# Markov chain Monte Carlo I

## ESS 575 Models for Ecological Data

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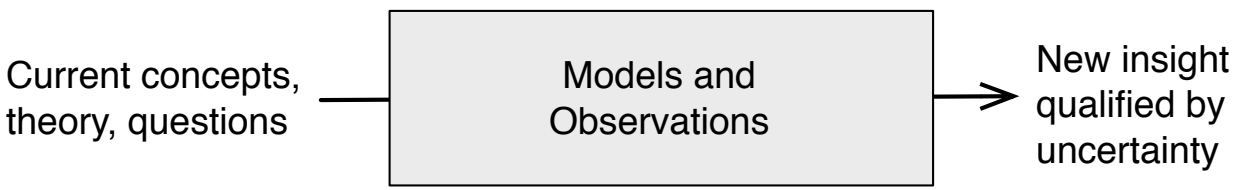
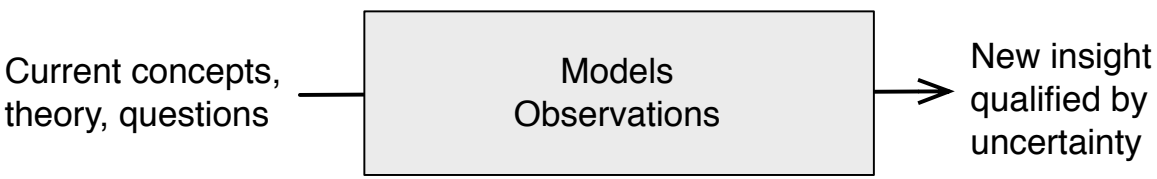
February 21, 2019

# What is this course about?

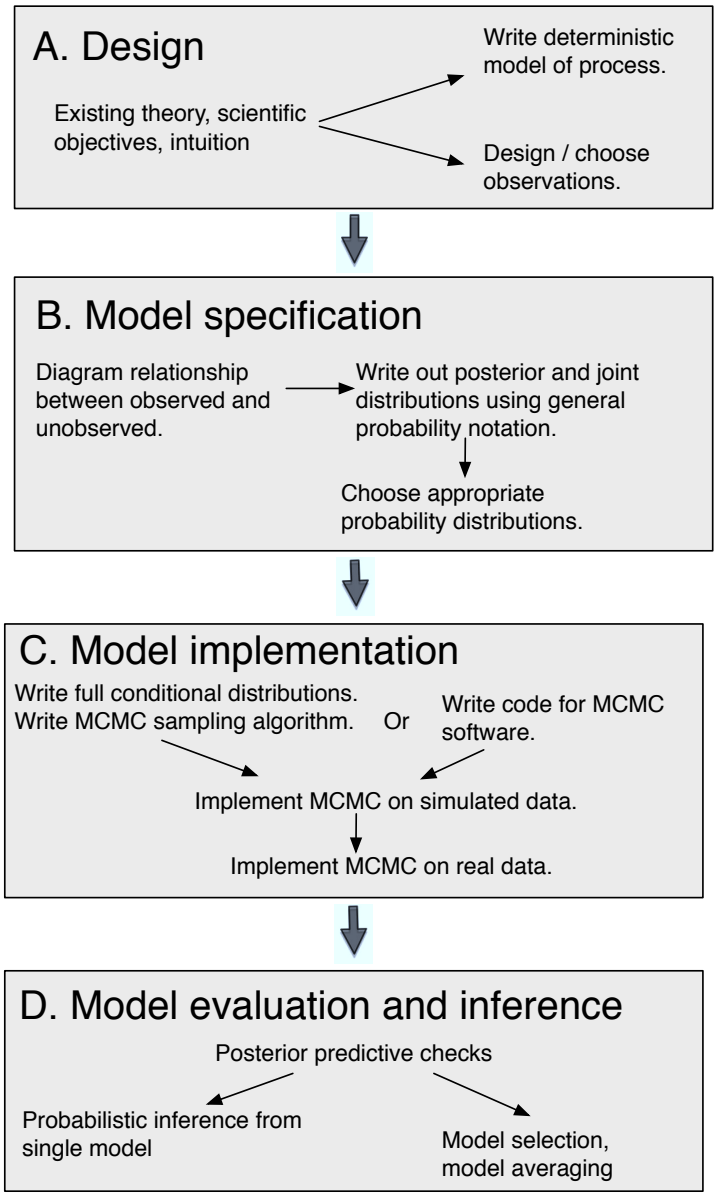


# You can understand it.

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



# The Bayesian method



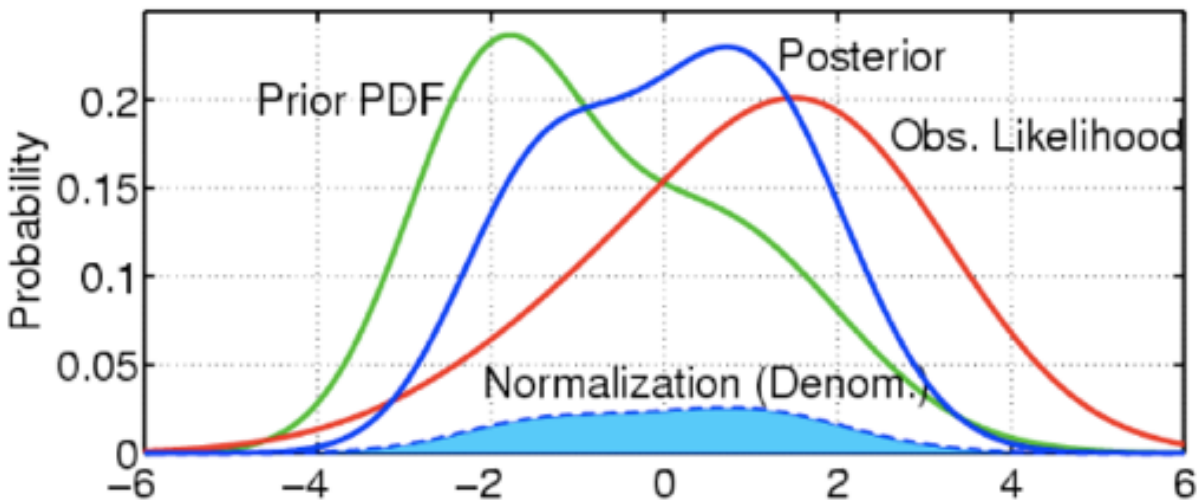
# The MCMC algorithm

- Why MCMC?
- Some intuition about how it works
- MCMC for multiple parameter models
  - Full-conditional distributions (today)
  - Gibbs sampling (today and lab next week)
  - Metropolis-Hastings algorithm (Thursday)
  - MCMC software (JAGS, next week)

# 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:

$$[\theta_1, \theta_{2,}\theta_3, \theta_4, z_i \mid \mathbf{y}, \mathbf{u}] =$$
$$\frac{\prod_{i=1}^{n}[y_i|\theta_1 z_i][u_i|\theta_2, z_i][z_i|\theta_3, \theta_4][\theta_1][\theta_2][\theta_3][\theta_4]}{\int \ldots . \int \prod_{i=1}^{n}[y_i|\theta_1 z_i][u_i|\theta_2, z_i][z_i|\theta_3, \theta_4][\theta_1][\theta_2][\theta_3][\theta_4] dz_i \, d\theta_1 \, d\theta_2 \, d\theta_3 \, d\theta_4}$$

