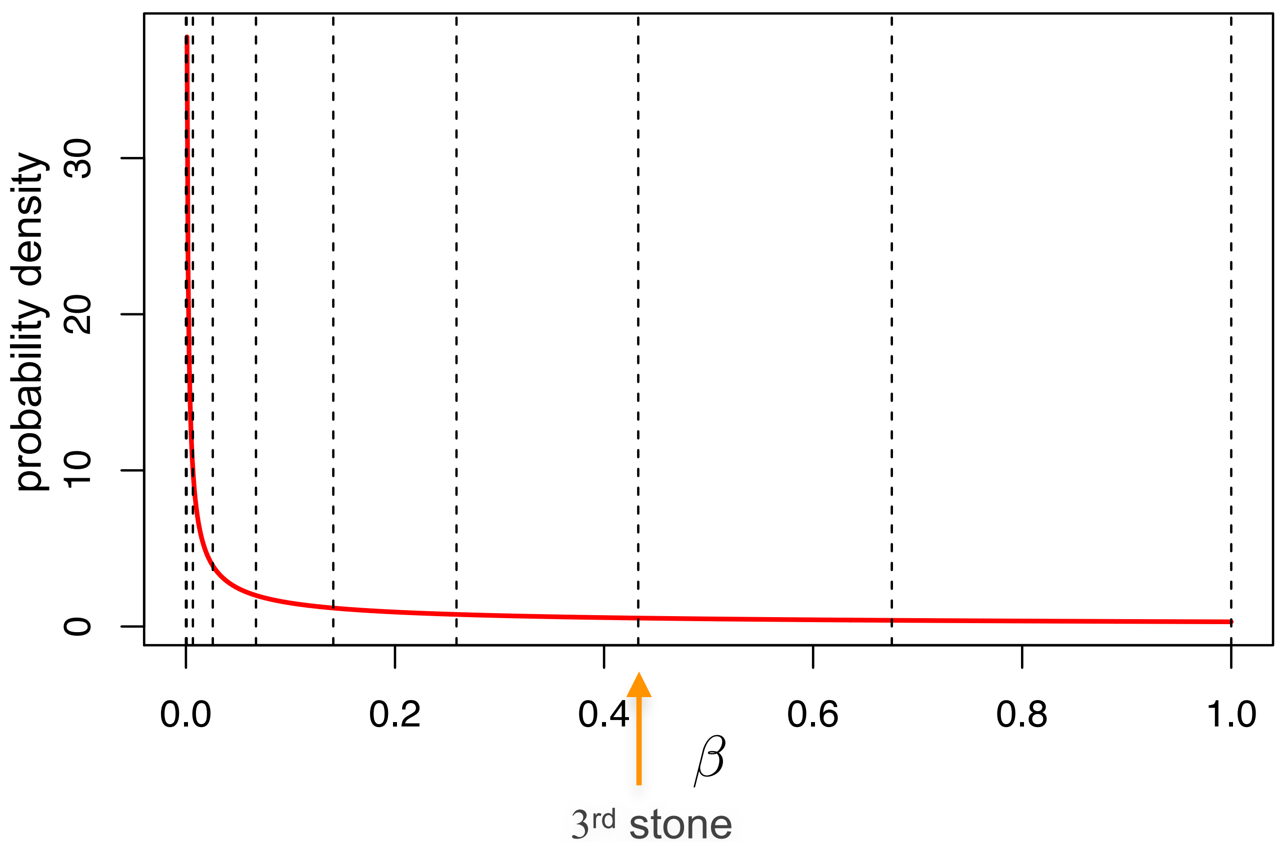

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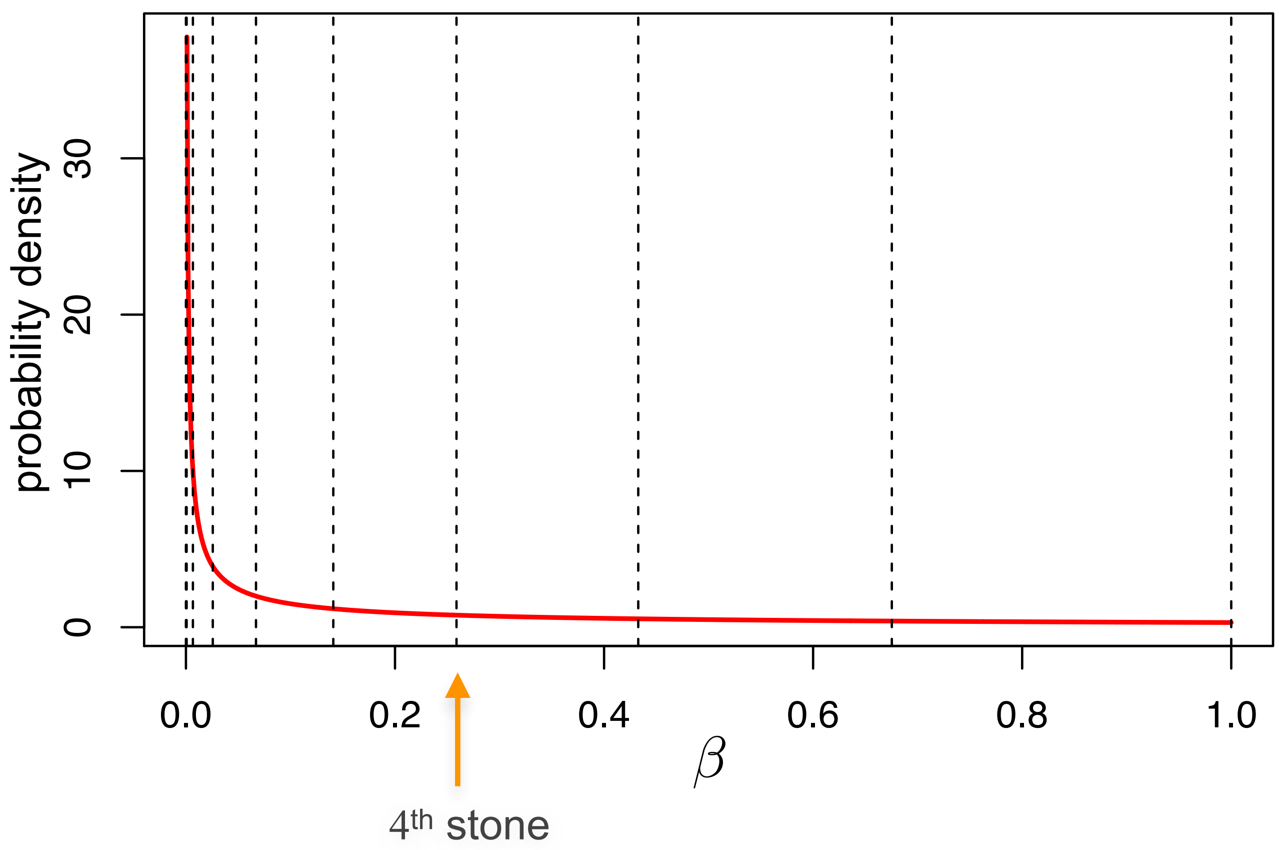

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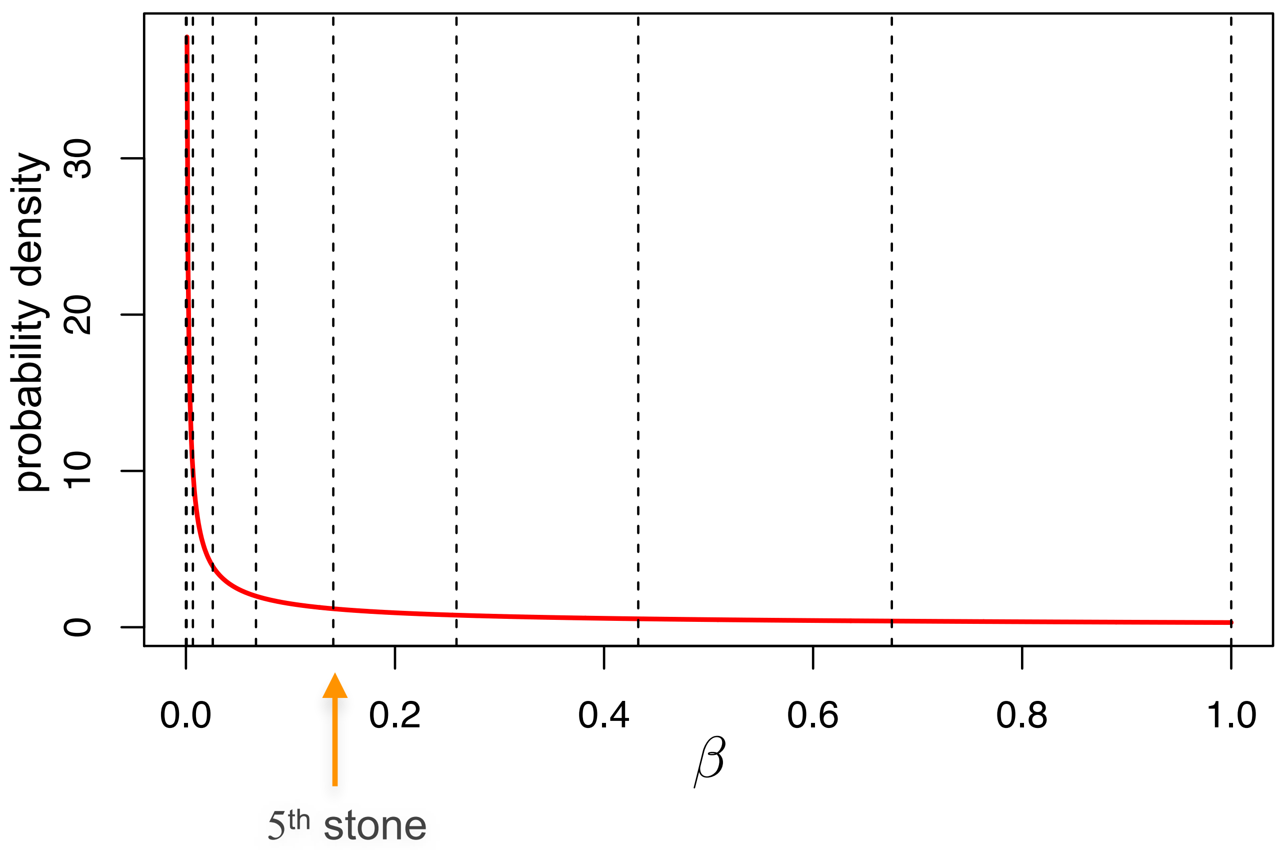

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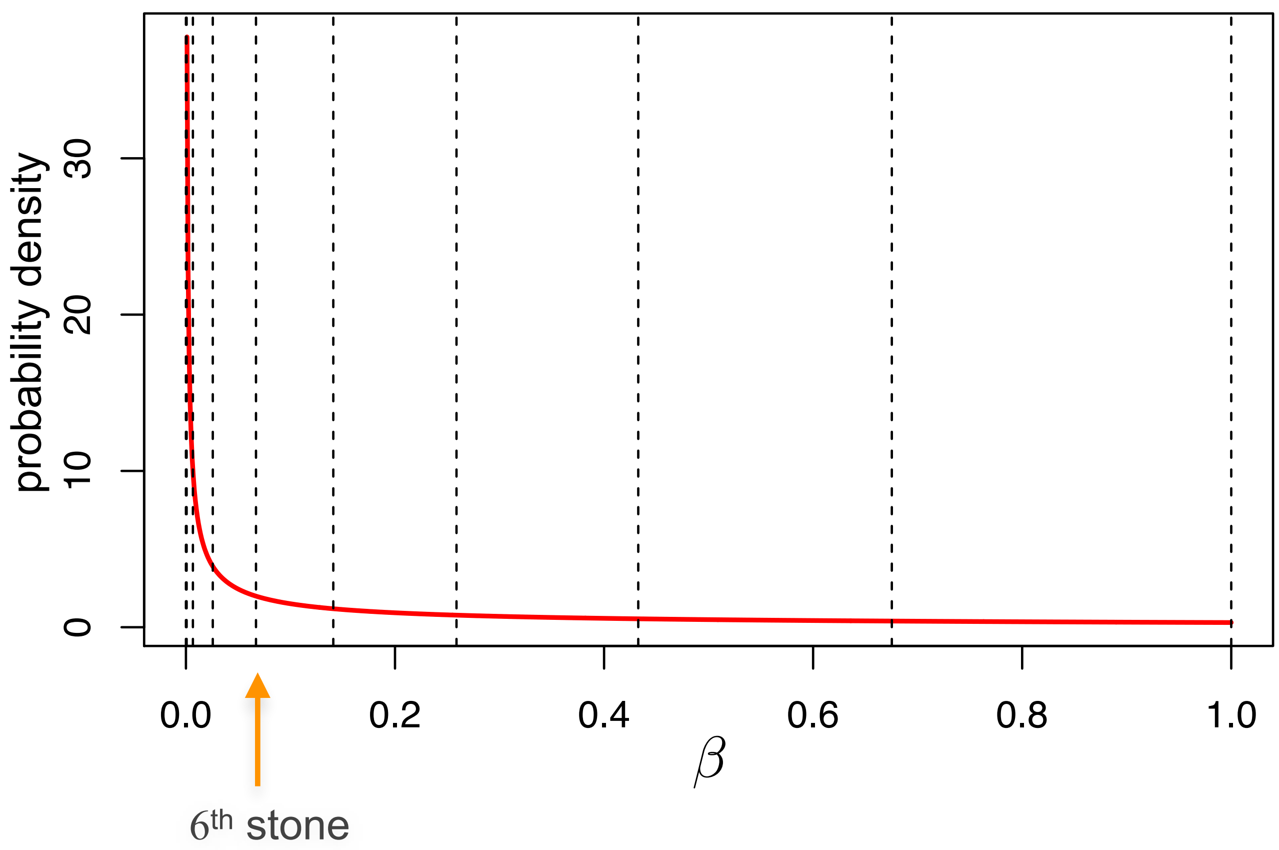

