Markov chain Monte Carlo I

Models for Socio-Environmental Data

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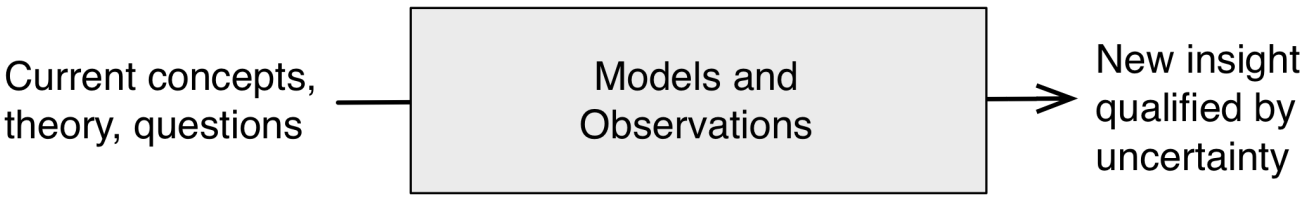
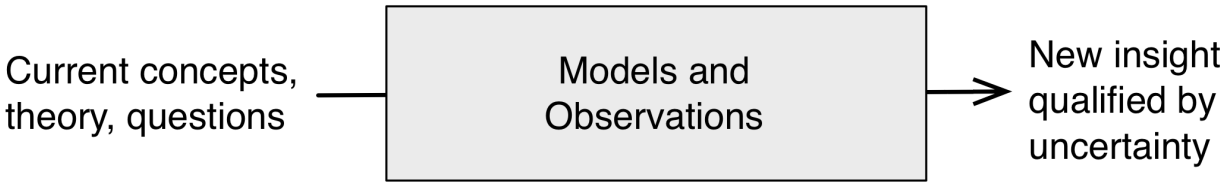
May 27, 2019

What is this course about?

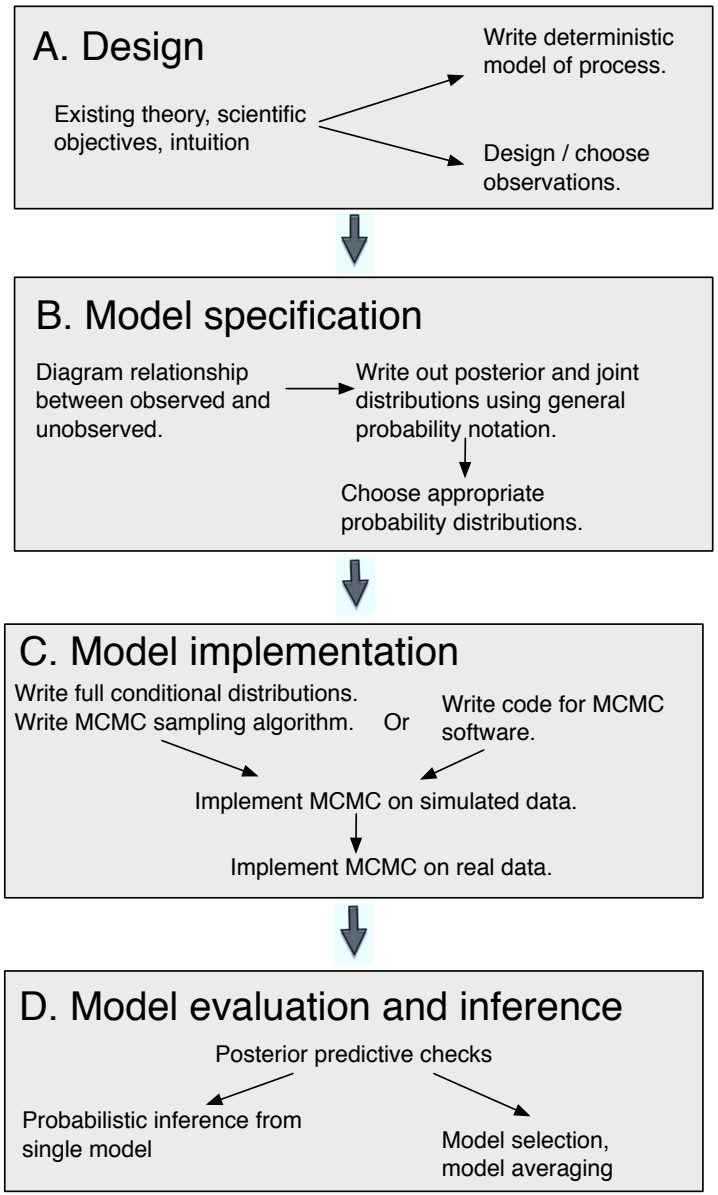


You can understand it.

- Rules of probability
  - Conditioning and independence
    - Law of total probability
    - Factoring joint probabilities
- Distribution theory
- Markov chain Monte Carlo



The Bayesian method



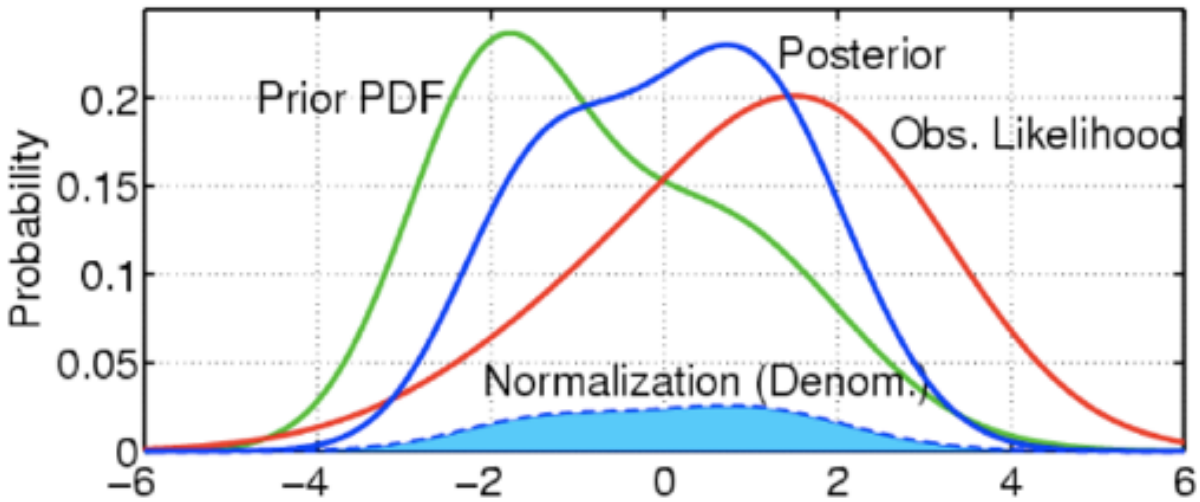
The MCMC algorithm

- Why MCMC?
- Some intuition about how it works for a single parameter model
- MCMC for multiple parameter models
  - Full-conditional distributions (today)
  - Gibbs sampling (today)
  - Metropolis-Hastings algorithm (optional lecture notes and reading)
  - MCMC software (JAGS, tomorrow)

MCMC learning outcomes

1. Develop a big picture understanding of how MCMC allows us to approximate the marginal posterior distributions of parameters and latent quantities.
2. Understand and be able to code a simple MCMC algorithm.
3. Appreciate the different methods that can be used within MCMC algorithms to make draws from the posterior distribution.
   - 3.1 Metropolis
   - 3.2 Metropolis-Hastings
   - 3.3 Gibbs
4. Understand concepts of burn-in and convergence.
5. Understand and be able to write full-conditional distributions.