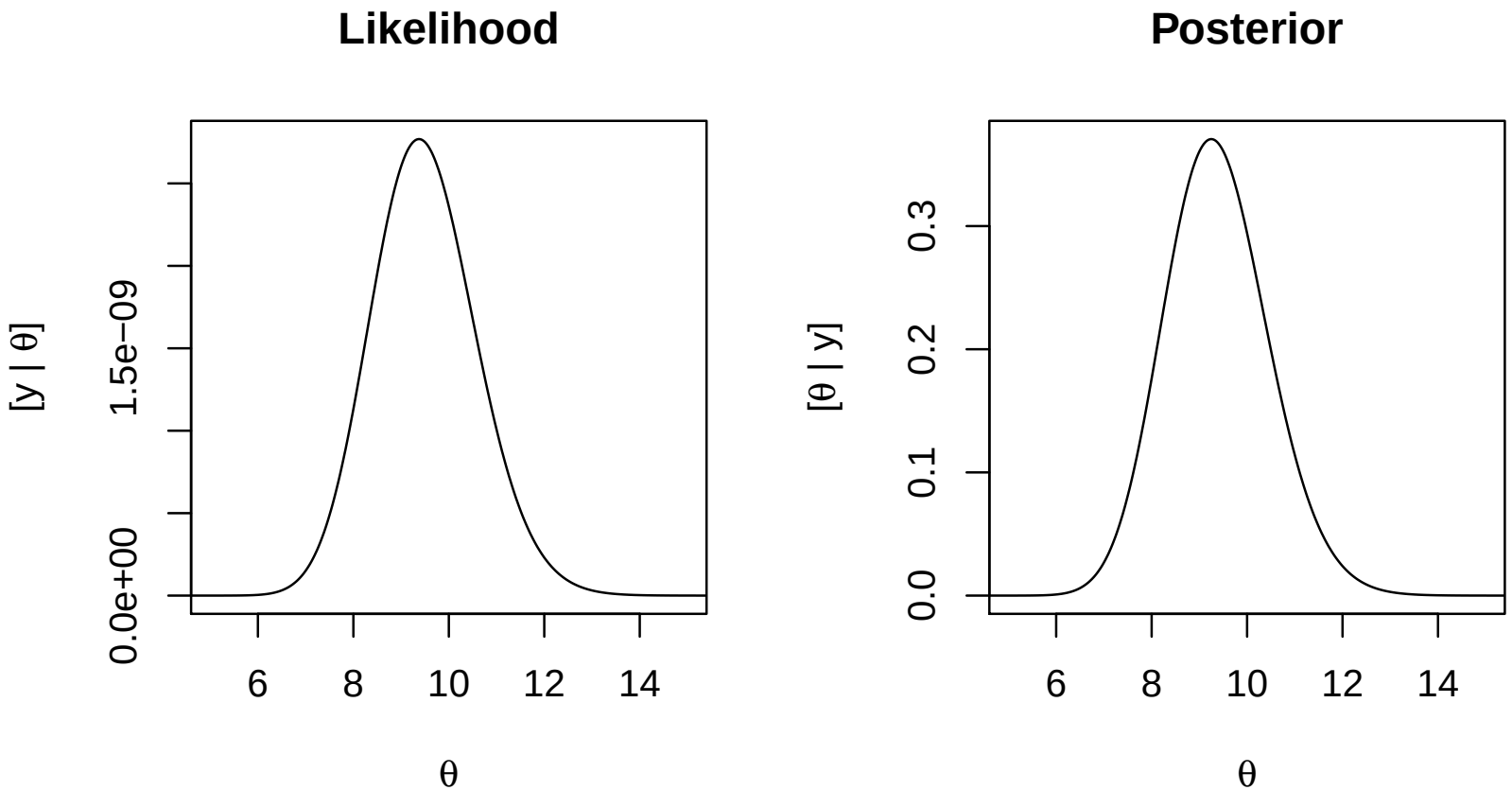
# What we are doing in MCMC?

Recall that the posterior distribution is proportional to the joint:

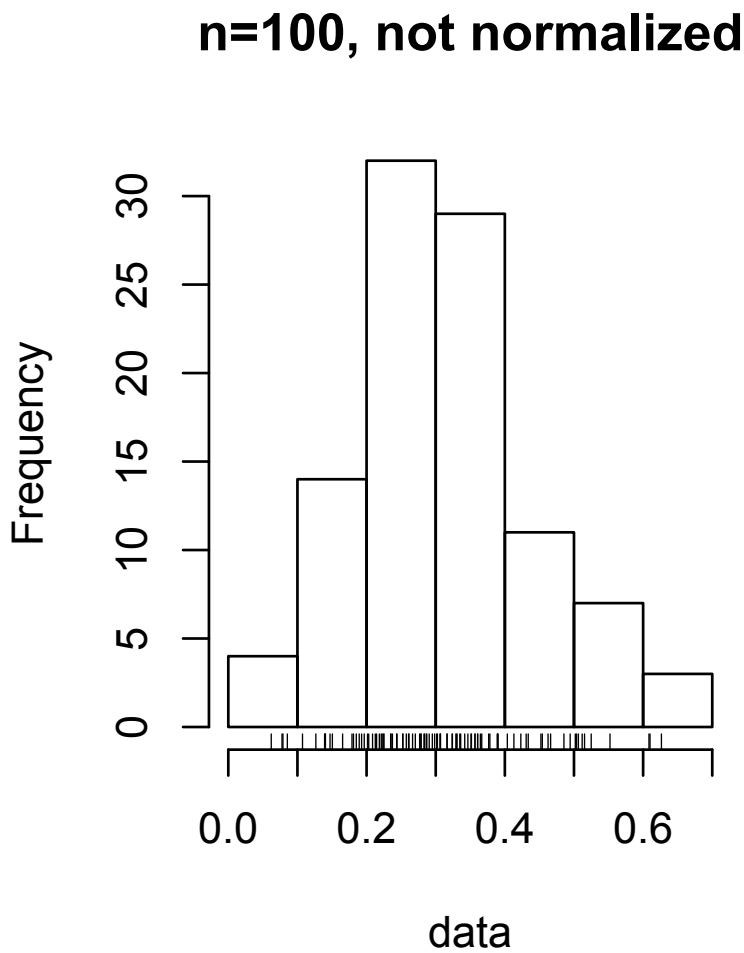
$$[\theta|y] \propto [y|\theta][\theta], \tag{1}$$