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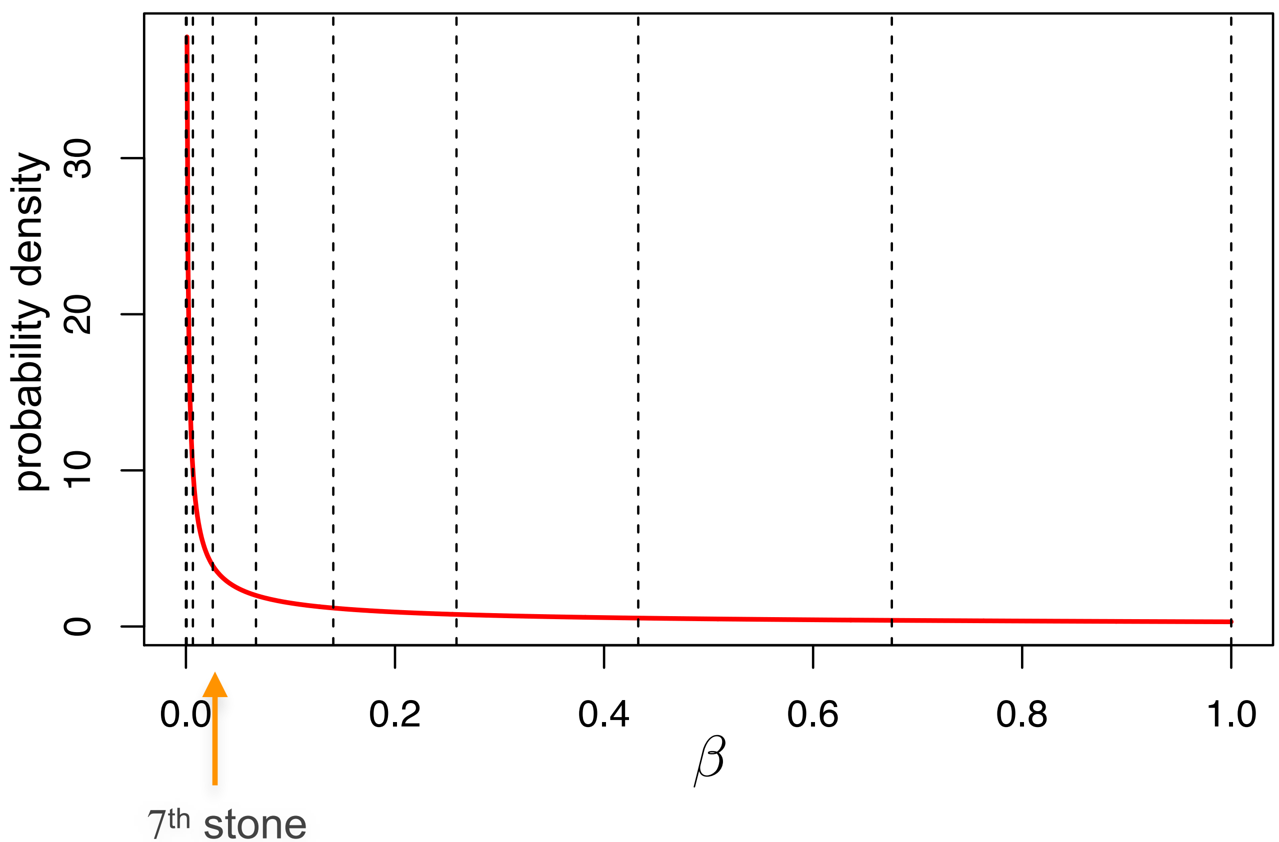

Model Selection: Bayesian Methods

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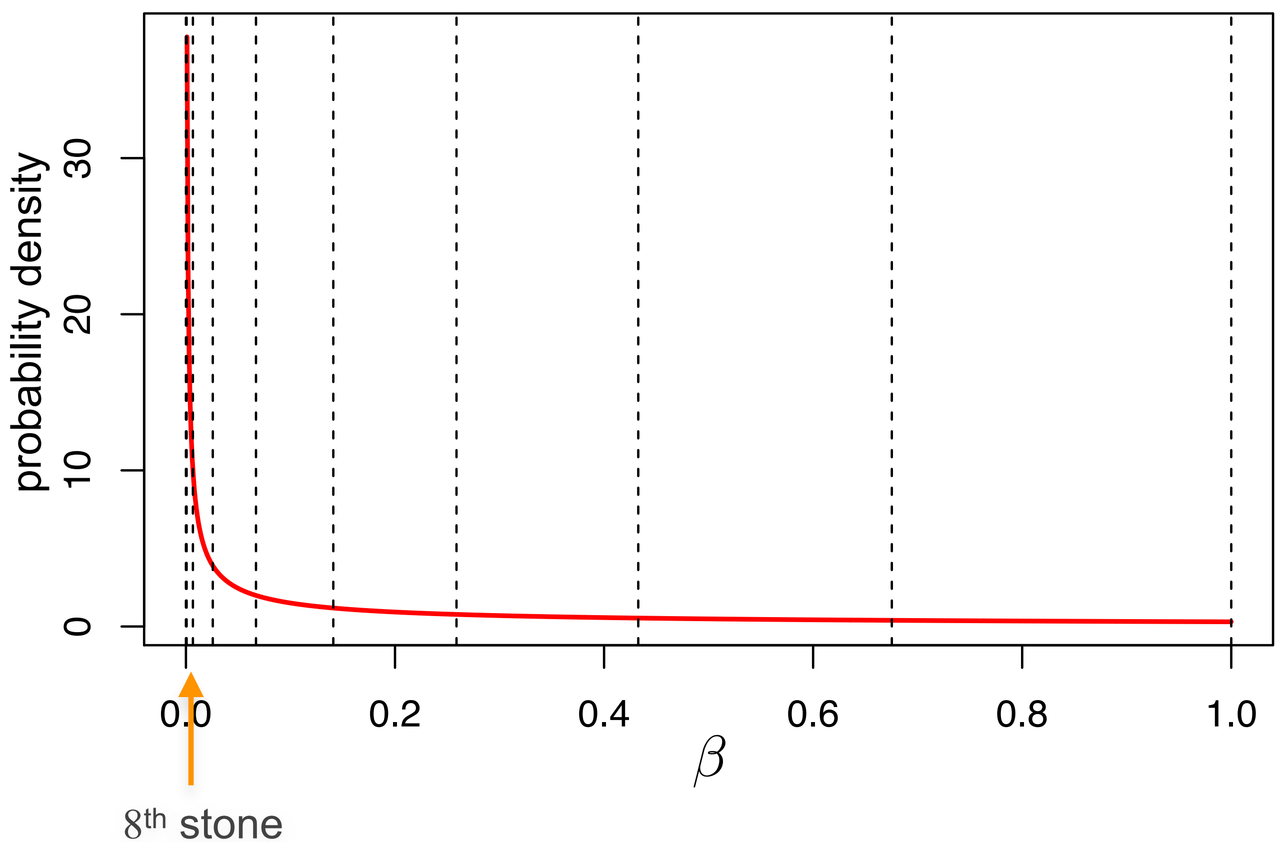

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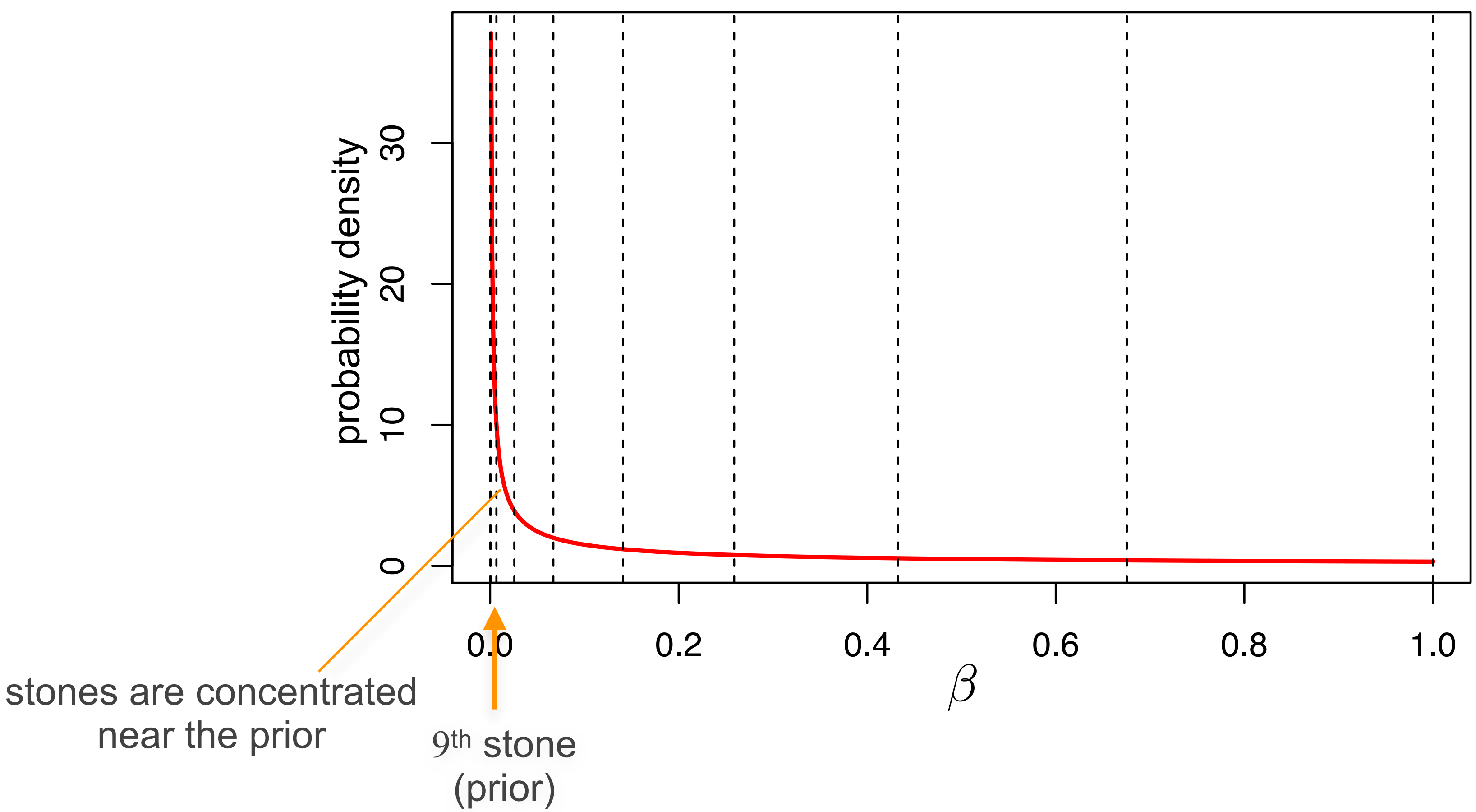

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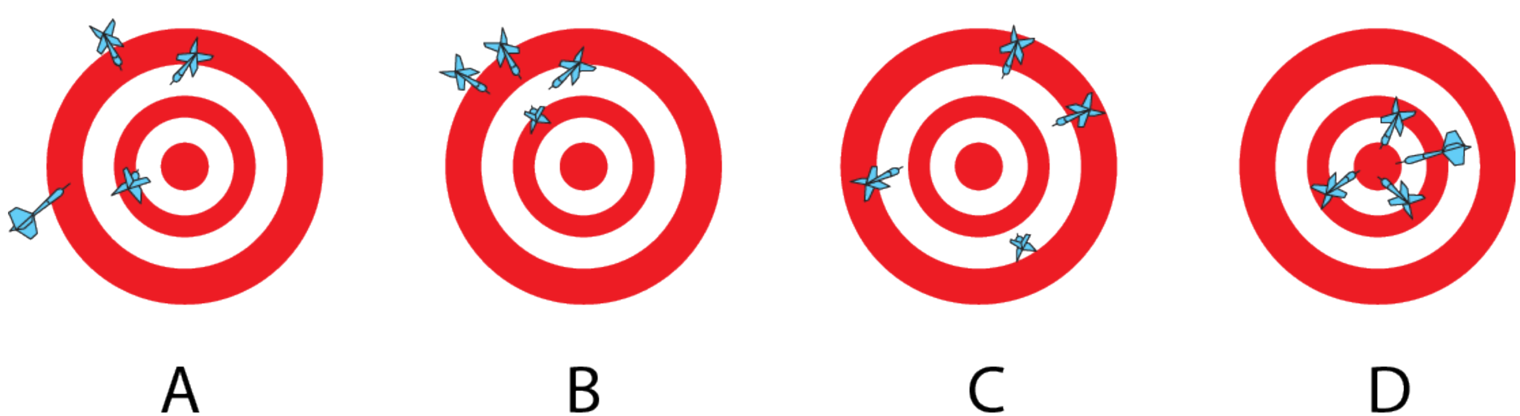

Outline

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Bayesian Evaluation of Model Adequacy

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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.