Remember the marginal distribution of the data



We have simple solutions for the posterior for simple models:

$$[\phi|y] = \text{beta}\left(\underbrace{\overbrace{\alpha}^{\text{The prior } \alpha} + y}_{\text{The new } \alpha}, \underbrace{\overbrace{\beta}^{\text{The prior} \beta} + n - y}_{\text{The new } \beta}\right)$$

Problems of high dimension do not have simple solutions:

$$[\theta_1, \theta_{2,} \theta_3, \theta_4, \mathbf{z} \mid \mathbf{y}, \mathbf{u}] =$$

$$\frac{\prod_{i=1}^{n} [y_i|\theta_1 z_i][u_i|\theta_2, z_i][z_i|\theta_3, \theta_4][\theta_1][\theta_2][\theta_3][\theta_4]}{\int .... \int \prod_{i=1}^{n} [y_i|\theta_1 z_i][u_i|\theta_2, z_i][z_i|\theta_3, \theta_4][\theta_1][\theta_2][\theta_3][\theta_4] dz_i \, d\theta_1 \, d\theta_2 \, d\theta_3 \, d\theta_4}$$

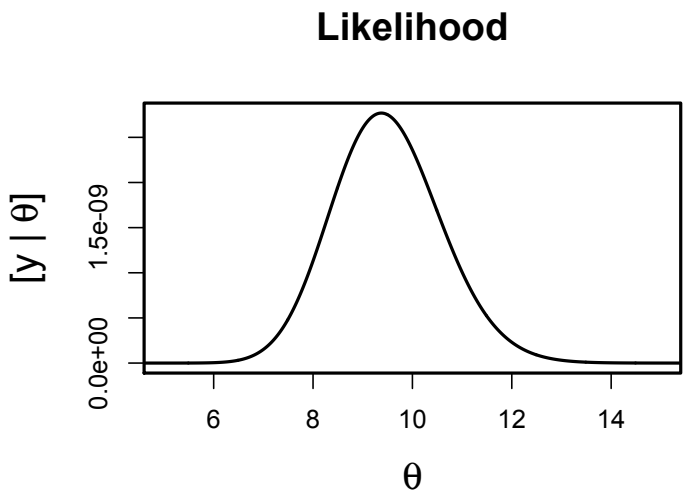
What we are doing in MCMC?

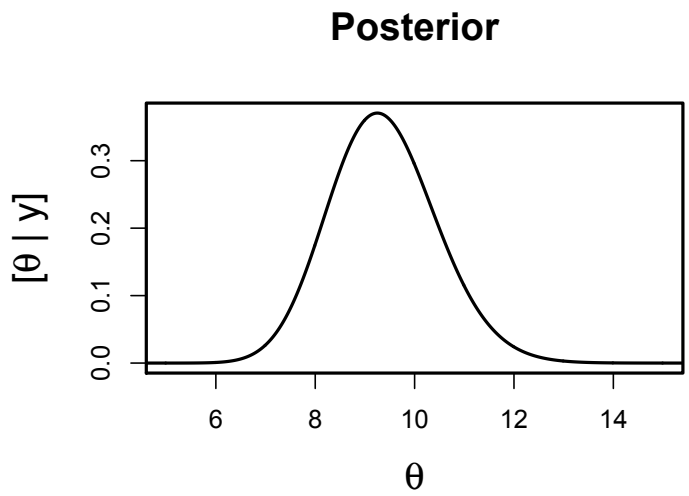
Recall that the posterior distribution is proportional to the joint:

$$[\theta|y] \propto [y|\theta][\theta], \tag{1}$$

because the marginal distribution of the data $\int [y|\theta][\theta] d\theta$ is a constant after the data have been observed.

What we are doing in MCMC?





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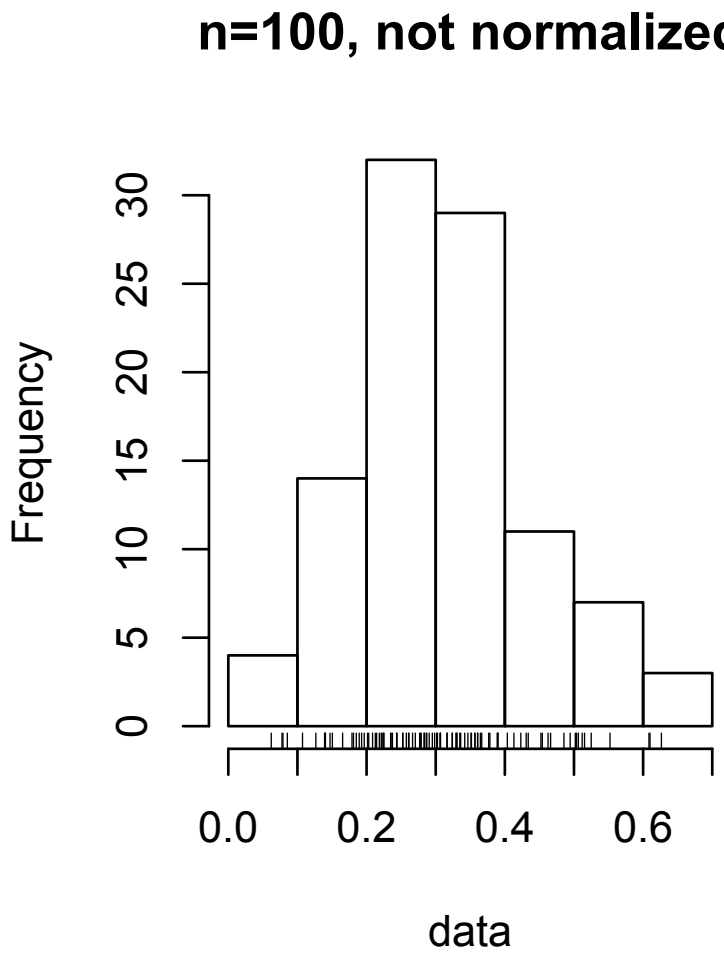
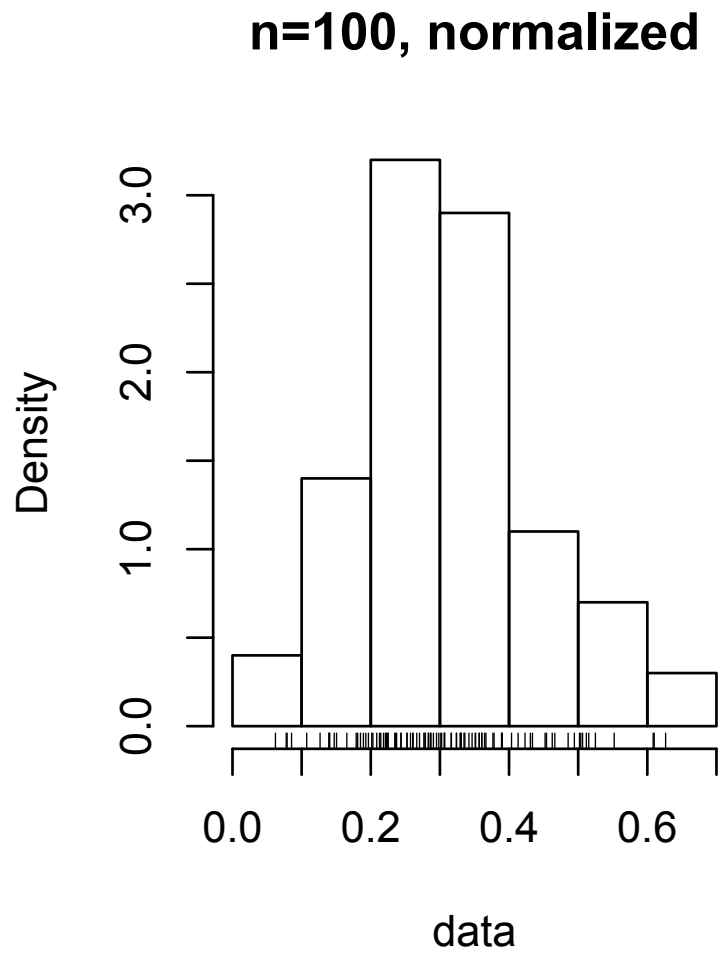