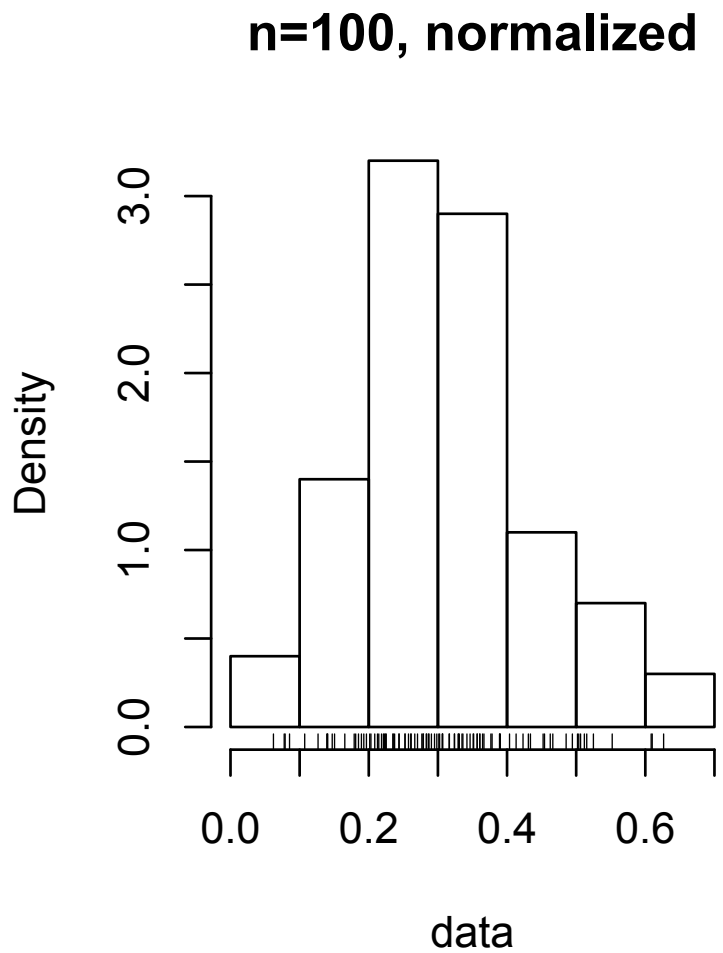
because the marginal distribution of the data $\int [y|\theta][\theta] d\theta$ is a constant after the data have been observed.

# What we are doing in MCMC?



# What we are doing in MCMC?



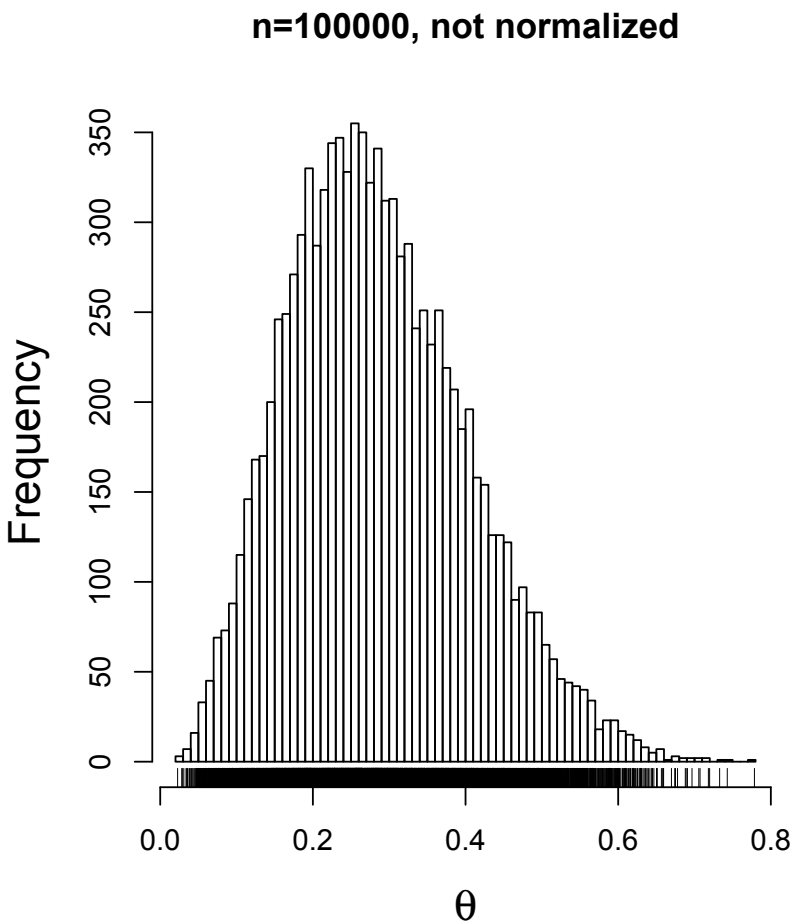



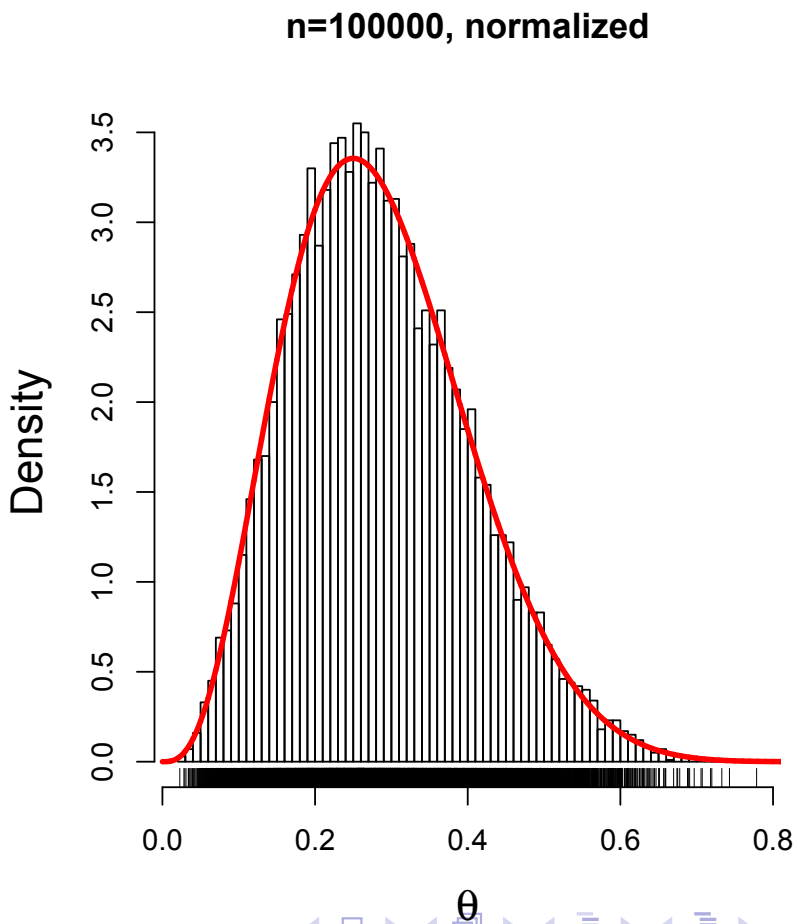
# What are we doing in MCMC?

- 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 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.