Bayesian Evaluation of Model Adequacy

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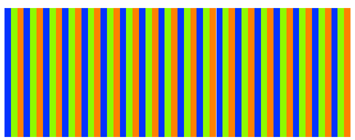
8. Compare T_{obs} to the distribution predicted from the posterior distribution.

Bayesian Evaluation of Model Adequacy

Posterior-predictive simulation

Original data matrix



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Bayesian Evaluation of Model Adequacy

Posterior-predictive simulation

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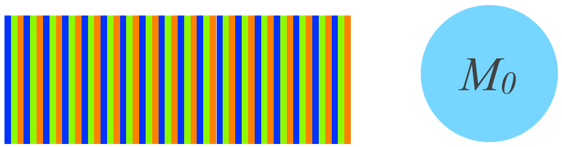
Candidate model

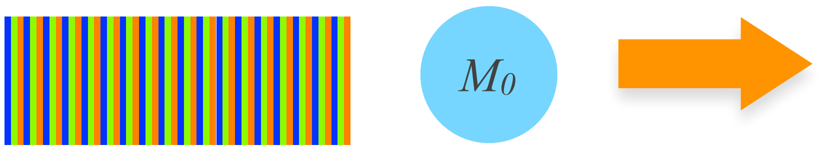


estimate the joint posterior probability distribution using MCMC

Bayesian Evaluation of Model Adequacy

Posterior-predictive simulation

Original data matrix | Candidate model | MCMC simulation



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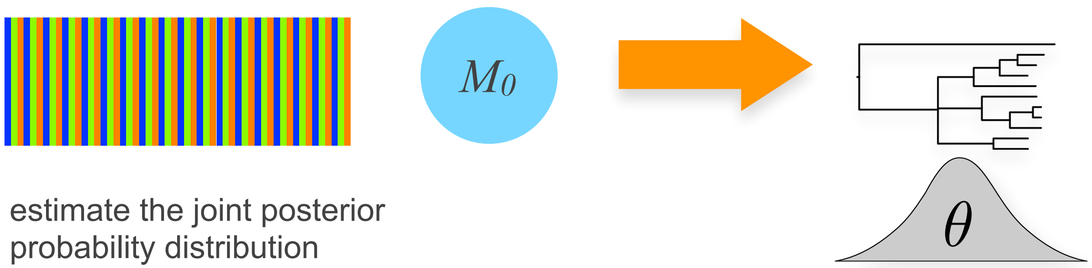
Original data matrix | Candidate model | MCMC simulation | Posterior samples



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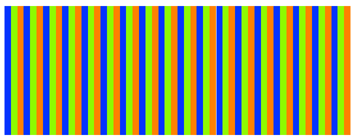
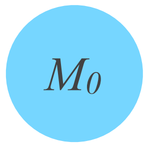
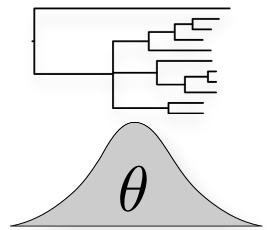
Simulate







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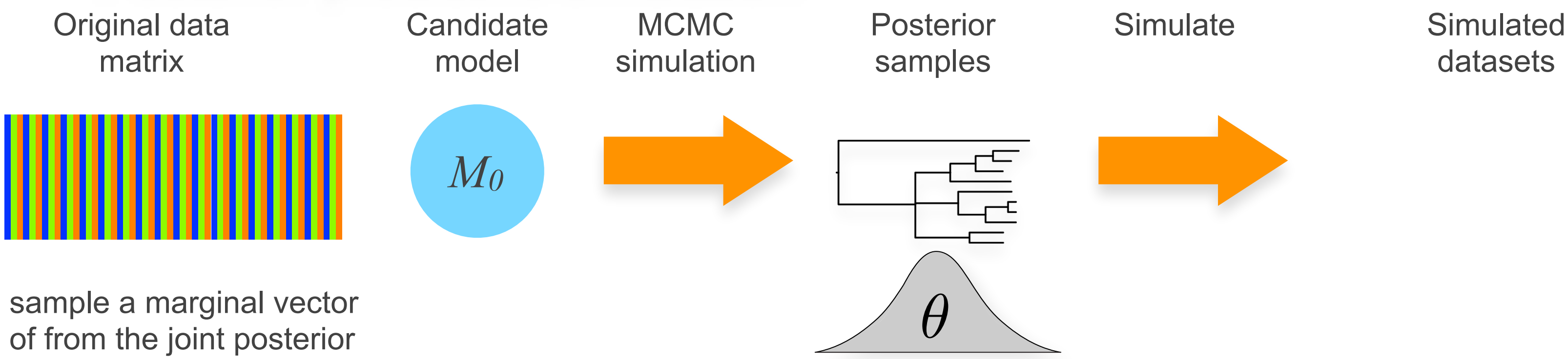

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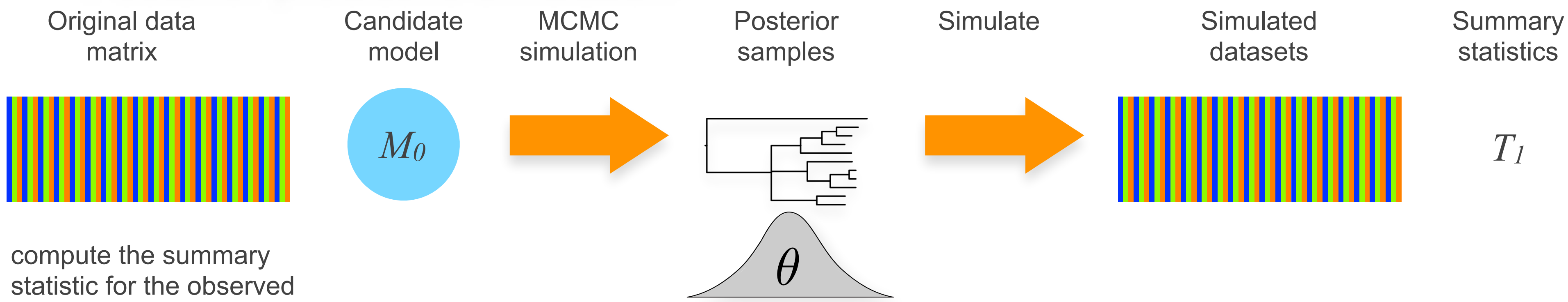

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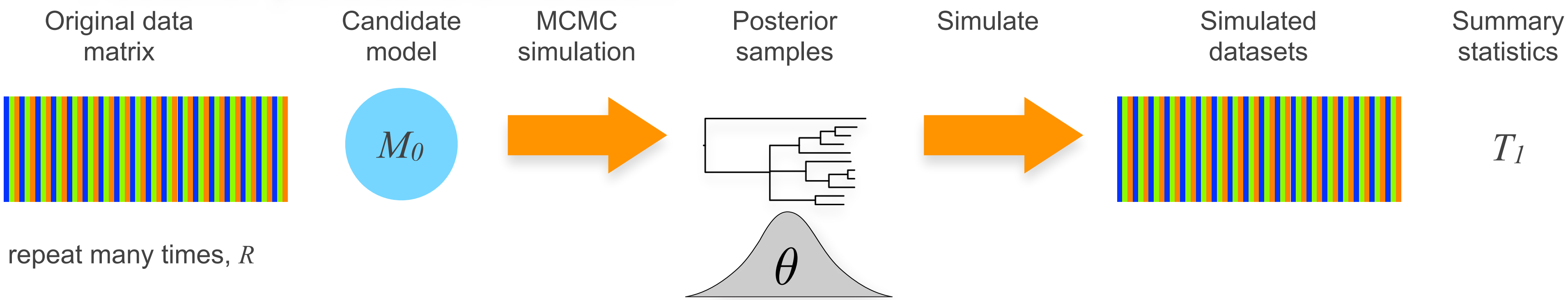

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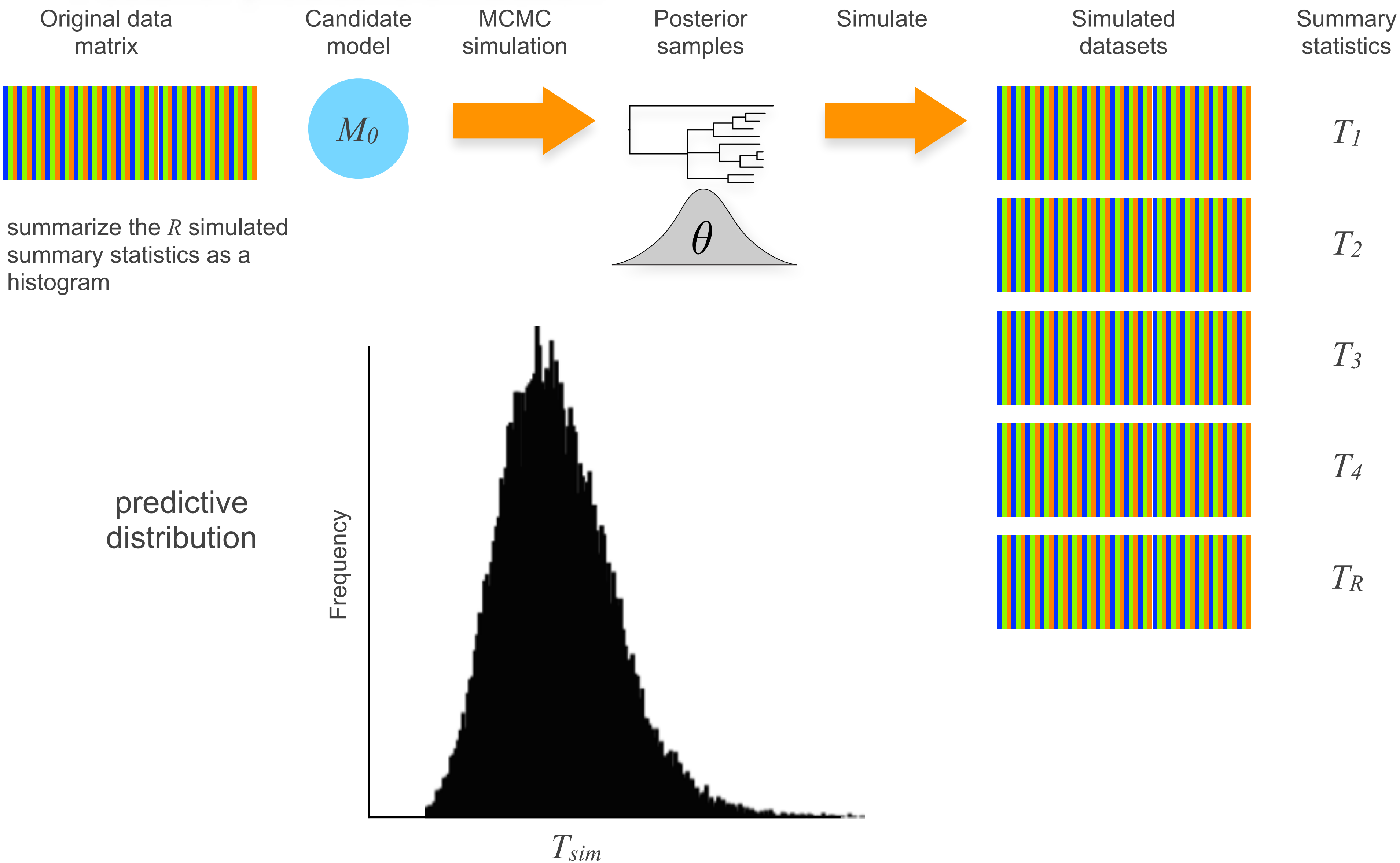