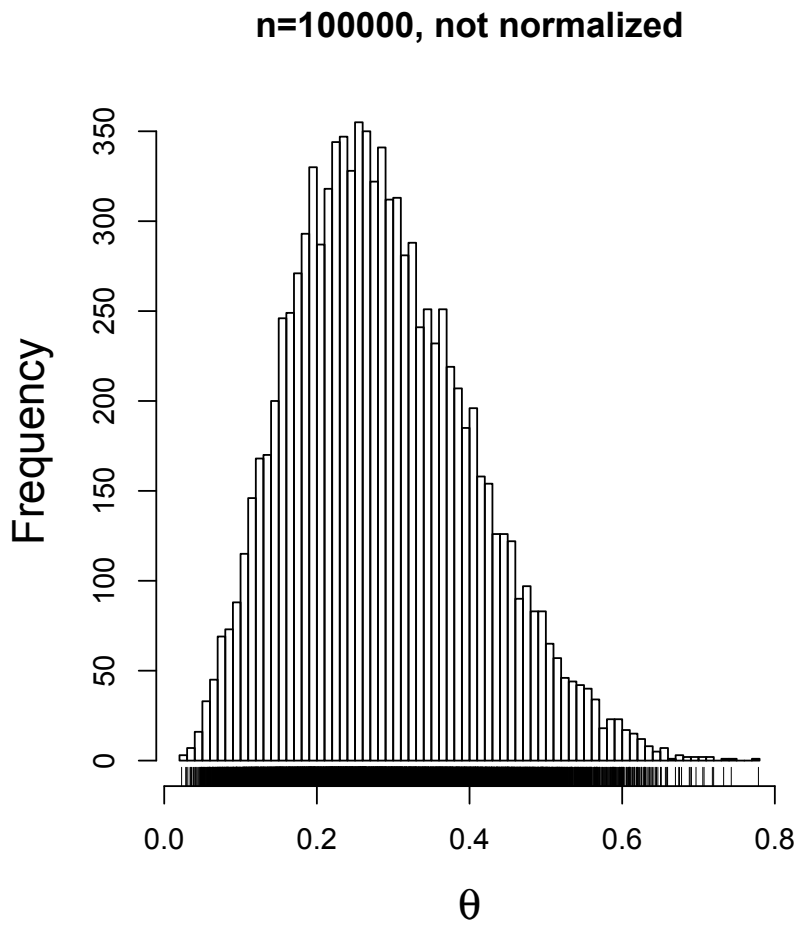


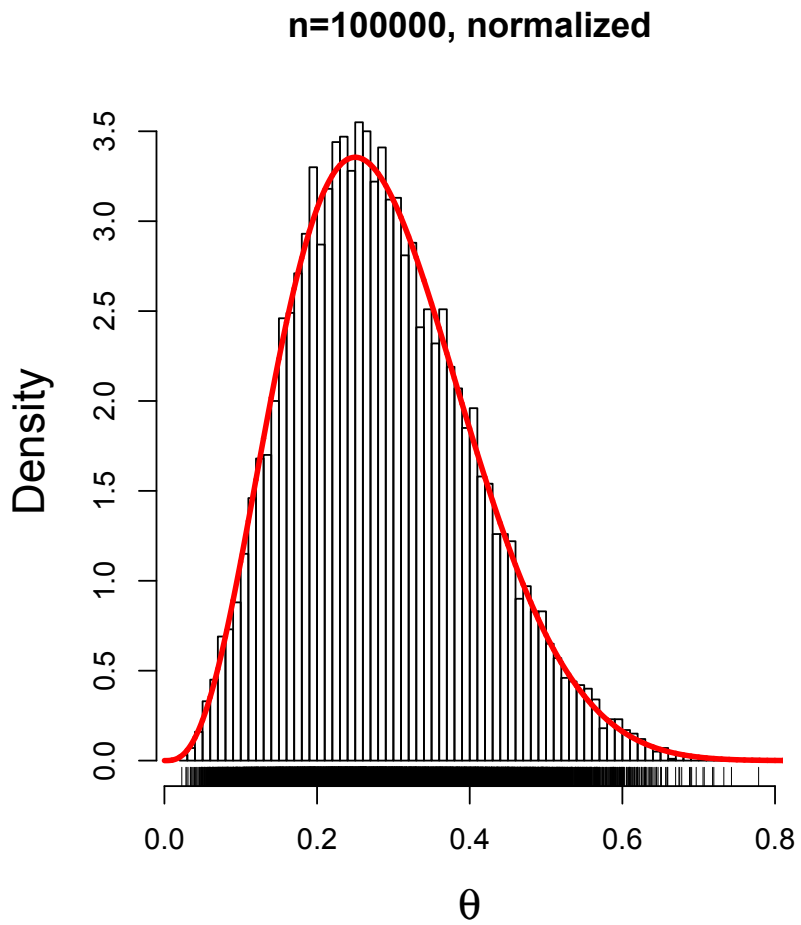
What are we doing in MCMC?

- The posterior distribution is unknown, but the likelihood is known as a likelihood profile and we know the priors.
- We want to accumulate many, many values that represent random samples proportionate to their density in the *marginal* posterior distribution.
- MCMC generates these samples using the likelihood and the priors to decide which samples to keep and which to throw away.
- We can then use these samples to calculate statistics describing the distribution: means, medians, variances, credible intervals etc.

What are we doing in MCMC?

The marginal posterior distribution of each unobserved quantity is approximated by samples accumulated in the chain.





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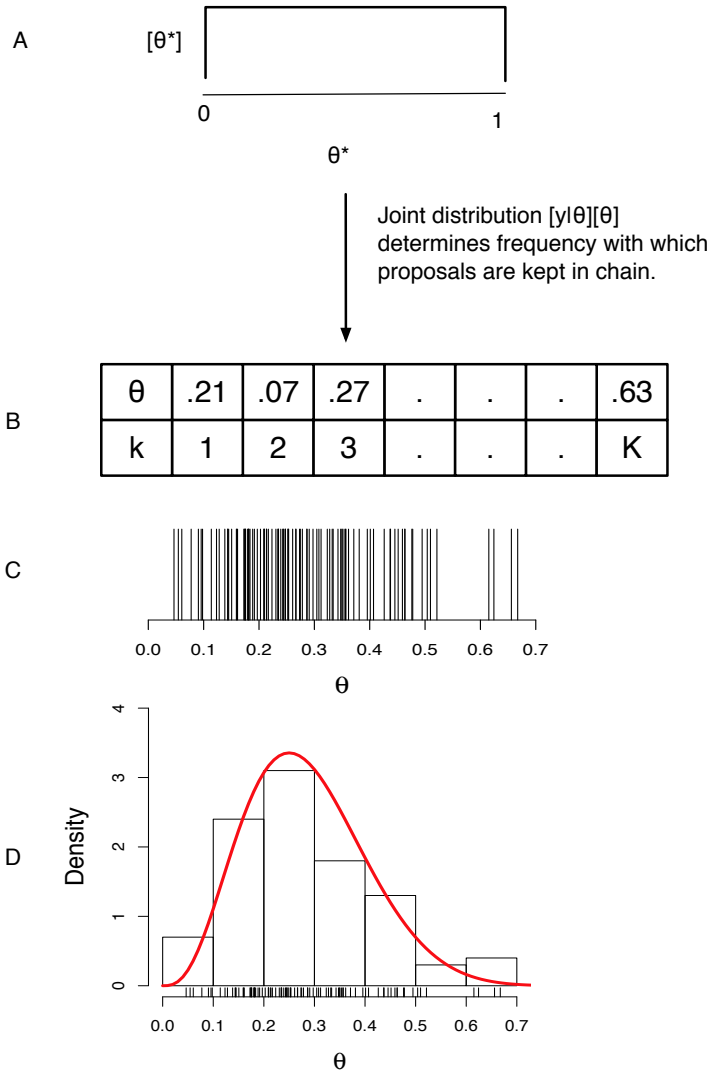