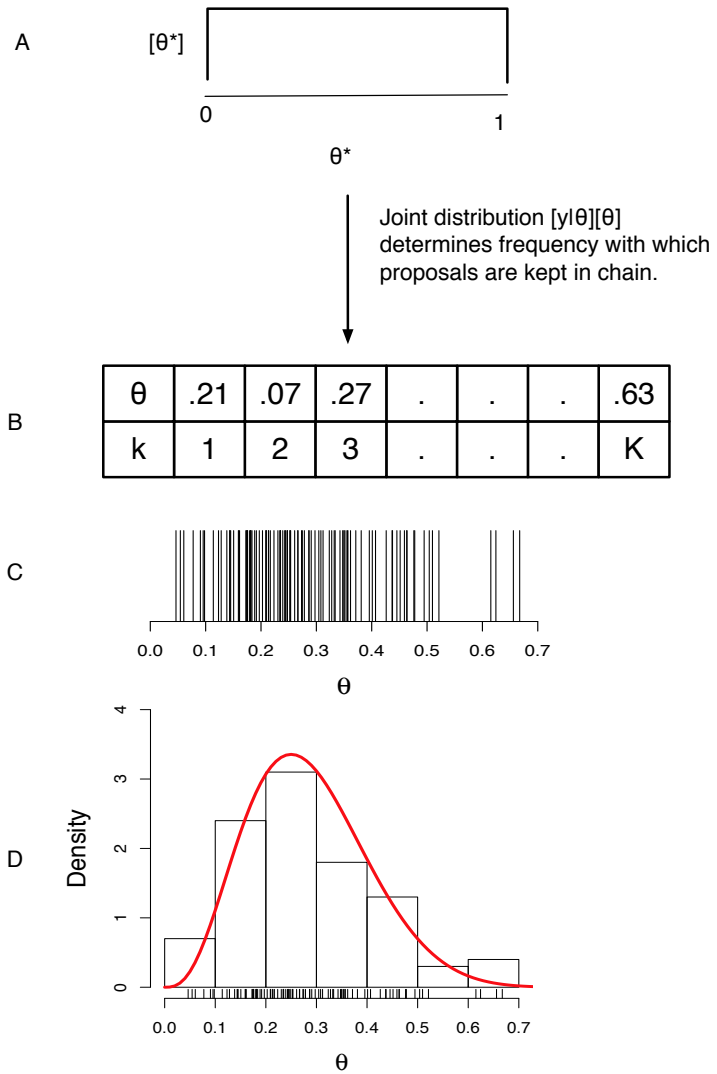
# What are we doing in MCMC?

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



# What are we doing in MCMC?



# 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 $\theta^{*k+1}$ | | $\theta^{*2}$ |
| Test | | $P(\theta^{*2}) > P(\theta^1)$ |
| Chain($\theta^k$) | $\theta^1$ | $\theta^2 = \theta^{*2}$ |

# 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 $\theta^{*k+1}$ | | $\theta^{*2}$ | $\theta^{*3}$ |
| Test | | $P(\theta^{*2}) > P(\theta^1)$ | $P(\theta^2) > P(\theta^{*3})$ |
| Chain$(\theta^k)$ | $\theta^1$ | $\theta^2 = \theta^{*2}$ | $\theta^3 = \theta^2$ |

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

# 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 $\theta^{*k+1}$ as the next value in the chain with probability $P_R$ and keep $\theta^k$ 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 $\theta^{*k+1}$ as the next value in the chain.
3. Otherwise, we retain $\theta^k$ as the next value.