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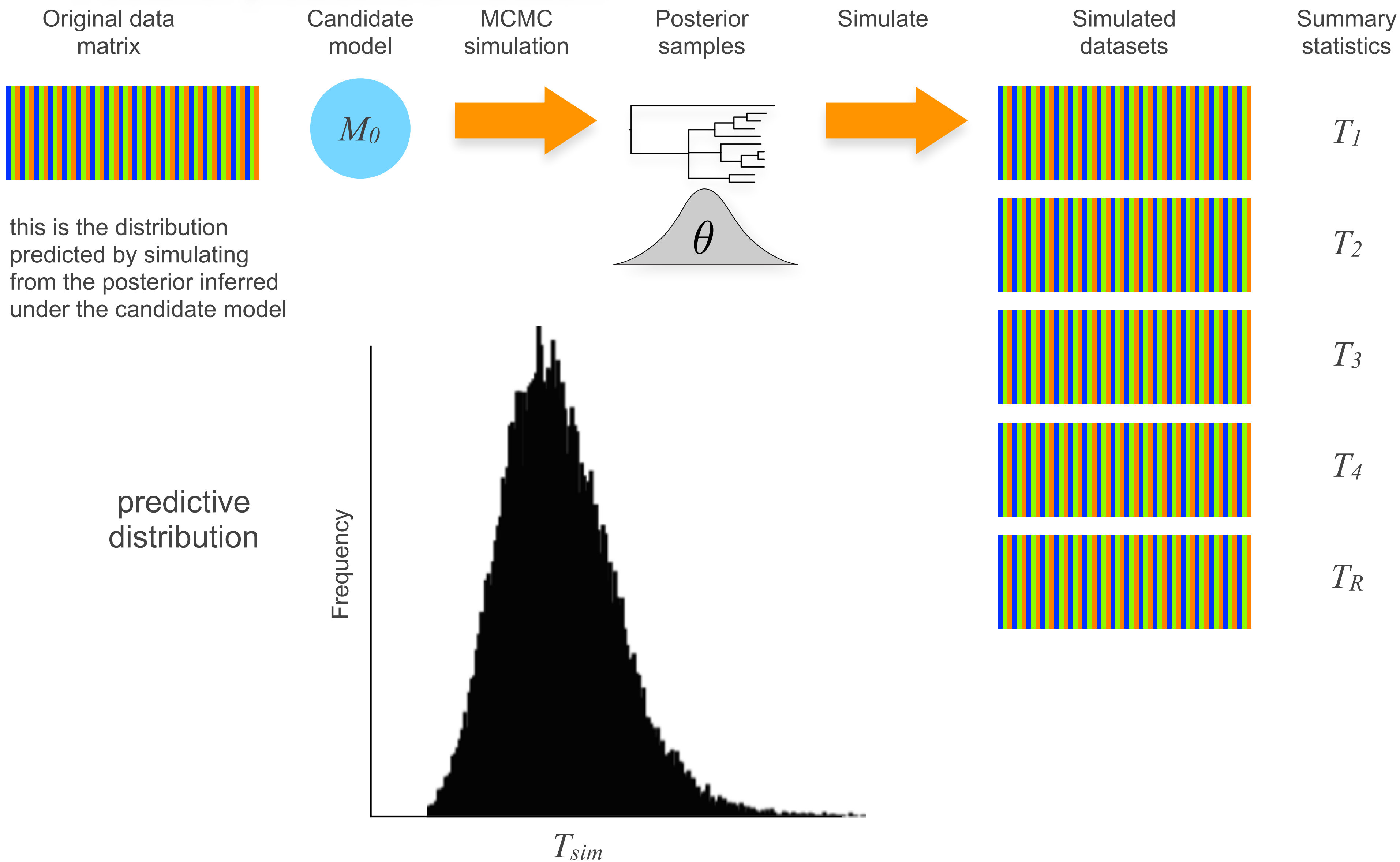

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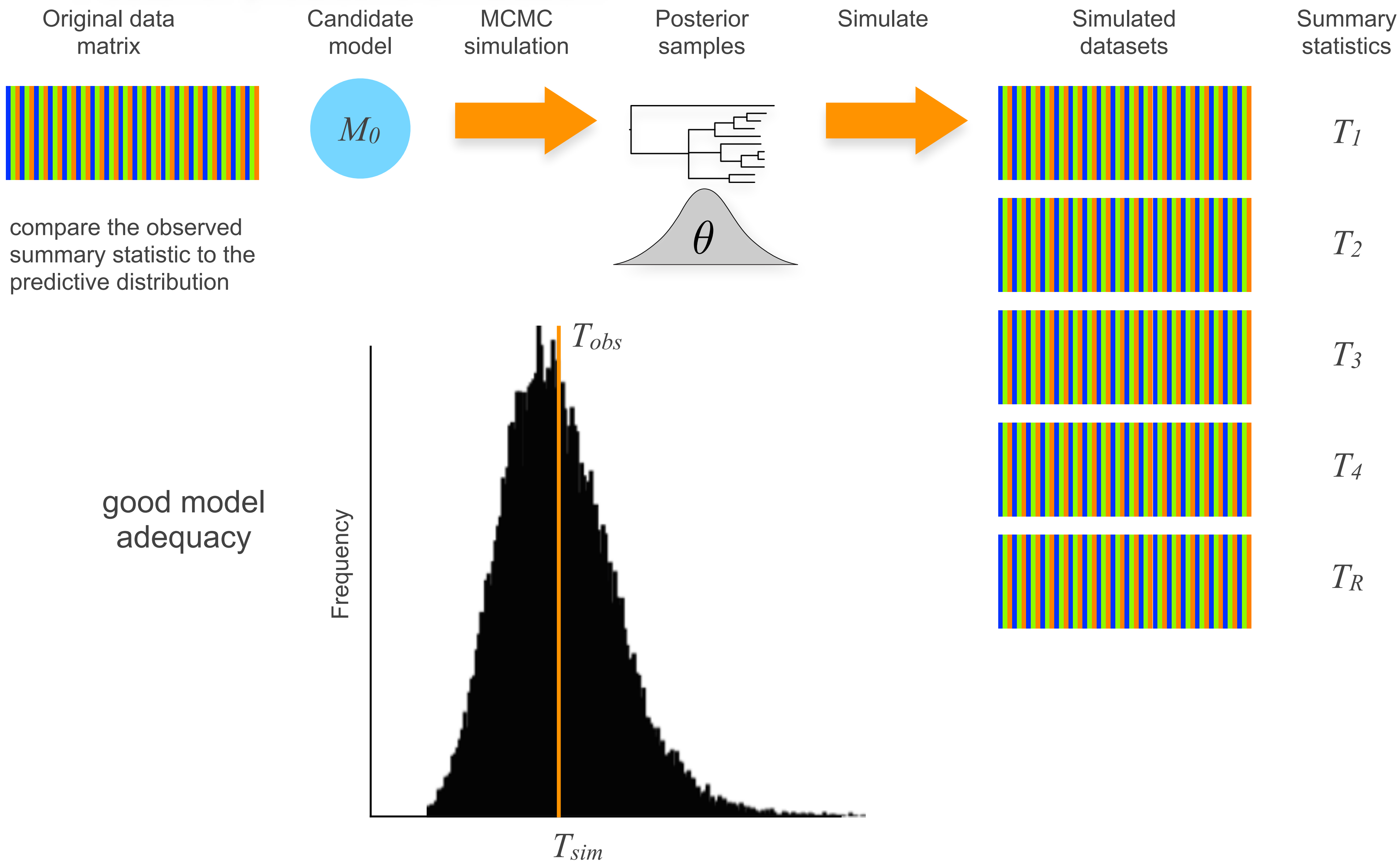

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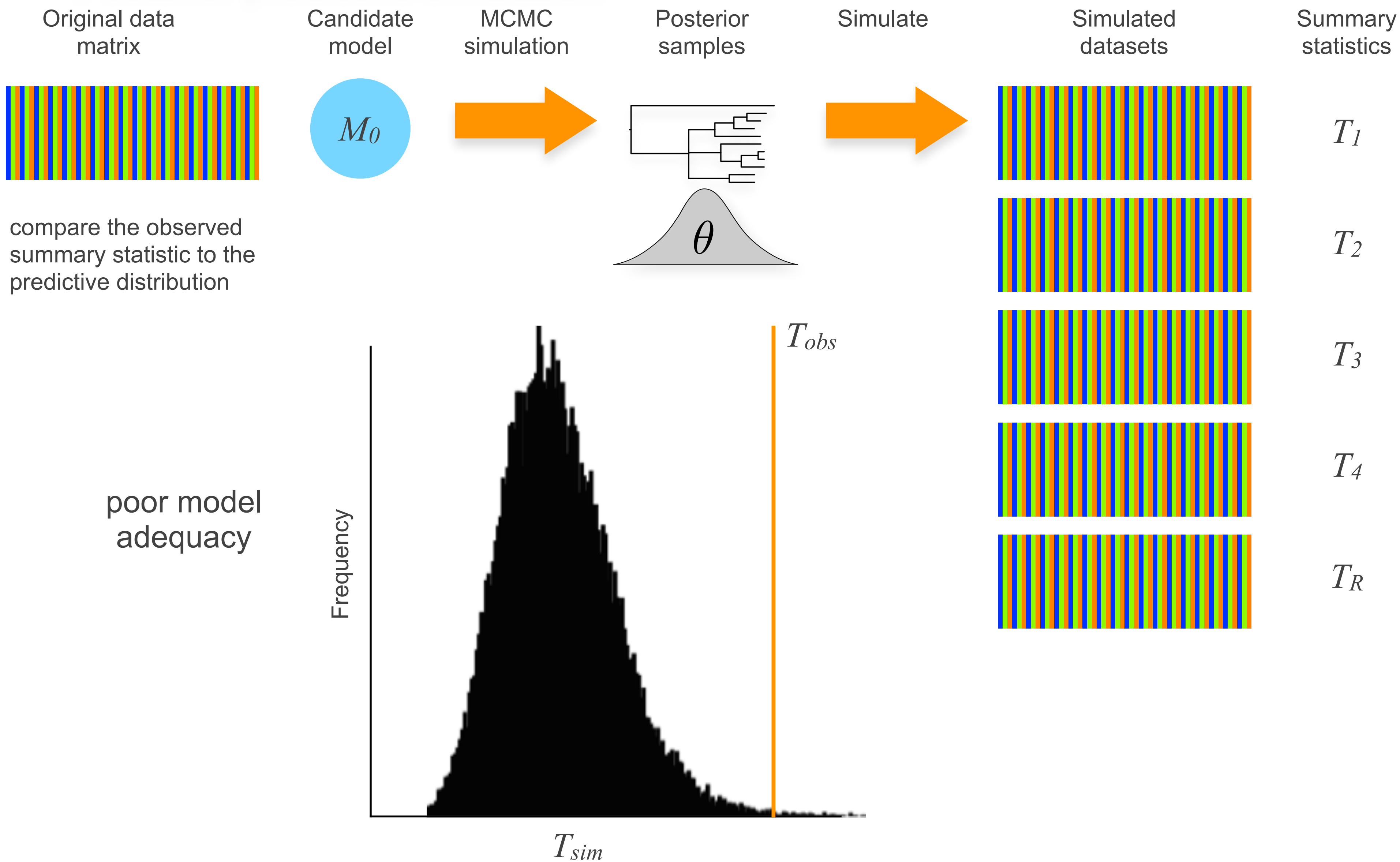

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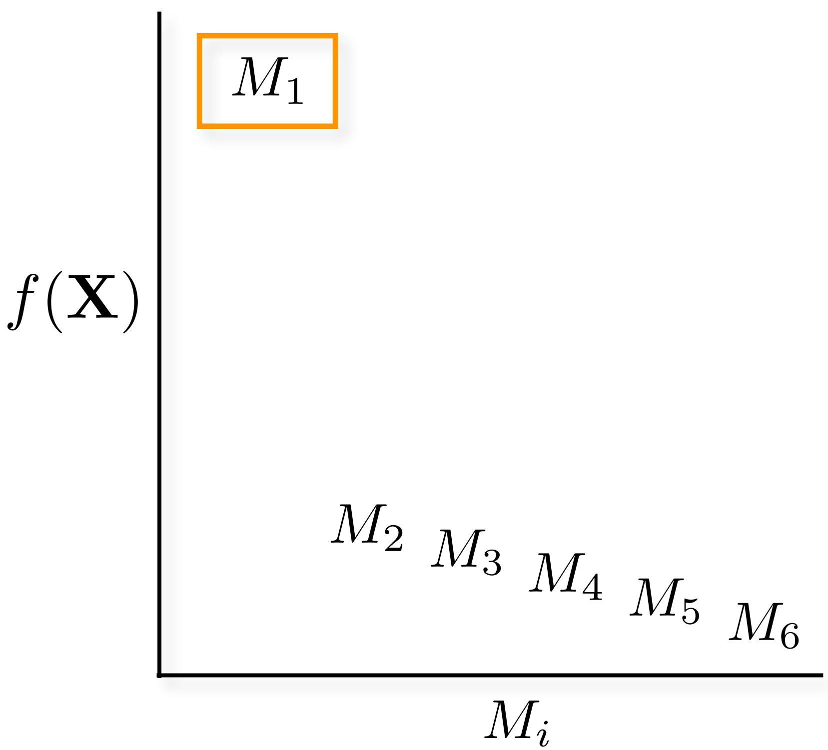

If the fit of the data to the selected mixed model is vastly better than other candidate models, conditioning on the best model may be justified.