Metropolis updates

We keep the more probable members of the posterior distribution by comparing a proposal with the current value in the chain.

k	1	2
Proposal $\boldsymbol{\theta}^{*k+1}$		$\boldsymbol{\theta}^{*2}$
Test		$P(\boldsymbol{\theta}^{*2}) > P\left(\boldsymbol{\theta}^{1}\right)$
Chain$(\boldsymbol{\theta}^{k})$	$\boldsymbol{\theta}^{1}$	$\boldsymbol{\theta}^{2} = \boldsymbol{\theta}^{*2}$

Metropolis updates

We keep the more probable members of the posterior distribution by comparing a proposal with the current value in the chain.

k	1	2	3
Proposal $\boldsymbol{\theta}^{*k+1}$		$\boldsymbol{\theta}^{*2}$	$\boldsymbol{\theta}^{*3}$
Test		$P(\boldsymbol{\theta}^{*2}) > P\left(\boldsymbol{\theta}^{1}\right)$	$P(\boldsymbol{\theta}^{2}) > P\left(\boldsymbol{\theta}^{*3}\right)$
Chain$(\boldsymbol{\theta}^{k})$	$\boldsymbol{\theta}^{1}$	$\boldsymbol{\theta}^{2} = \boldsymbol{\theta}^{*2}$	$\boldsymbol{\theta}^{3} = \boldsymbol{\theta}^{2}$

Metropolis updates

We keep the more probable members of the posterior distribution by comparing a proposal with the current value in the chain.

k	1	2	3	4				K
Proposal θ^{*k+1}		θ^{*2}	θ^{*3}	θ^{*4}	.	.	.	.
Test		$P(\theta^{*2}) > P(\theta^1)$	$P(\theta^2) > P(\theta^{*3})$	$P(\theta^3) > P(\theta^{*4})$	.	.	.	.
Chain(θ^k)	θ^1	$\theta^2 = \theta^{*2}$	$\theta^3 = \theta^2$	$\theta_4 = \theta_3$				

Metropolis updates

$$[\theta^{*k+1}|y] = \frac{\overbrace{[y|\theta^{*k+1}]}^{\text{likelihood}}\overbrace{[\theta^{*k+1}]}^{\text{prior}}}{\int [y|\theta][\theta]d\theta}$$

$$[\theta^{k}|y] = \frac{\overbrace{[y|\theta^{k}]}^{\text{likelihood}}\overbrace{[\theta^{k}]}^{\text{prior}}}{\int [y|\theta][\theta]d\theta}$$

$$R = \frac{[\theta^{*k+1}|y]}{[\theta^{k}|y]}$$

The cunning idea behind Metropolis updates

$$[\theta^{*k+1}|y] = \frac{\overbrace{[y|\theta^{*k+1}]}^{\text{likelihood}}\overbrace{[\theta^{*k+1}]}^{\text{prior}}}{\cancel{\int [y|\theta][\theta]d\theta}}$$

$$[\theta^{k}|y] = \frac{\overbrace{[y|\theta^{k}]}^{\text{likelihood}}\overbrace{[\theta^{k}]}^{\text{prior}}}{\cancel{\int [y|\theta][\theta]d\theta}}$$

$$R = \frac{[\theta^{*k+1}|y]}{[\theta^{k}|y]}$$

When do we keep the proposal?

$$P_R = \min(1, R)$$

Keep θ^{*k+1} as the next value in the chain with probability P_R and keep θ^k with probability $1 - P_R$.

When do we keep the proposal?

1. Calculate R based on likelihoods and priors.
2. Draw a random number, U from uniform distribution 0,1 If $R > U$, we keep the proposal θ^{*k+1} as the next value in the chain.
3. Otherwise, we retain θ^{k} as the next value.

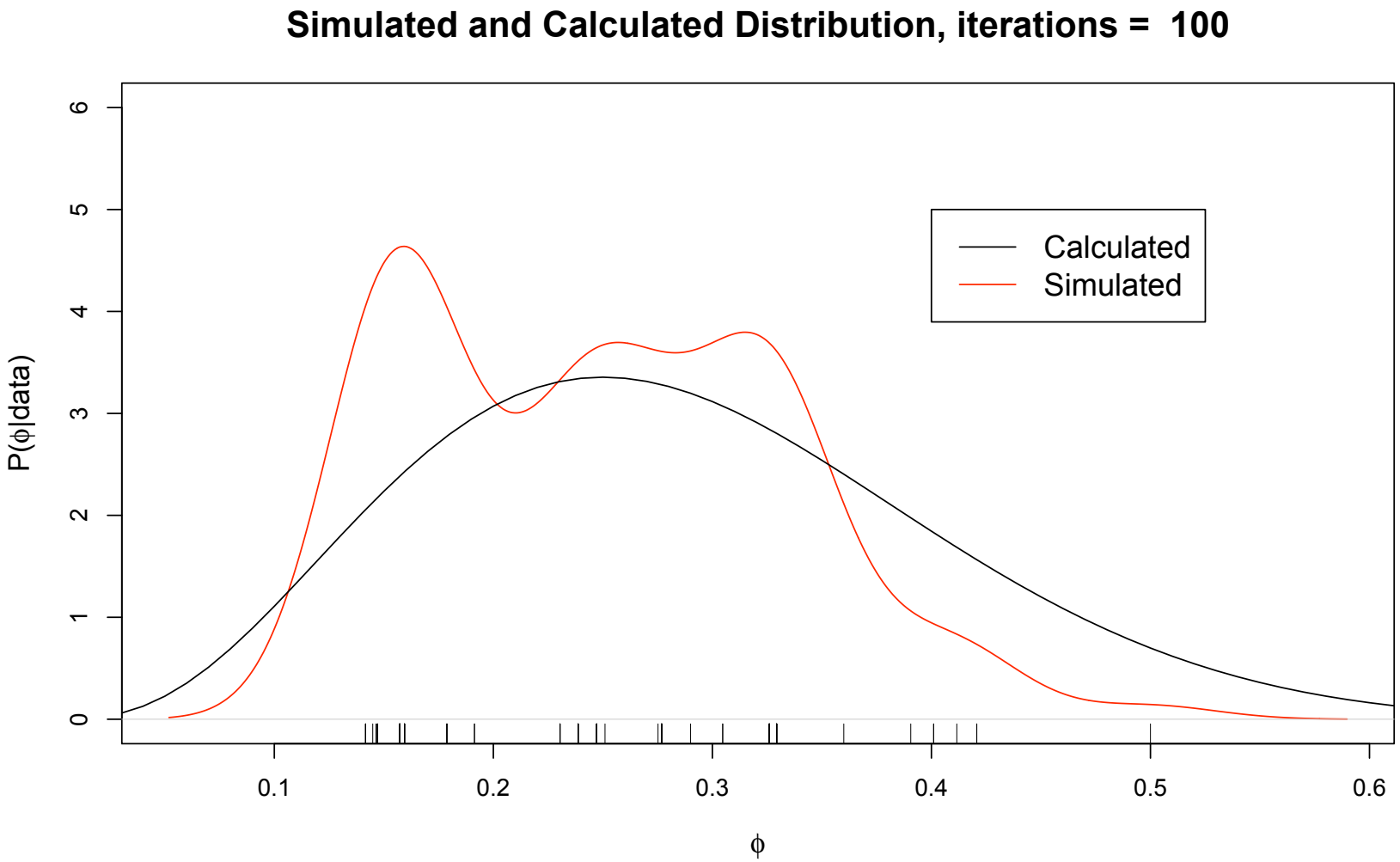
A simple example for one parameter

- Tawni is interested in estimating the prevalence of bacterial kidney disease in a population of trout in Colorado.
- She is a bit lazy, so she only samples 12 fish, 3 of which have the disease.
- How could she calculate the parameters of the posterior distribution of prevalence on the back of a cocktail napkin?