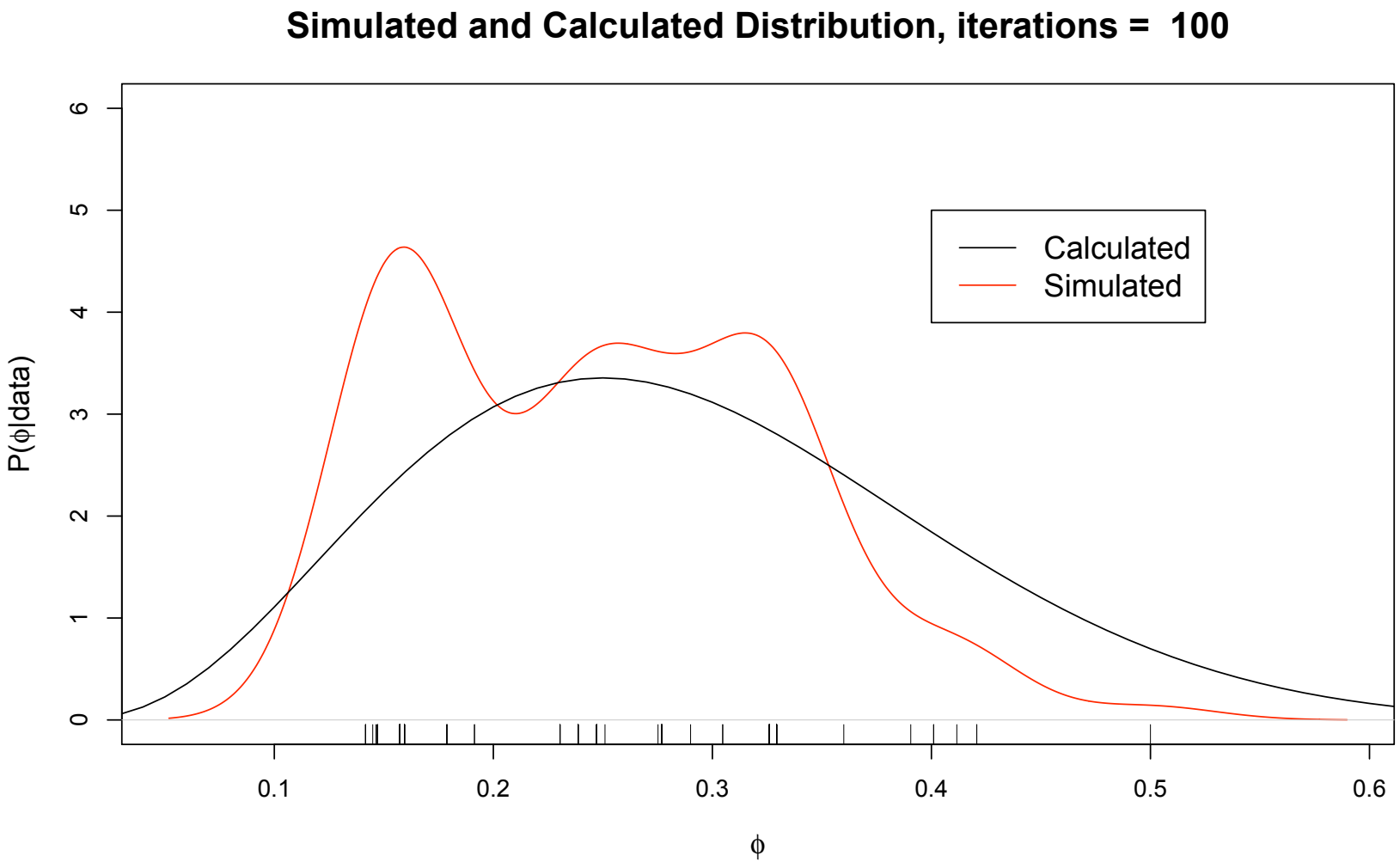
# A simple example for one parameter

- 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



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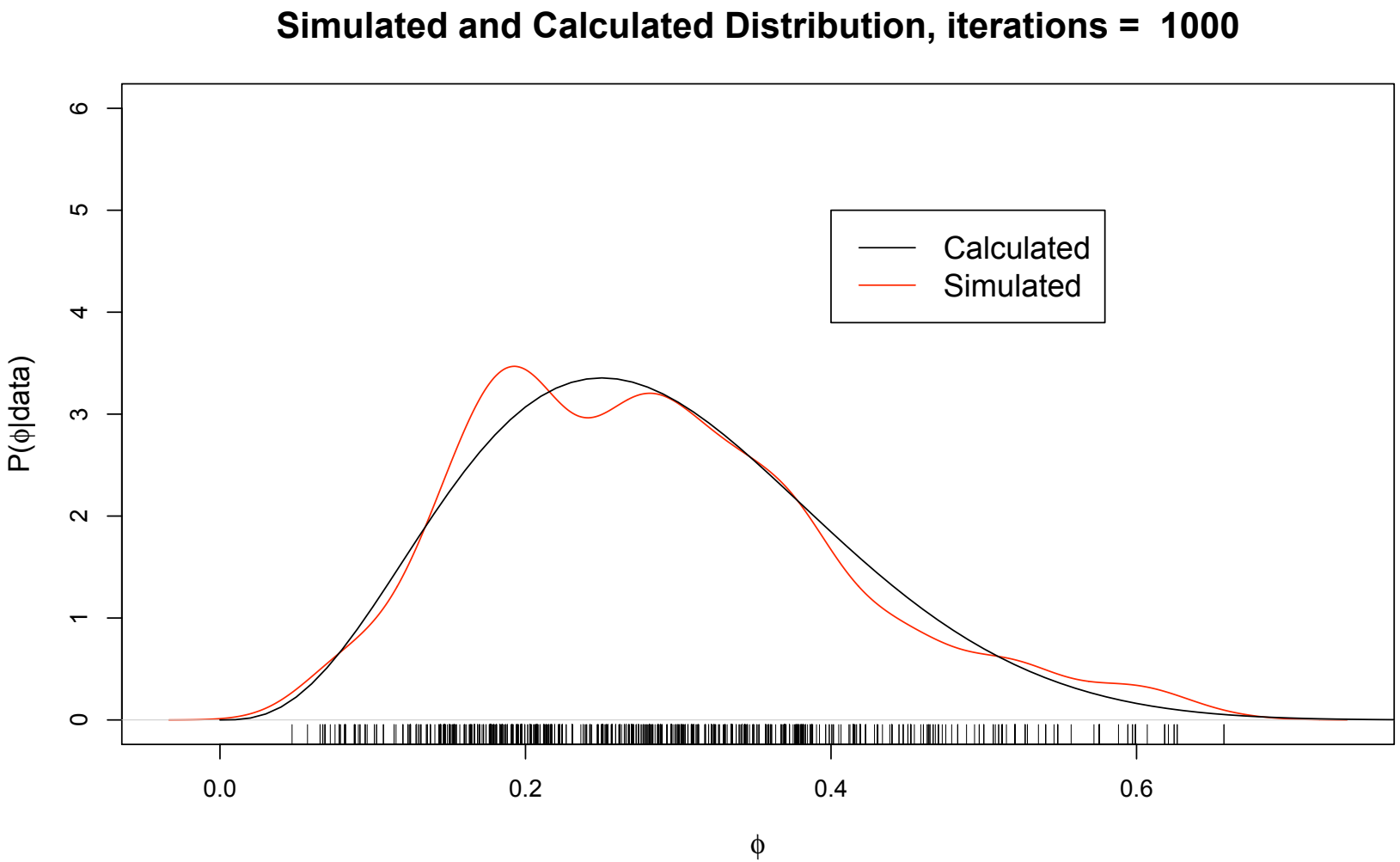

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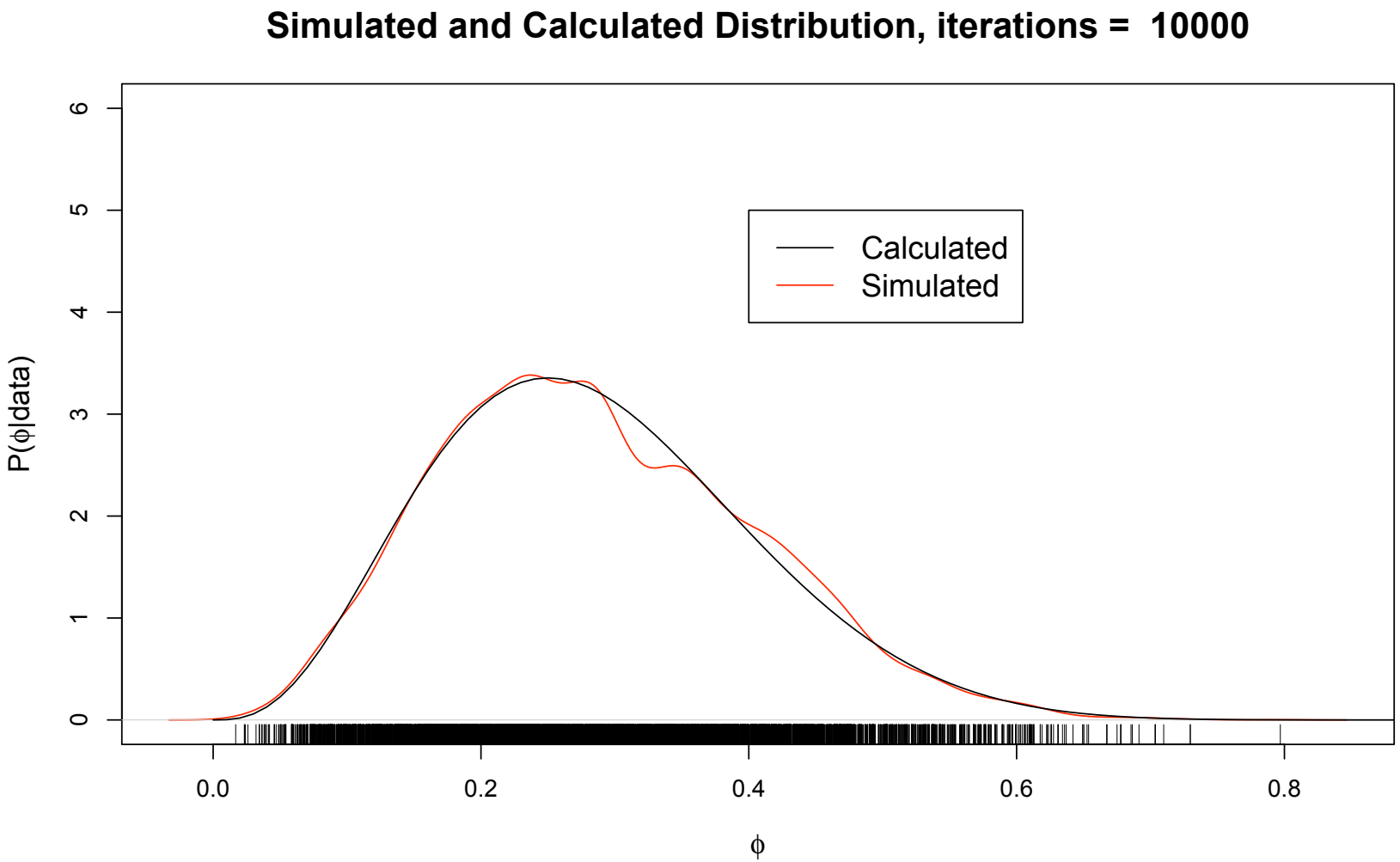