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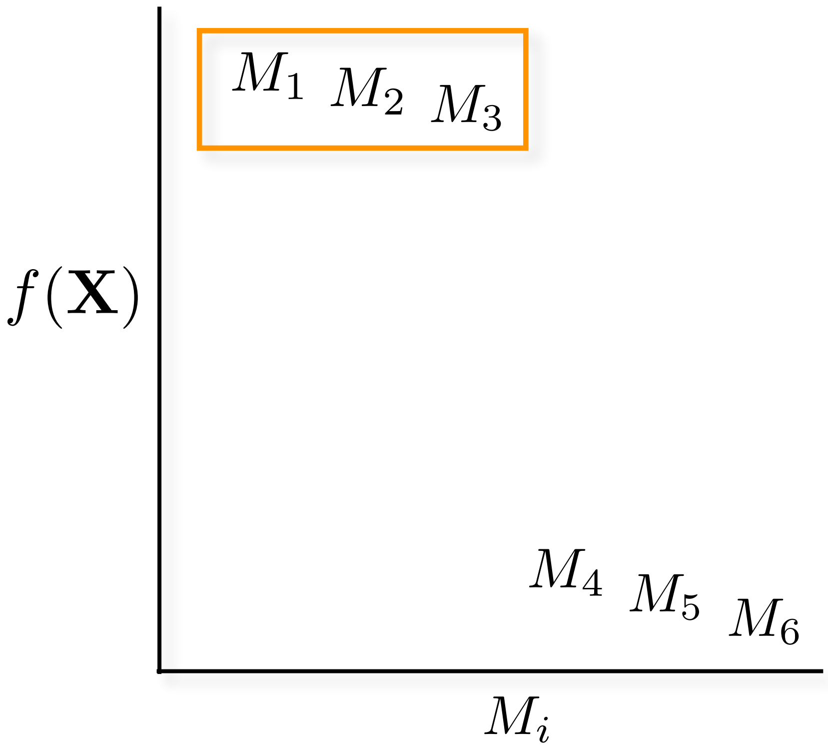

Conversely, if the fit of the data to the selected model is only marginally better than other candidate models, it would be unwise to condition on the best model.

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Bayesian model averaging: reversible-jump MCMC (rjMCMC)

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

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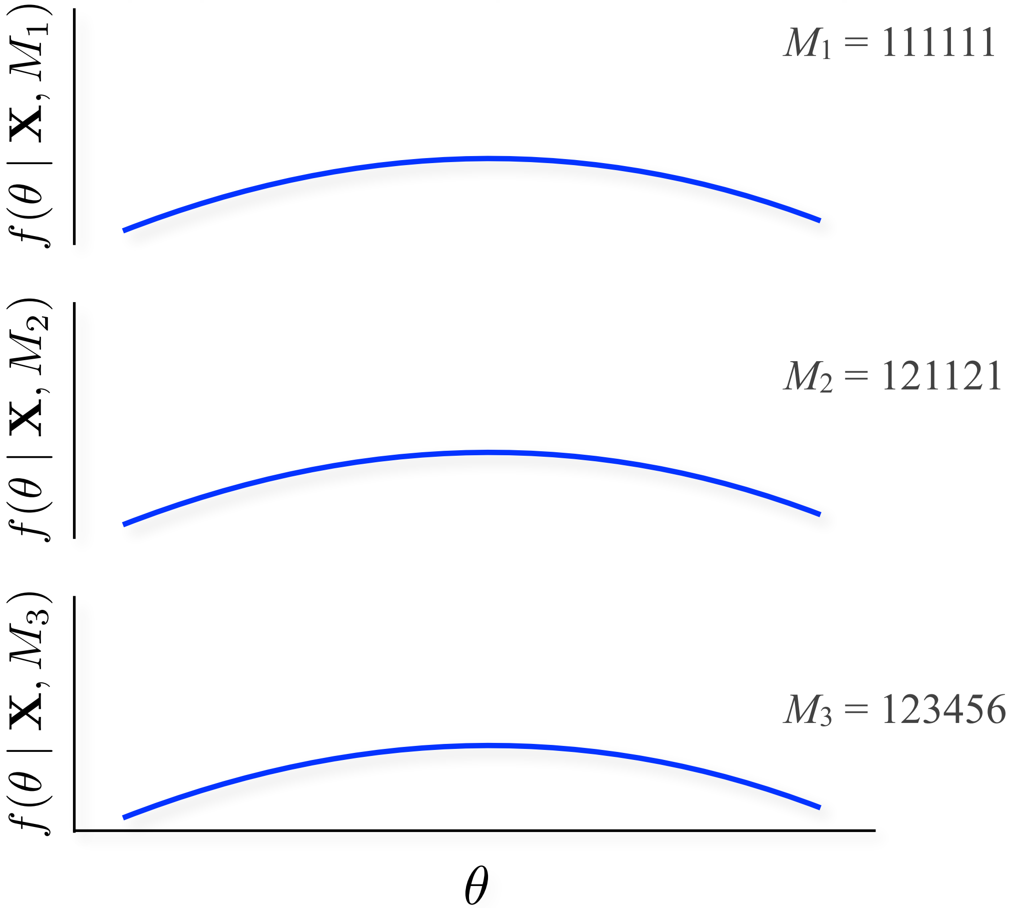

We infer the joint posterior probability distribution by averaging over a set of models, M_i.

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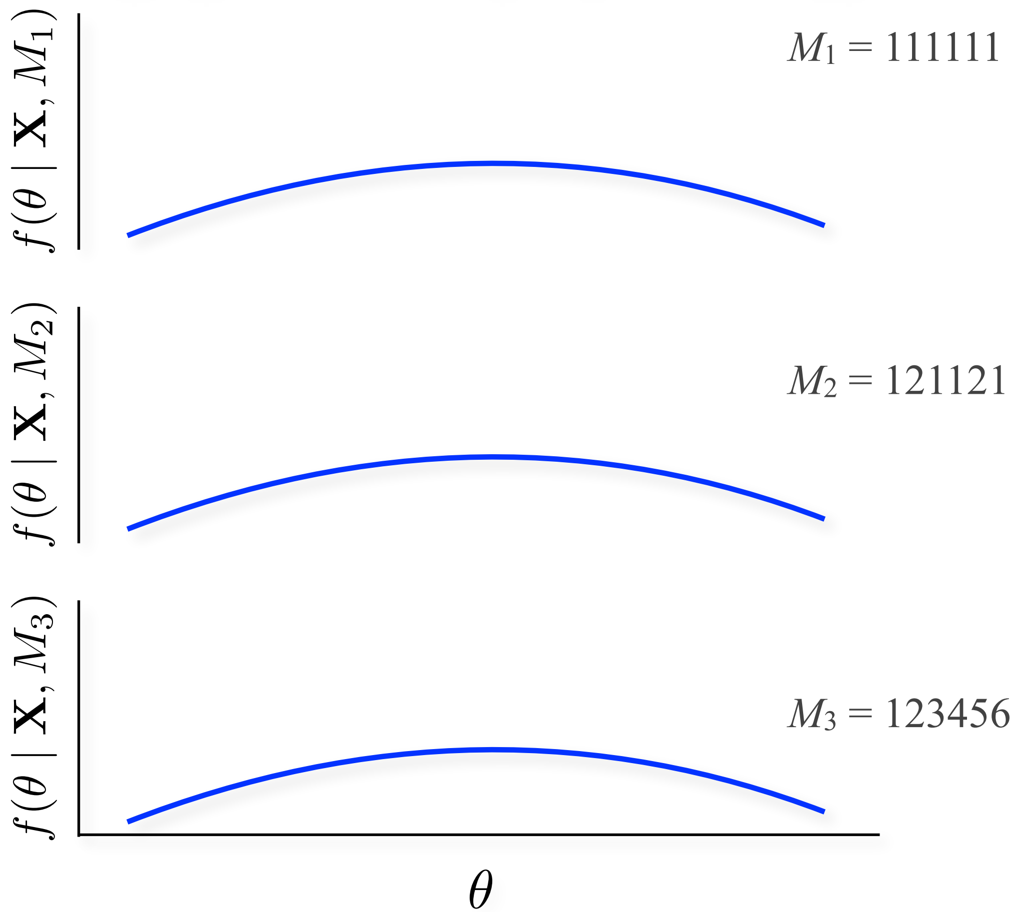

Like other variables, we specify the prior probability distribution for the models.

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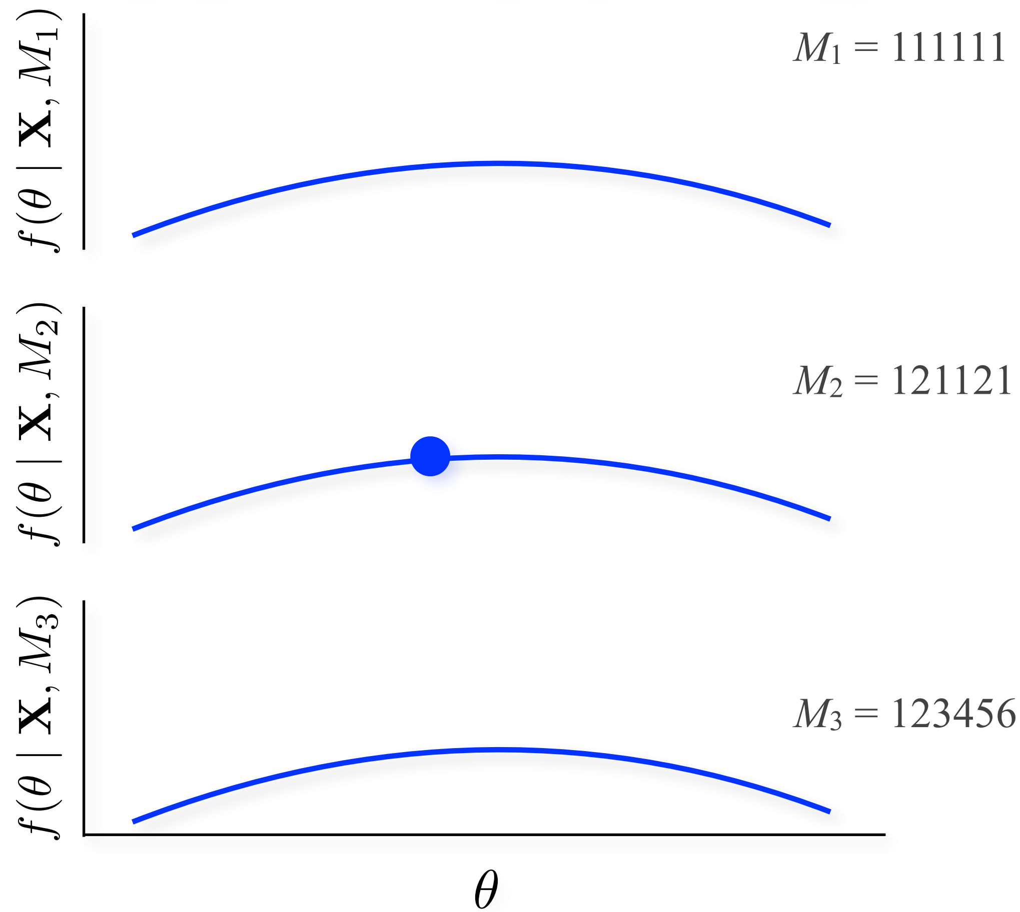

Within a model, we sample parameter values in the normal way.