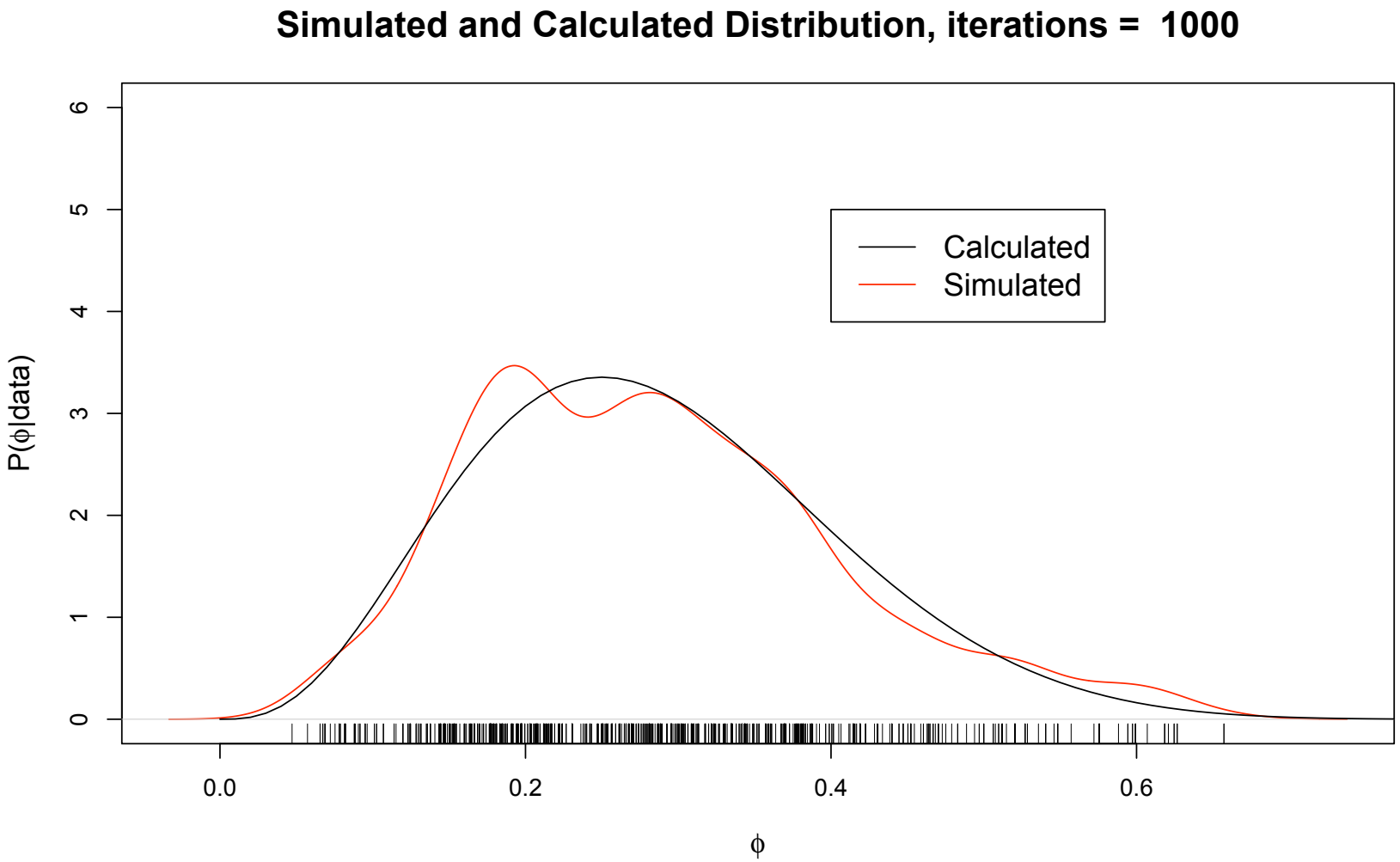
The model

$$[\phi|y] \propto \text{binomial}(y|n,\phi)\text{beta}(\phi|1,1)$$

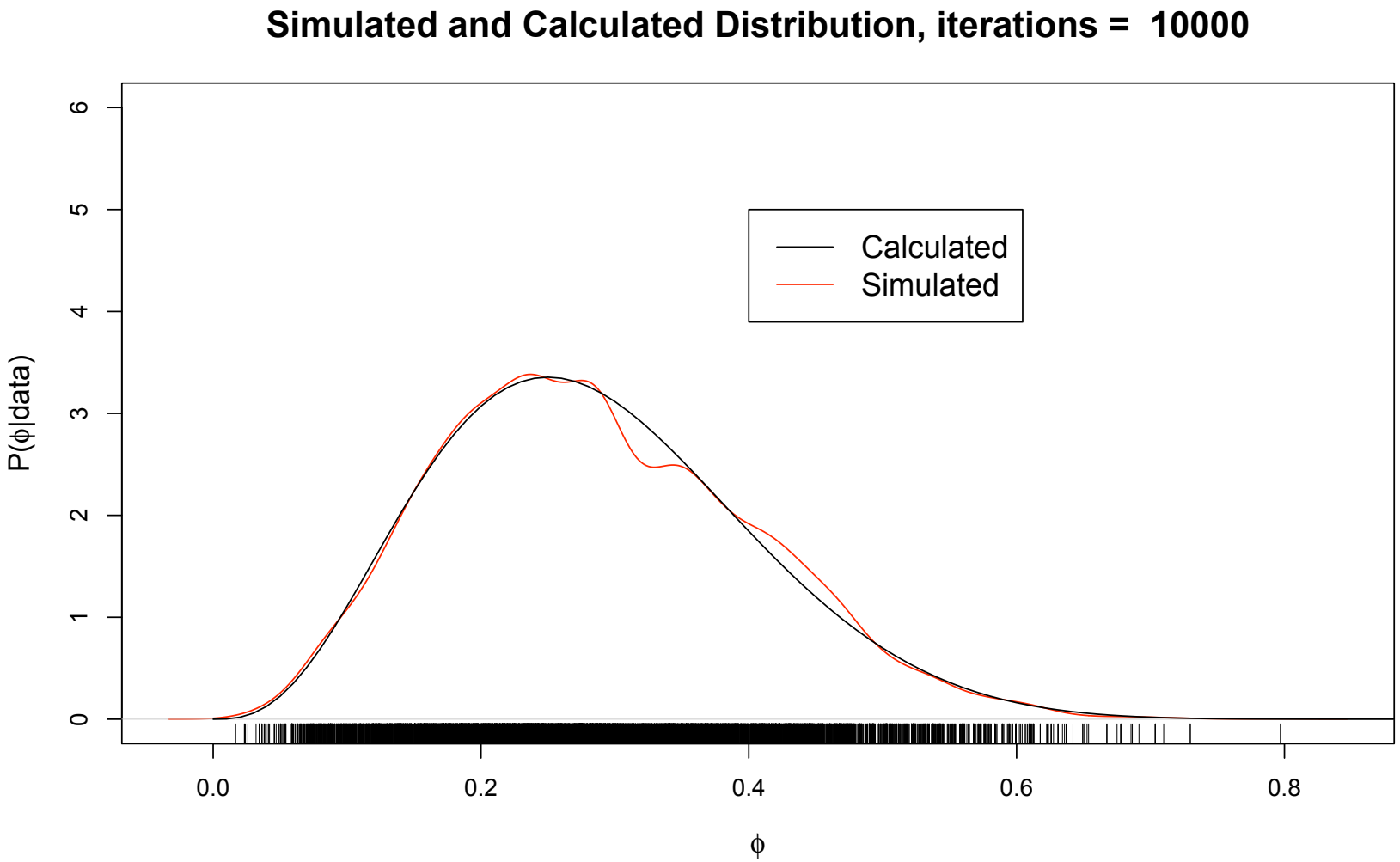
Sampling from the posterior



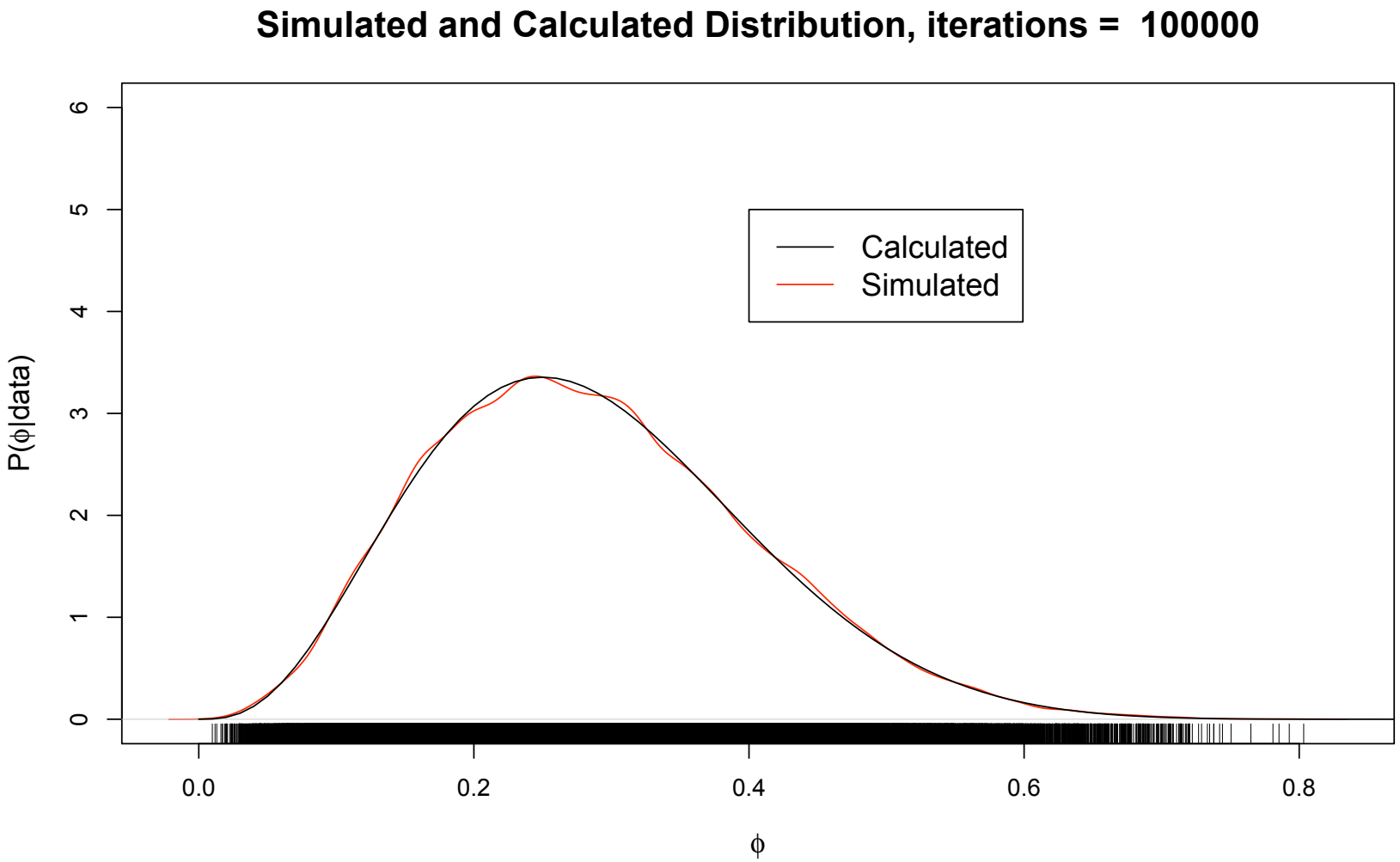
Sampling from the posterior



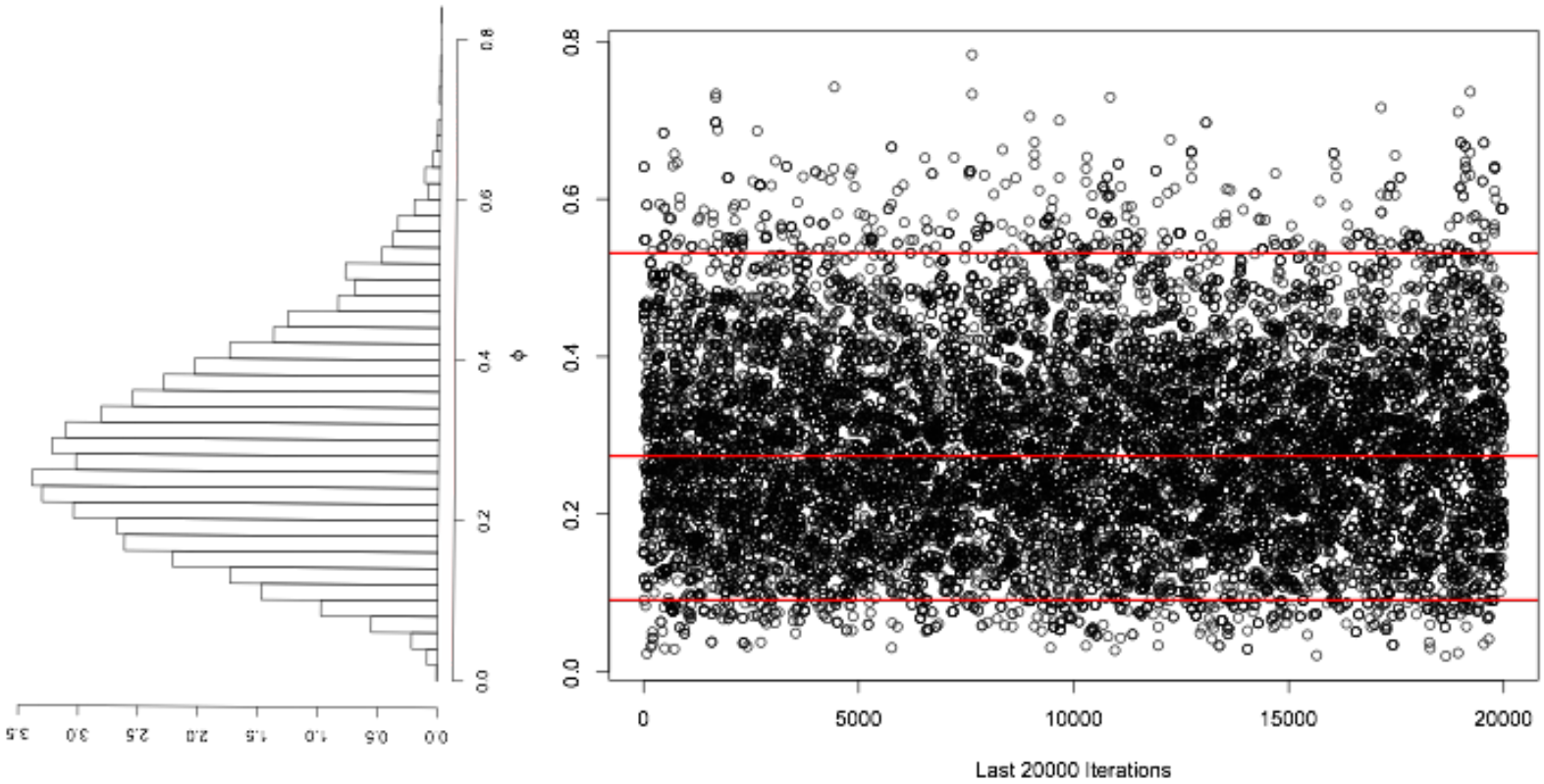
Sampling from the posterior



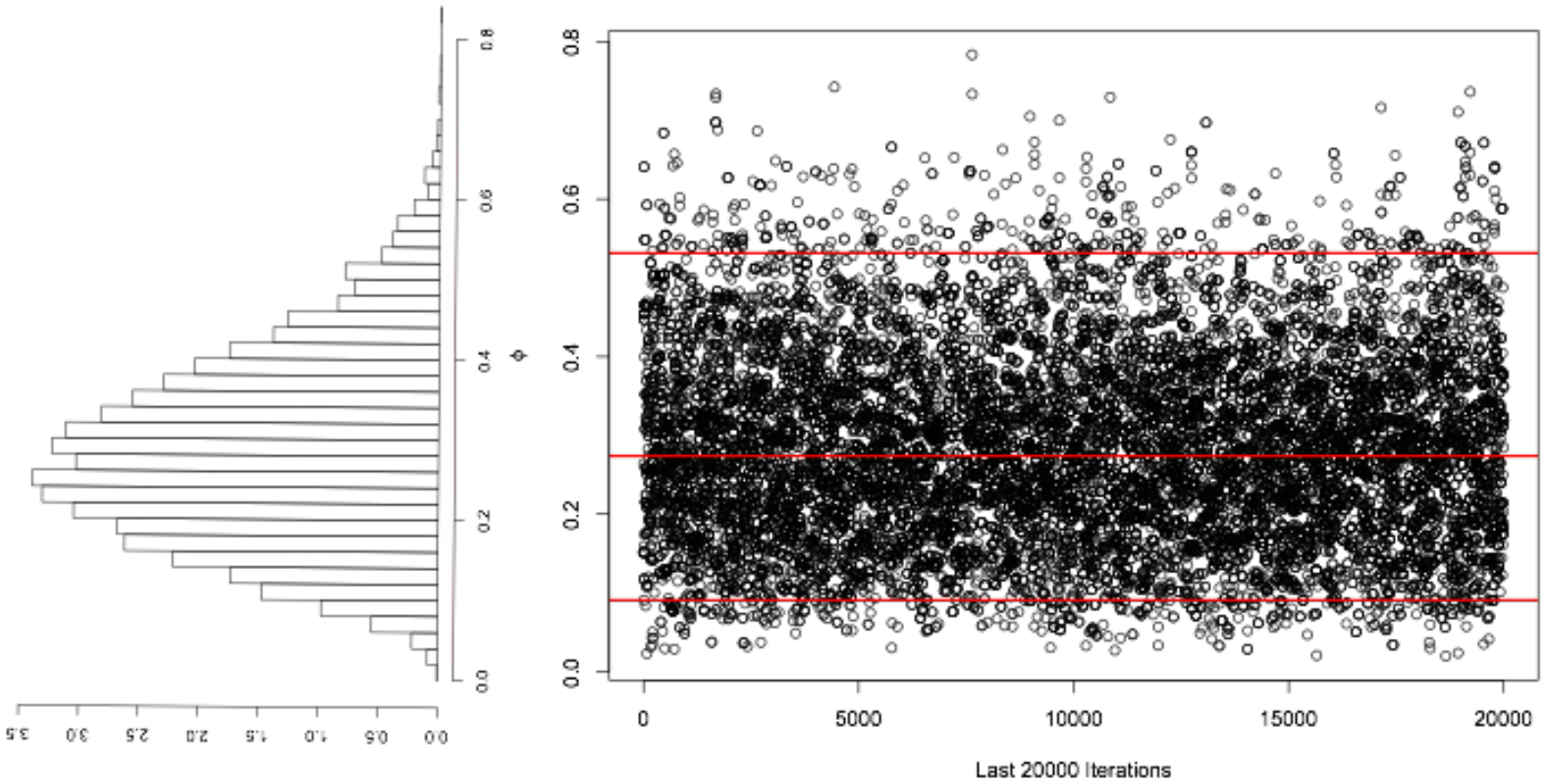
Sampling from the posterior



Sampling from the posterior

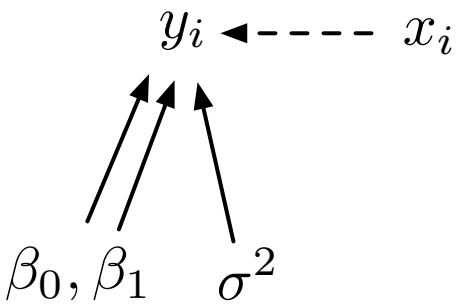


Sampling from the posterior



The chain has *converged* when adding more samples does not change the shape of the posterior distribution. We throw away samples that are accumulated before convergence (burn-in).

Intuition for MCMC for multi-parameter models



$$g(\beta_0, \beta_1, x_i) = \beta_0 + \beta_1 x_i$$

$$[\beta_0, \beta_1, \sigma^2 \mid y_i] \propto [\beta_0, \beta_1, \sigma^2, y_i]$$

factoring rhs using DAG:

$$[\beta_0, \beta_1, \sigma^2 \mid y_i] \propto [y_i \mid g(\beta_0, \beta_1, x_i), \sigma^2][\beta_0], [\beta_1][\sigma^2]$$

joint for all data :

$$[\beta_0, \beta_1, \sigma^2 \mid \boldsymbol{y}] \propto \prod_{i=1}^{n} [y_i \mid g(\beta_0, \beta_1, x_i), \sigma^2][\beta_0][\beta_1][\sigma^2]$$

choose specific distributions:

$$\begin{aligned}[\beta_0, \beta_1, \sigma^2 \mid \boldsymbol{y}] \propto & \prod_{i=1}^{n} \text{normal}(y_i \mid g(\beta_0, \beta_1, x_i), \sigma^2) \\ & \times \text{normal}(\beta_0 \mid 0, 10000)\text{normal}(\beta_1 \mid 0, 10000) \\ & \times \text{uniform}(\sigma^2 \mid 0, 500)\end{aligned}$$

Intuition for MCMC for multi-parameter models

$$
\begin{aligned}
[\beta_0, \beta_1, \sigma^2 \mid \mathbf{y}] &\propto \prod_{i=1}^{n} \text{normal}(y_i | g(\beta_0, \beta_1, x_i), \sigma^2) \\
&\times \text{normal}(\beta_0 \mid 0, 10000)\text{normal}(\beta_1 \mid 0, 10000)\text{uniform}(\sigma^2 \mid 0, 10
\end{aligned}
$$

1. Set initial values for $\beta_0, \beta_1, \sigma^2$
2. Assume β_1, σ^2 are known and constant. Make a draw for β_0. Store the draw.
3. Assume β_0, σ^2 are known and constant. Make a draw for β_1. Store the draw.
4. Assume β_0, β_1 are known and constant. Make a draw for σ^2. Store the draw.
5. Do this many times. The stored values for each parameter approximate its marginal posterior distribution after convergence.

Implementing MCMC for multiple parameters and latent quantities

- Write an expression for the posterior and joint distribution using a DAG as a guide. Always.
- If you are using MCMC software (e.g. JAGS) use expression for the posterior and joint distribution as template for writing code. You are done.
- If you are writing your own MCMC sampler *and* to understand what JAGS is doing for you:
  - Decompose the expression of the multivariate joint distribution into a series of univariate distributions called *full-conditional distributions*.
  - Choose a sampling method for each full-conditional distribution.
  - Cycle through each unobserved quantity, sampling from its full-conditional distribution, treating the others as if they were known and constant.
  - The accumulated samples approximate the marginal posterior distribution of each unobserved quantity.
  - Note that this takes a complex, multivariate problem and turns it into a series of simple, univariate problems that we solve, as in the example above, one at a time.

Definition of full-conditional distribution

Let $\boldsymbol{\theta}$ be a vector of length k containing all of the unobserved quantities we seek to understand. Let $\boldsymbol{\theta}_{-j}$ be a vector of length $k-1$ that contains all of the unobserved quantities *except* θ_j. The full-conditional distribution of θ_j is

$$[\theta_j | y, \boldsymbol{\theta}_{-j}],$$

which we notate as

$$[\theta_j | \cdot].$$

It is the posterior distribution of θ_j conditional on all of the other parameters and the data, which we assume are *known*.