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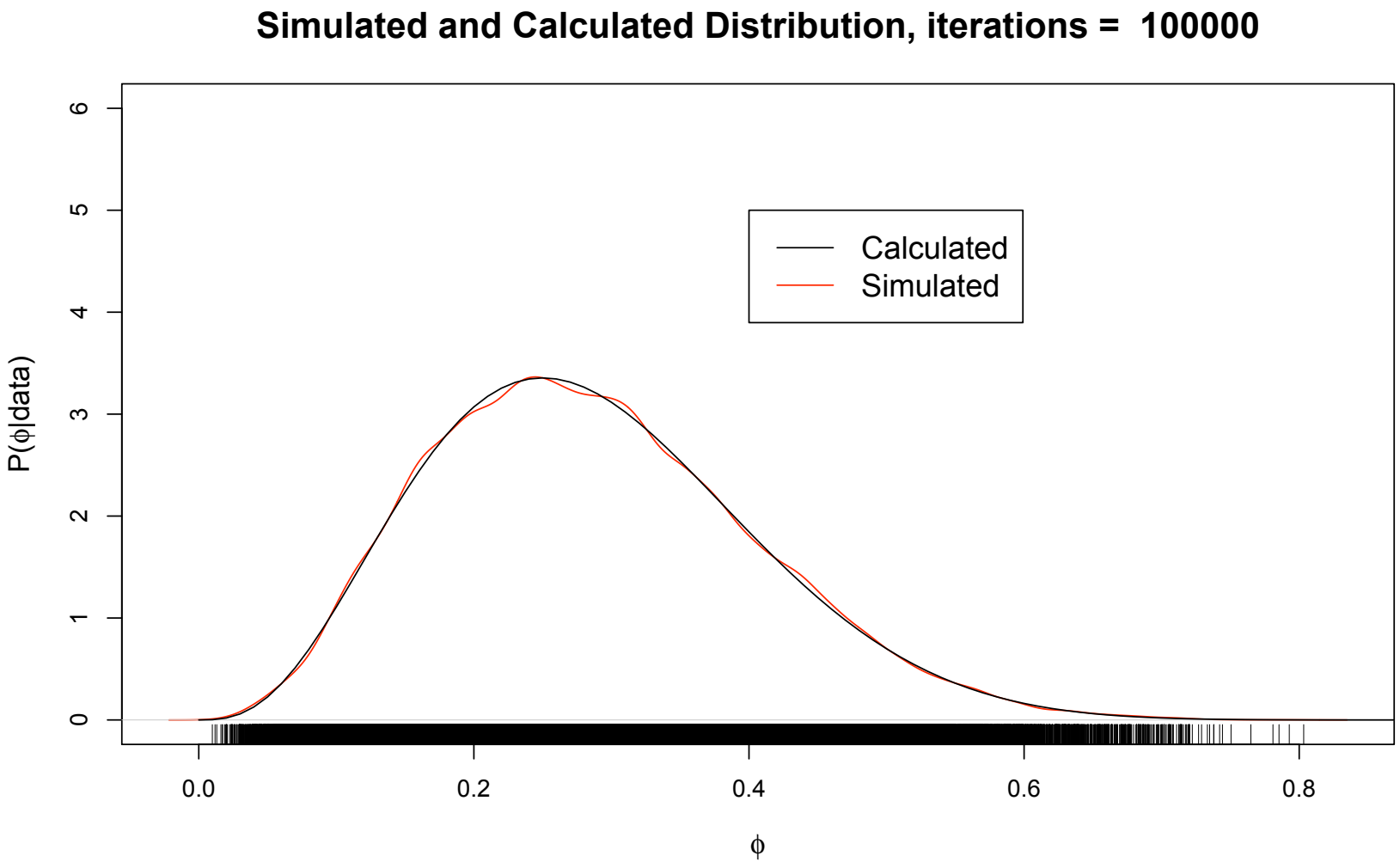