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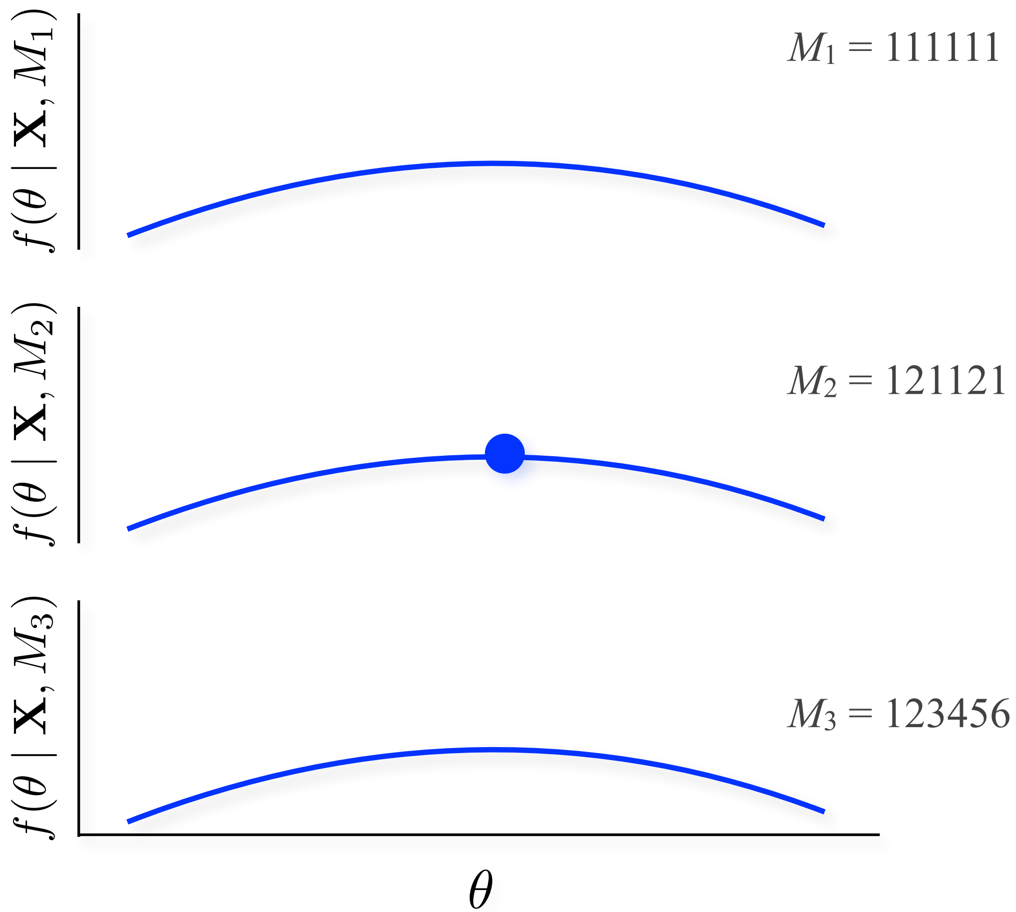

Within a model, we sample parameter values in the normal way.

Bayesian Model Selection

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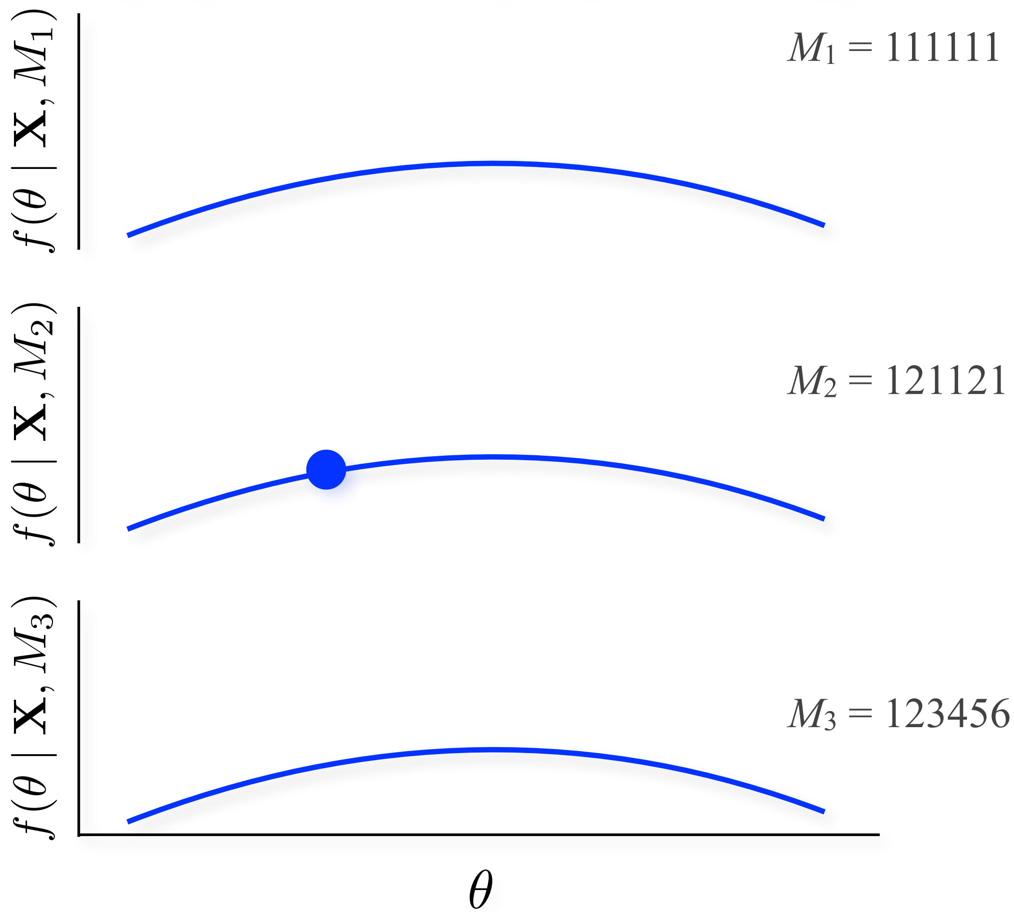

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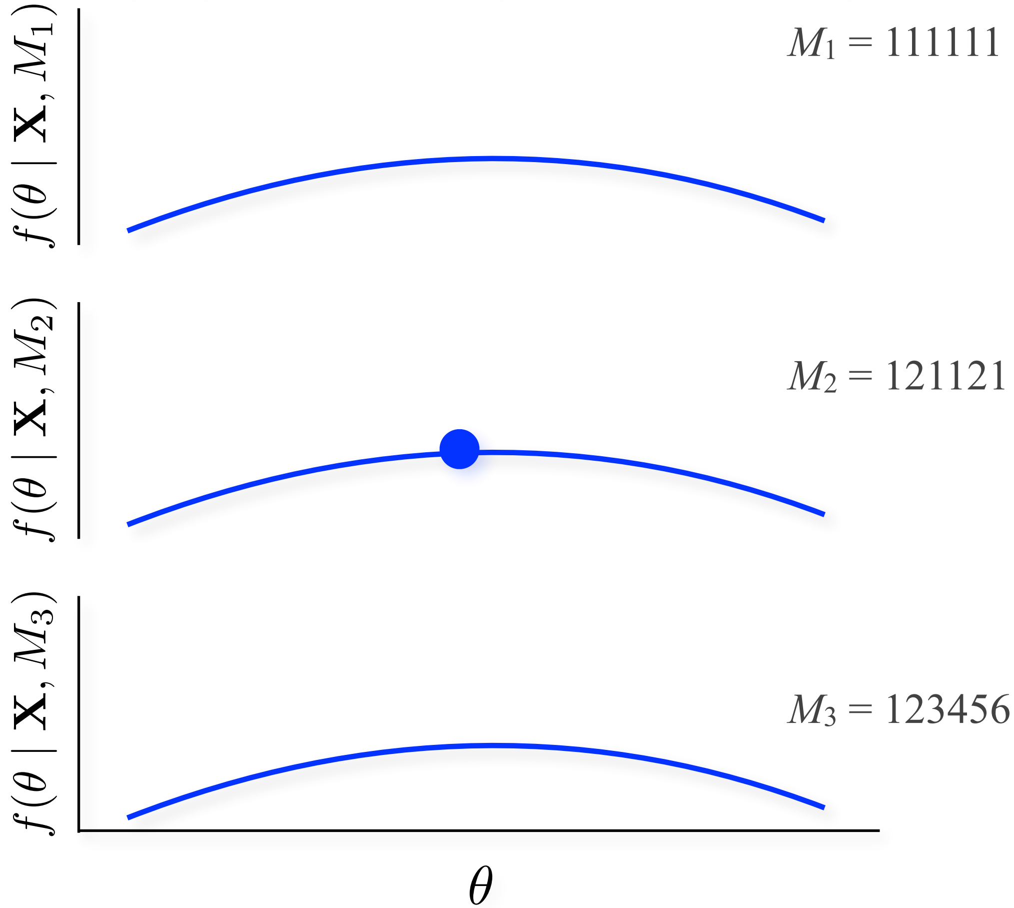

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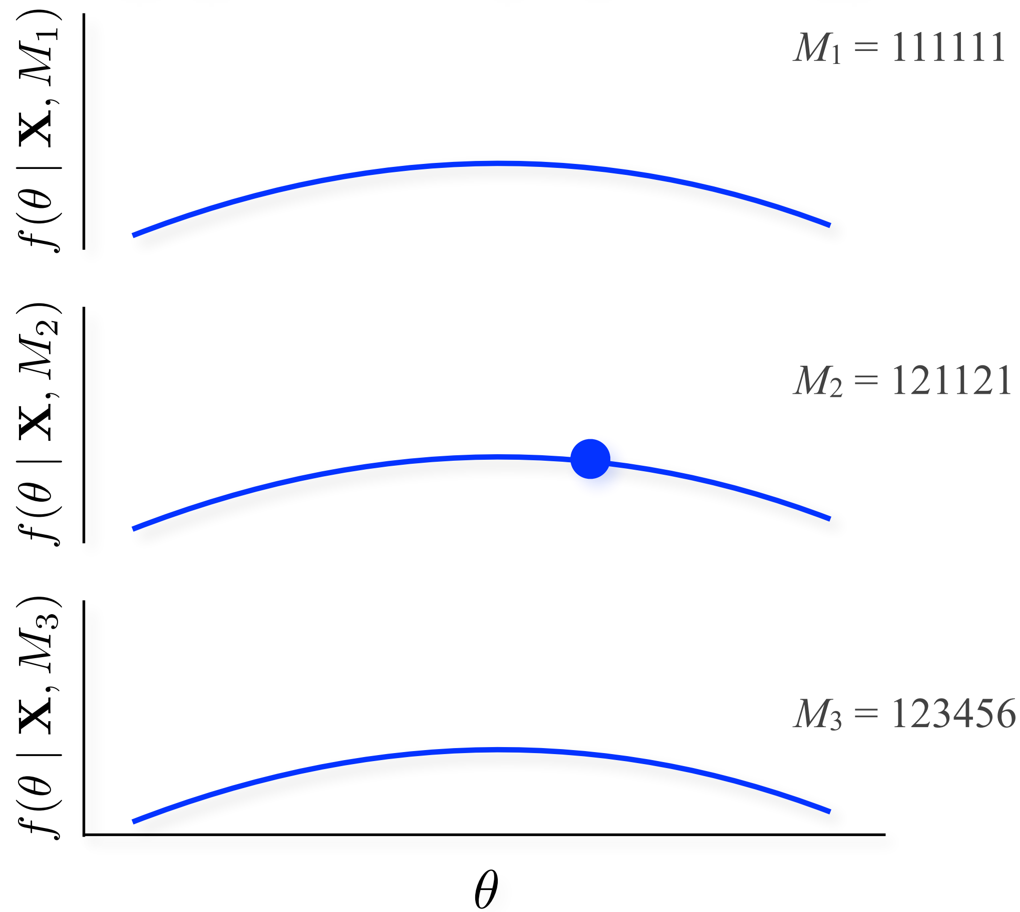