Writing full-conditional distributions

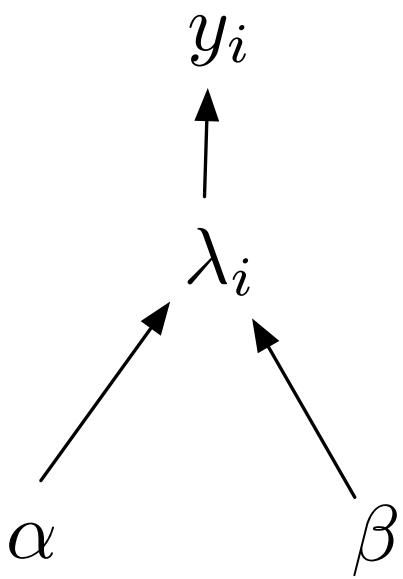
- You will have one full-conditional for each unobserved quantity in the posterior.
- For each unobserved quantity, write the distributions where it appears.
- Ignore the other distributions.
- Simple.

Example

- Clark 2003 considered the problem of modeling fecundity of spotted owls and the implication of individual variation in fecundity for population growth rate.
- Data were number of offspring produced by per pair of owls with sample size $n = 197$.

Clark, J. S. 2003. Uncertainty and variability in demography and population growth: A hierarchical approach. Ecology 84:1370-1381.

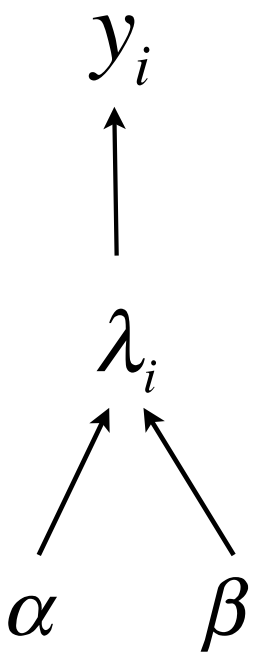
Example



$$
\begin{aligned}
[\boldsymbol{\lambda}, \alpha, \beta | \mathbf{y}] &\propto \prod_{i=1}^{n} \text{Poisson}\left(y_i | \lambda_i\right) \text{gamma}\left(\lambda_i | \alpha, \beta\right) \\
&\times \text{gamma}\left(\alpha | .001, .001\right) \text{gamma}\left(\beta | .001, .001\right)
\end{aligned}
$$

Full-conditionals

$$[\boldsymbol{\lambda}, \alpha, \beta | \mathbf{y}] \propto \prod_{i=1}^{n} \text{Poisson}\left(y_i | \lambda_i\right) \text{gamma}\left(\lambda_i | \alpha, \beta\right) \text{gamma}\left(\beta | .001, .001\right) \text{ gamma}\left(\alpha | .001, .001\right)$$



We use the multivariate joint distribution to find univariate full-conditional distributions for all unobserved quantities.

How many full conditionals are there?

Writing full-conditional distributions

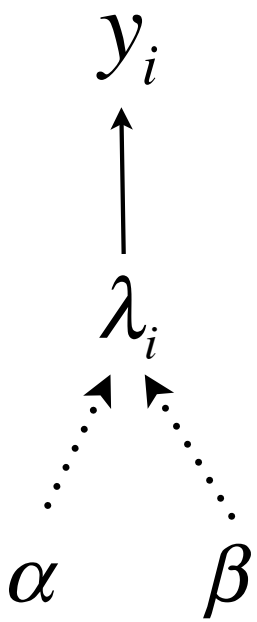
- You will have one full-conditional for each unobserved quantity in the posterior.
- For each unobserved quantity, write the distributions (including products) where it appears.
- Ignore the other distributions.
- Simple.

Full-conditional for each λ_i

$$[\boldsymbol{\lambda}, \alpha, \beta|\mathbf{y}] \propto \prod_{i=1}^{n} \text{Poisson}\,(y_i|\lambda_i)\,\text{gamma}\,(\lambda_i|\alpha,\beta)\,\text{gamma}\,(\beta|.001,.001)\;\;\text{gamma}\,(\alpha|.001,.001)$$

Writing the full-conditional distribution for λ_i:

$$[\lambda_i \mid .] \propto \text{Poisson}\left(y_i \mid \lambda_i\right)\text{gamma}\left(\lambda_i \mid \alpha,\beta\right)$$

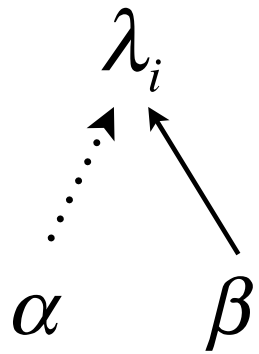


Full-conditional for β

$$[\boldsymbol{\lambda}, \alpha, \beta | \mathbf{y}] \propto \prod_{i=1}^{n} \text{Poisson}\left(y_i | \lambda_i\right) \text{gamma}\left(\lambda_i | \alpha, \beta\right) \text{gamma}\left(\beta | .001, .001\right) \text{ gamma}\left(\alpha | .001, .001\right)$$

Writing the full-conditional distribution for β:

$$[\beta | .] \propto \prod_{i=1}^{n} \text{gamma}\left(\lambda_i | \alpha, \beta\right) \text{gamma}\left(\beta | .001, .001\right)$$

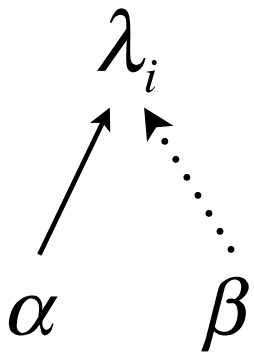


Full-conditional for α

$$[\boldsymbol{\lambda}, \alpha, \beta | \mathbf{y}] \propto \prod_{i=1}^{n} \text{Poisson}\left(y_i | \lambda_i\right) \text{gamma}\left(\lambda_i | \alpha, \beta\right) \text{gamma}\left(\beta | .001, .001\right) \text{gamma}\left(\alpha | .001, .001\right)$$

Writing the full-conditional distribution for α:

$$[\alpha \mid \cdot] \propto \prod_{i=1}^{n} \text{gamma}(\lambda_i \mid \alpha, \beta) \text{gamma}(\alpha \mid .001, .001)$$



Full-conditionals for the model

Posterior and joint:

$$\begin{aligned}[\boldsymbol{\lambda}, \alpha, \beta | \mathbf{y}] &\propto \prod_{i=1}^{n} \text{Poisson}\left(y_i | \lambda_i\right) \text{gamma}\left(\lambda_i | \alpha, \beta\right) \\ &\times \text{gamma}\left(\alpha | .001, .001\right) \text{gamma}\left(\beta | .001, .001\right)\end{aligned}$$

Full conditionals:

$$[\lambda_i | .] \propto \text{Poisson}\left(y_i | \lambda_i\right) \text{gamma}\left(\lambda_i | \alpha, \beta\right)$$

$$[\beta | .] \propto \prod_{i=1}^{n} \text{gamma}\left(\lambda_i | \alpha, \beta\right) \text{gamma}\left(\beta | .001, .001\right)$$

$$[\alpha | .] \propto \prod_{i=1}^{n} \text{gamma}\left(\lambda_i | \alpha, \beta\right) \text{gamma}\left(\alpha | .001, .001\right)$$

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  - Note that this takes a complex, multivariate problem and turns it into a series of simple, univariate problems that we solve, as in the example above, one at a time.

Choosing a sampling method

1. Acept-reject:
   - 1.1 Metropolis: requires a symmetric proposal distribution (e.g., normal, uniform). This is what we used above in the example for one parameter.
   - 1.2 Metropolis-Hastings: allows asymmetric proposal distributions (e.g., beta, gamma, lognormal). See optional notes.
2. Gibbs: accepts all proposals because they are especially well chosen. In lab today.