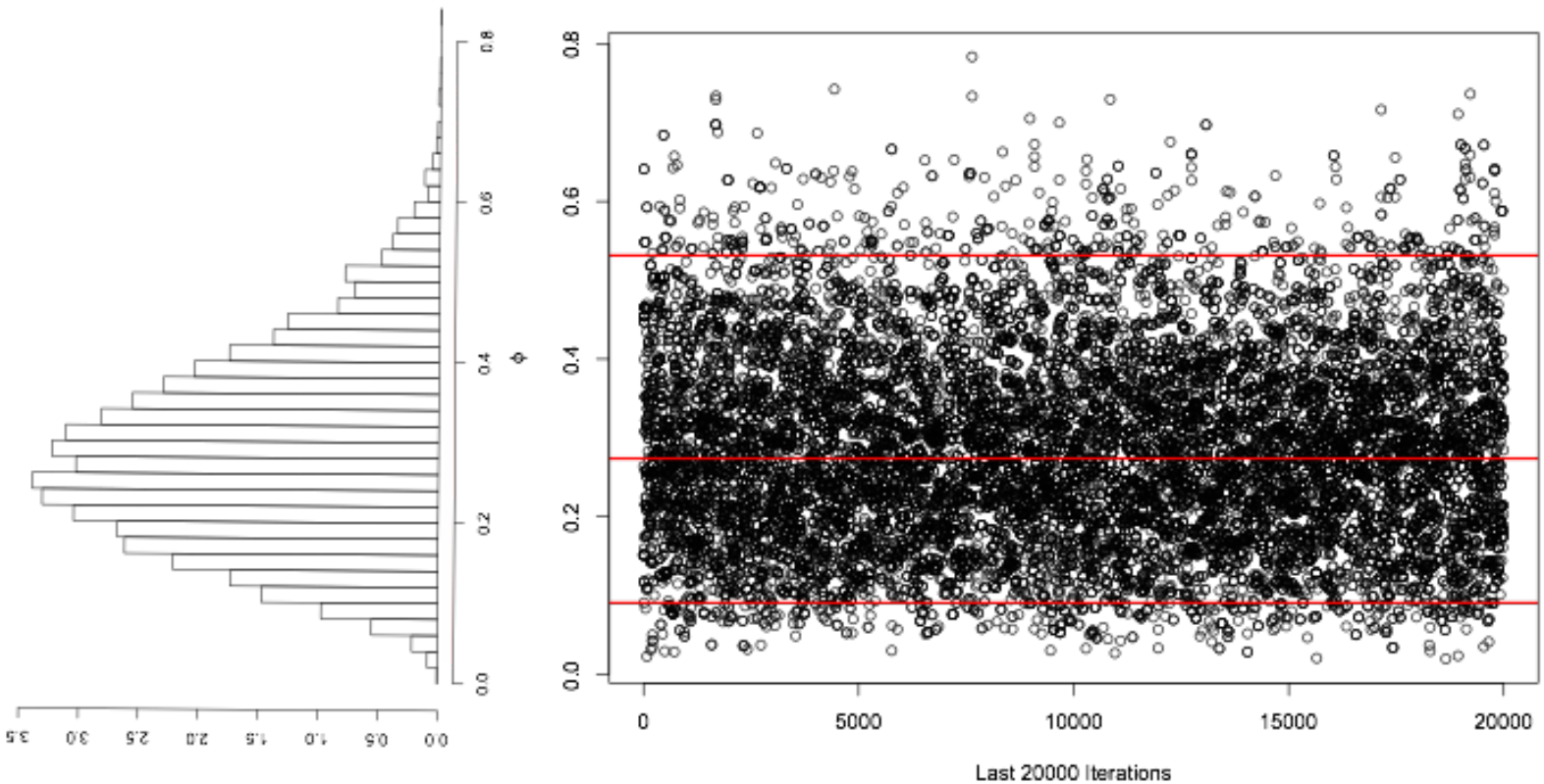
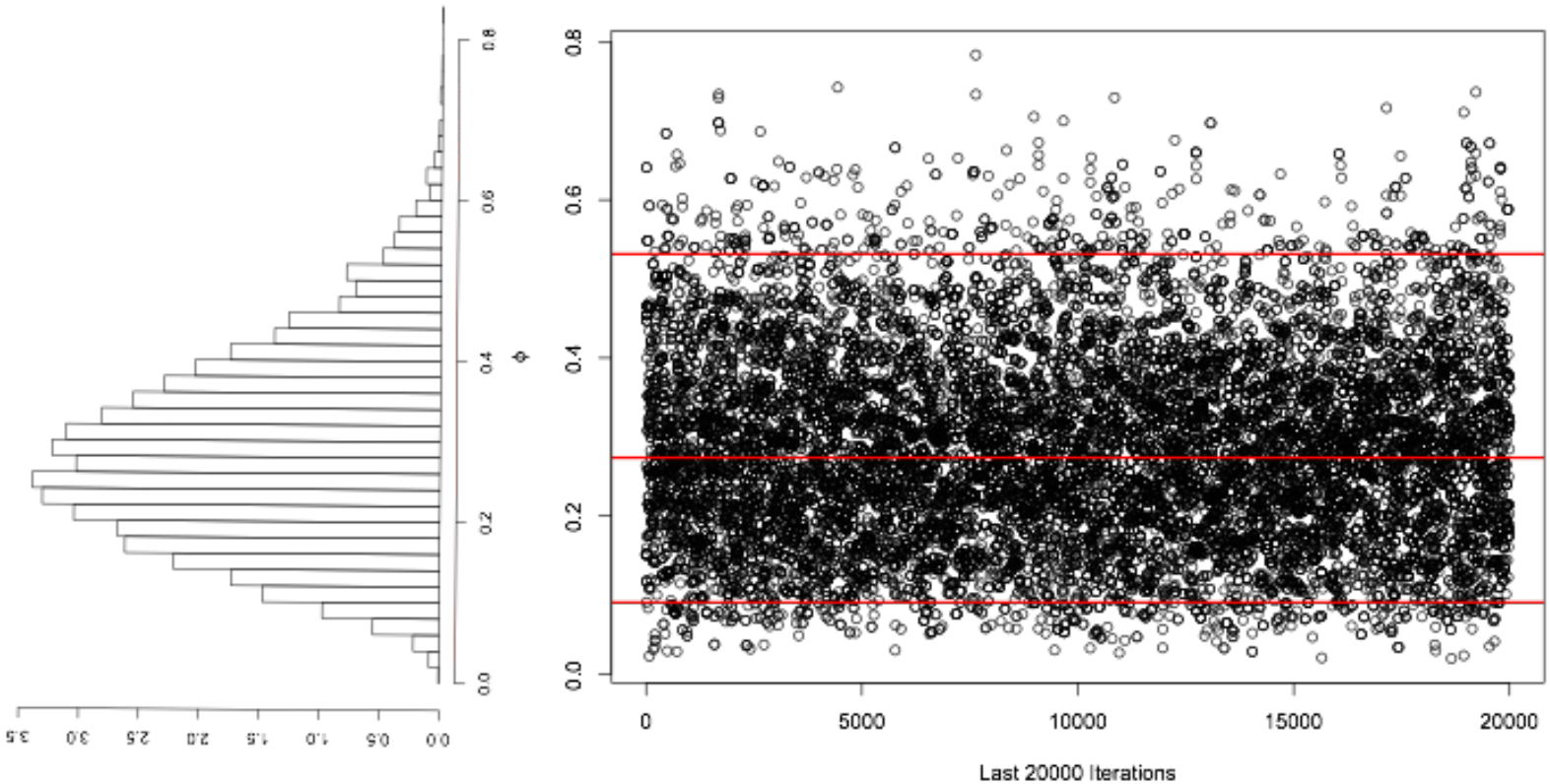