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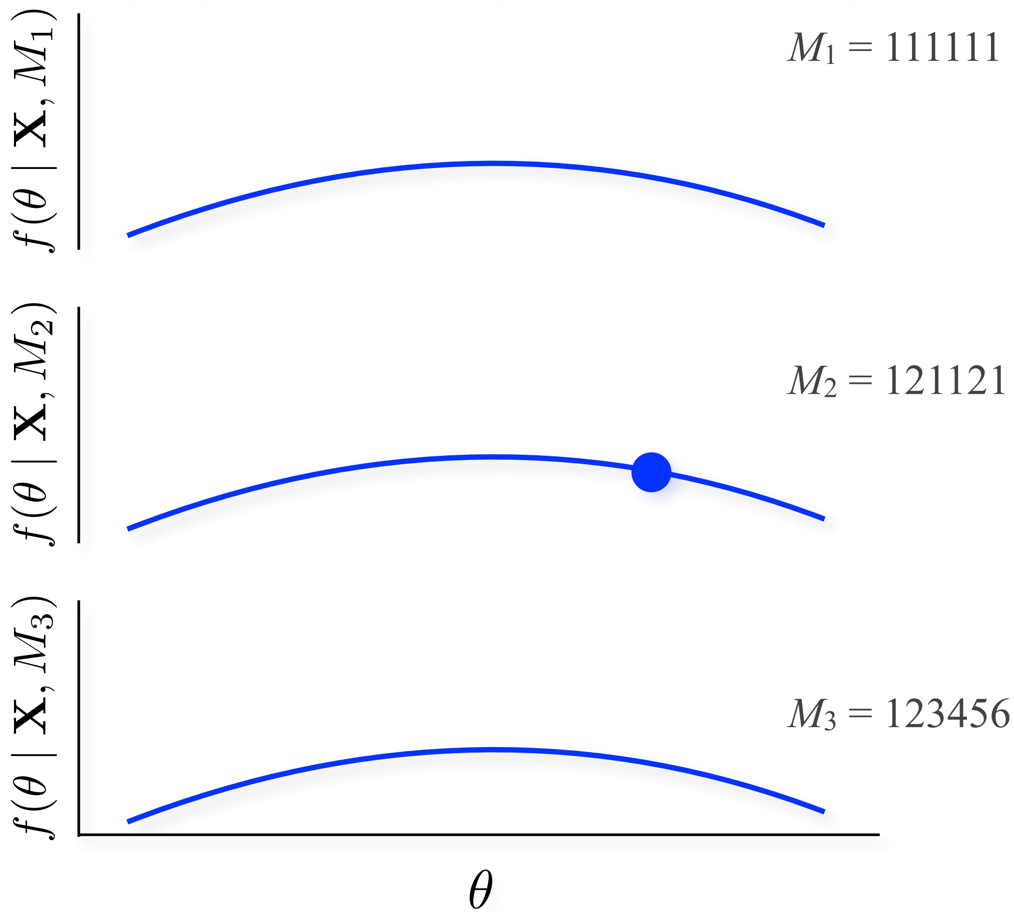

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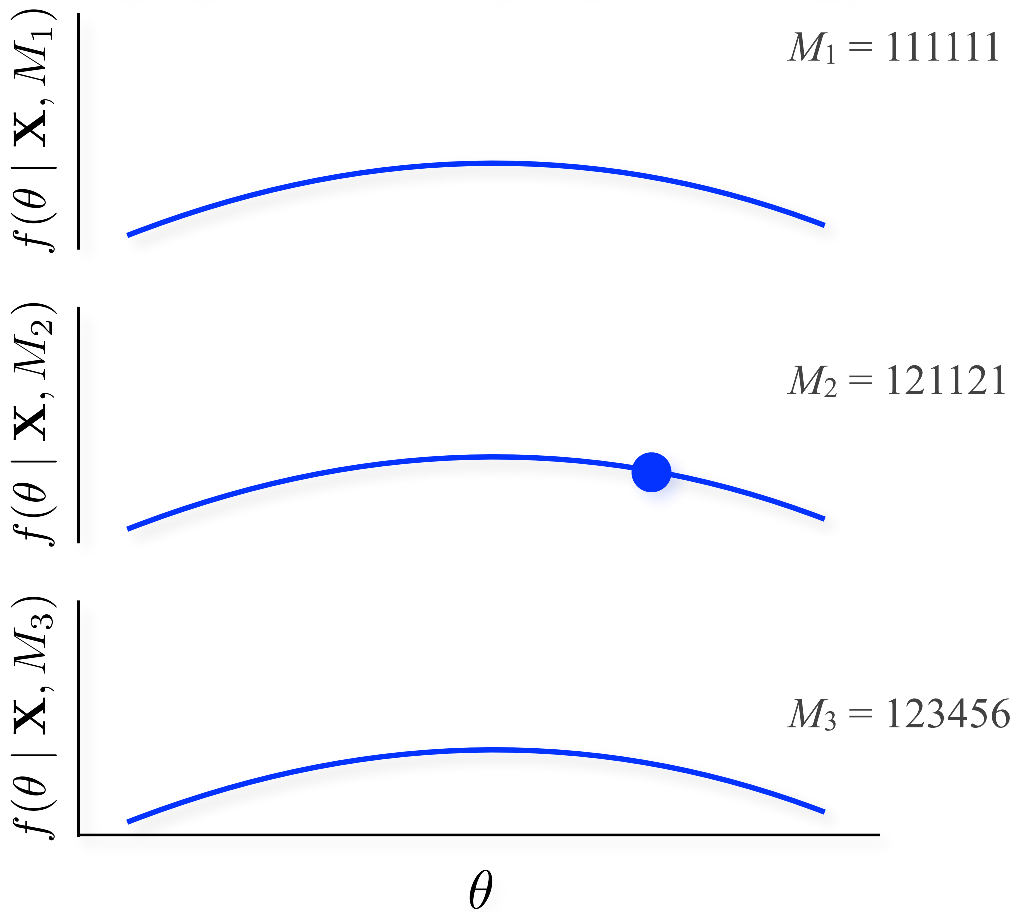

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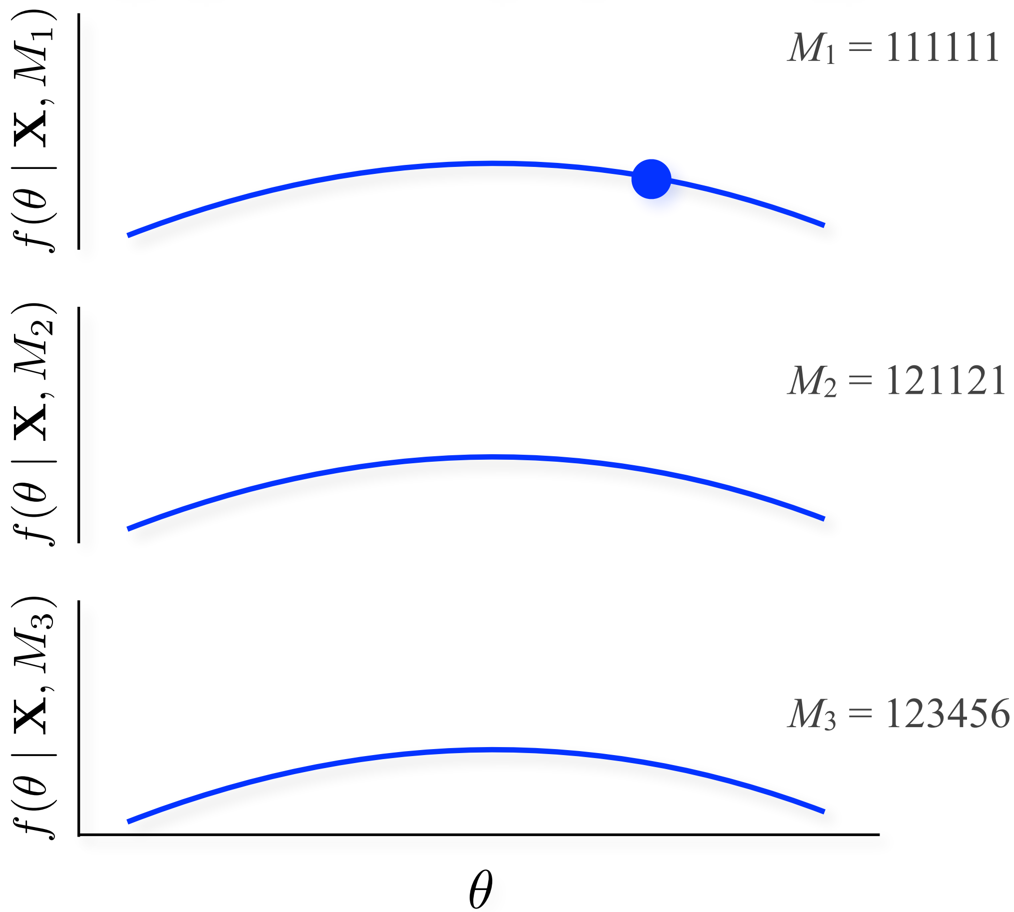

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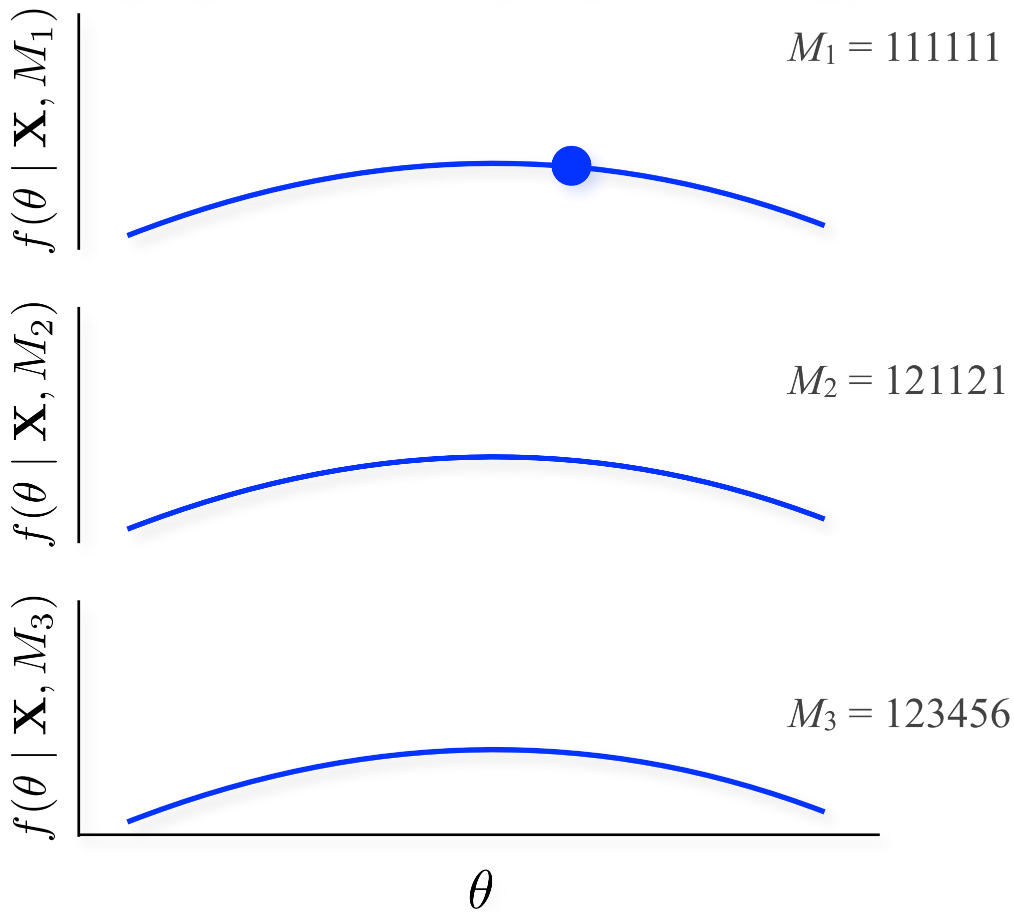

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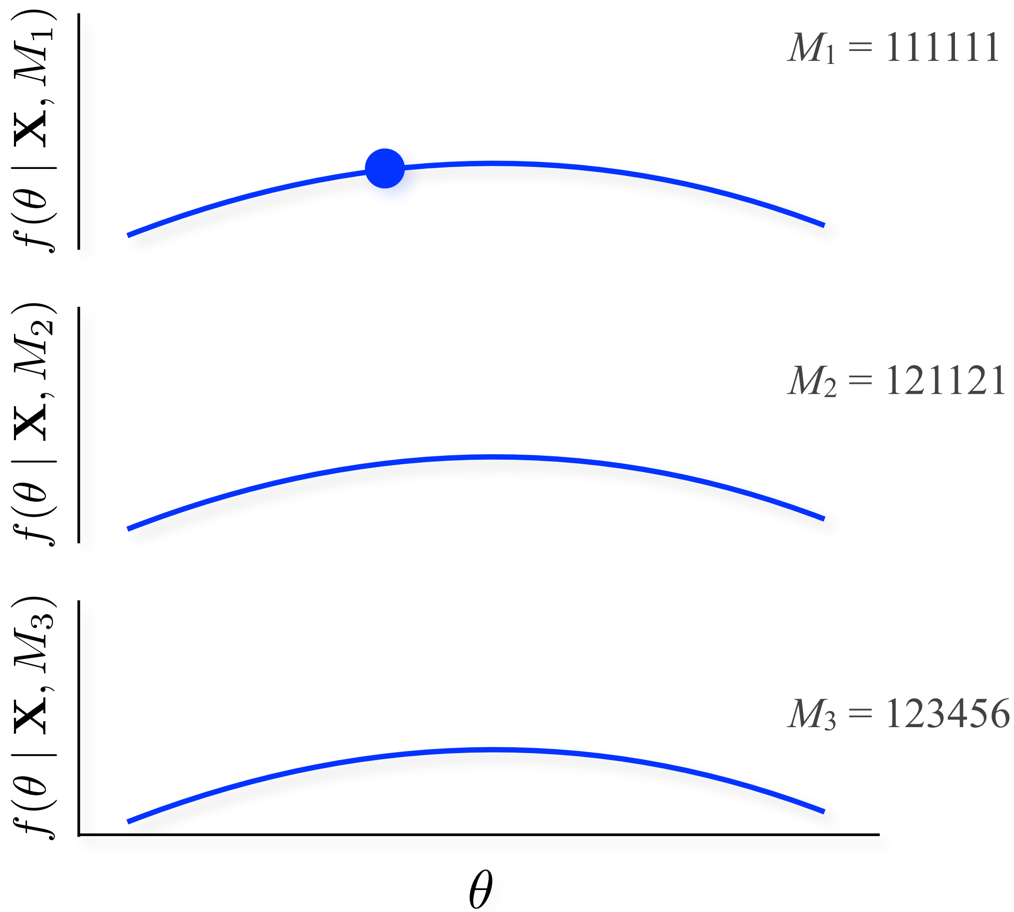

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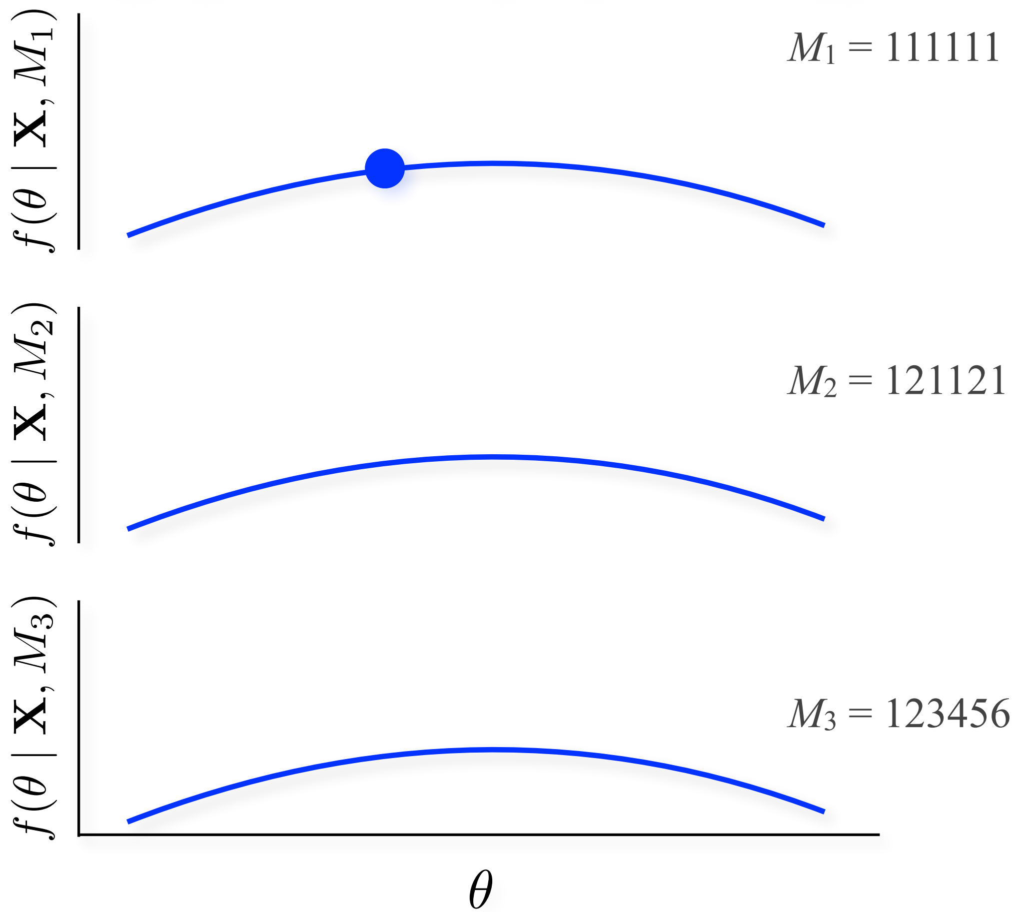

Parameter estimates for all parameters are therefore averaged over all models.

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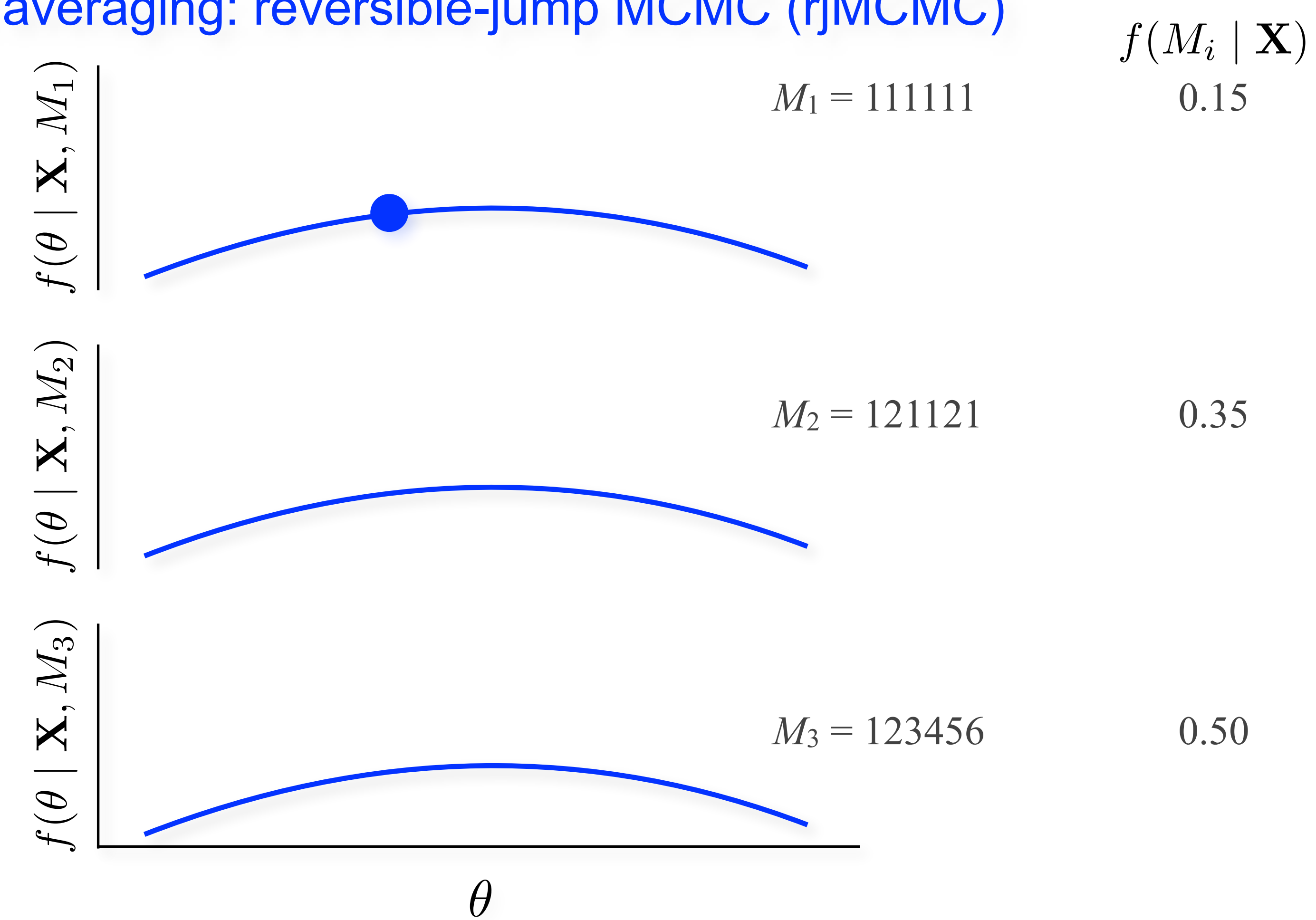

The proportion of time the jMCMC spends visiting each model is an estimate of its marginal posterior probability.

Bayesian Model Selection

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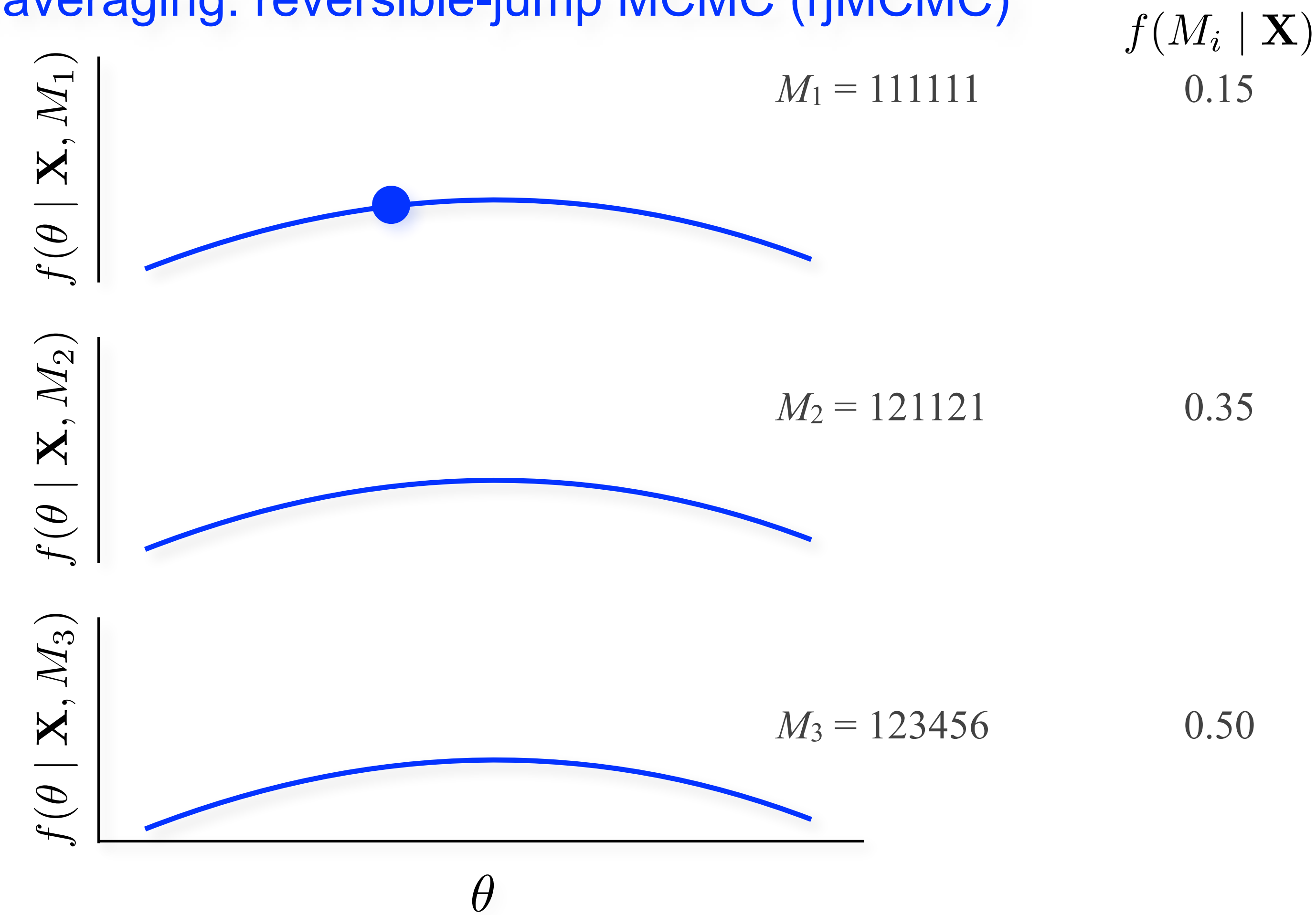

The proportion of time the jMCMC spends visiting each model is an estimate of its marginal posterior probability, so we get model selection for free!

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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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