# Sampling from the posterior

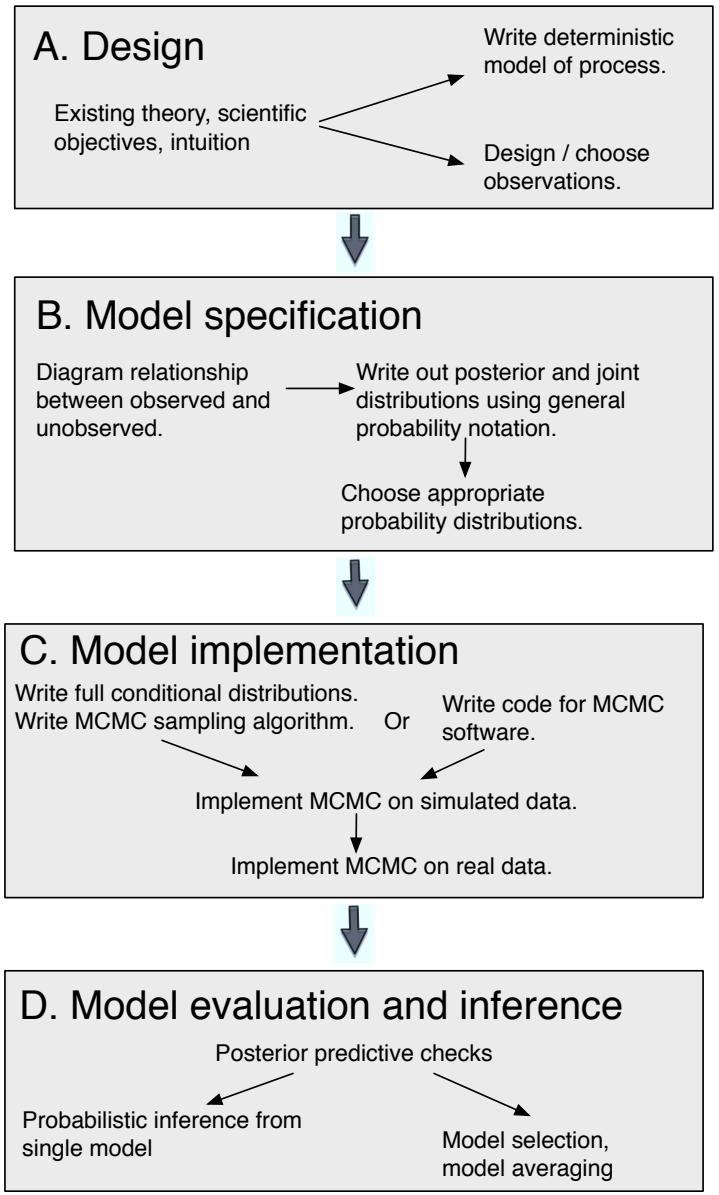


# Sampling from the posterior

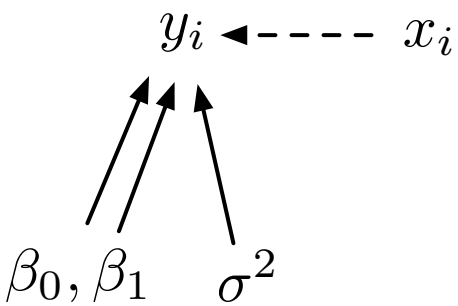



The chain has *converged* when adding more samples does not change the shape of the posterior distribution. We throw away samples that are accumulated before convergence (burn-in).

# The Bayesian method



# 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:

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

# Intuition for MCMC for multi-parameter models

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

1. Set initial values for $\beta_0, \beta_1, \sigma^2$
2. Assume $\beta_1, \sigma^2$ are known and constant. Make a draw for $\beta_0$. Store the draw.
3. Assume $\beta_0, \sigma^2$ are known and constant. Make a draw for $\beta_1$. Store the draw.
4. Assume $\beta_0, \beta_1$ are known and constant. Make a draw for $\sigma^2$. 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.
- If you are writing your own MCMC sampler:
  - 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* $\theta_j$. The full-conditional distribution of $\theta_j$ is

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

which we notate as

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

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

# Writing full-conditional distributions

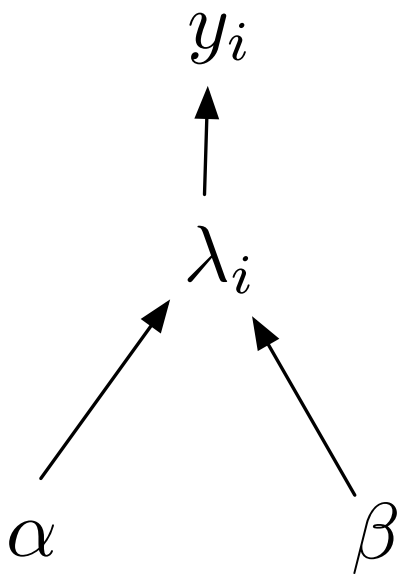
- You will have one full-conditional for each unobserved quantity in the posterior.
- For each unobserved quantity, write the distributions where it appears.
- Ignore the other distributions.
- Simple.

# 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.

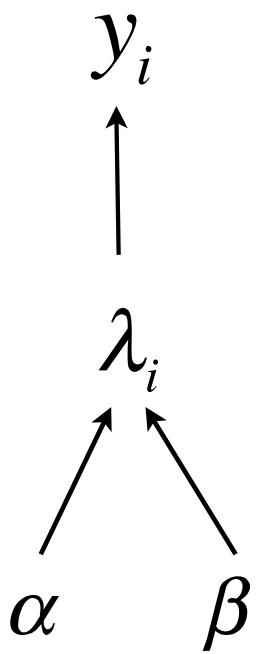
# Example




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

# 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

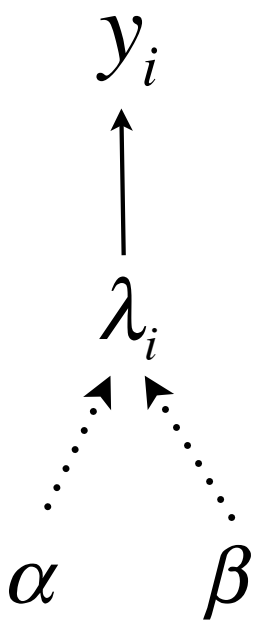
- You will have one full-conditional for each unobserved quantity in the posterior.
- For each unobserved quantity, write the distributions (including products) where it appears.
- Ignore the other distributions.
- Simple.

# Full-conditional for each $\lambda_i$

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

Writing the full-conditional distribution for $\lambda_i$:

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

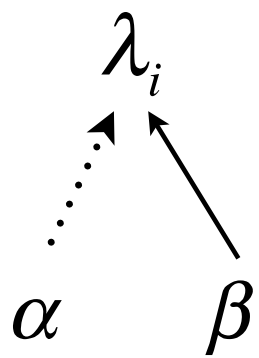


# Full-conditional for $\beta$

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

Writing the full-conditional distribution for β:

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

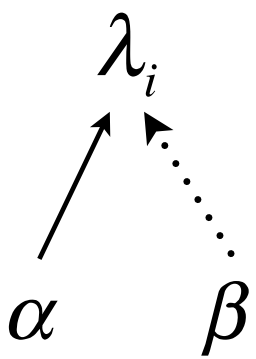


# Full-conditional for $\alpha$

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

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:

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

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

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

# Implementing MCMC for multiple parameters and latent quantities

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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. Accept-reject:
   1.1 Metropolis: requires a symmetric proposal distribution (e.g., normal, uniform). This is what we used above in the *Chytrid* example for one parameter.
   1.2 Metropolis-Hastings: allows asymmetric proposal distributions (e.g., beta, gamma, lognormal). Thursday.
2. Gibbs: accepts all proposals because they are especially well chosen. Now.

# Why do you need to understand conjugate priors?

- A easy way to find parameters of posterior distributions for simple problems as you learned in lab last week.
- Critical to understanding Gibbs updates in Markov chain Monte Carlo as you are about to learn.

# What are conjugate priors?

Assume we have a likelihood and a prior:

$$\overbrace{[\theta|y]}^{\text{posterior}} = \frac{\overbrace{[y|\theta]}^{\text{likelihood}}\overbrace{[\theta]}^{\text{prior}}}{[y]}.$$

If the form of the distribution of the posterior

$[\theta|y]$

is the same as the form of the distribution of the prior,

$[\theta]$

then the likelihood and the prior are said to be conjugates

$$\underbrace{[y|\theta][\theta]}_{\text{congugates}}$$

and the prior is called a conjugate prior for $\theta$.

# Gibbs updates

When priors and likelihoods are conjugate, we *know* all but one of the parameters of the full-conditional because they are *assumed to be known* at each iteration. We make a draw of the single unknown *directly* from its posterior distribution as if the other parameters were fixed.

Wickedly clever.

# Gamma-Poisson conjugate relationship for $\lambda$

The conjugate prior distribution for a Poisson likelihood is gamma$(\lambda|\alpha,\beta)$. Given $n$ observations $y_i$ of new data, the posterior distribution of $\lambda$ is

$$[\lambda|\mathbf{y}] = \text{gamma}\left(\underbrace{\overbrace{\alpha_0}^{\text{The prior } \alpha} + \sum_{i=1}^{n} y_i}_{\text{The new } \alpha}, \underbrace{\overbrace{\beta_0}^{\text{The prior } \beta} + n}_{\text{The new } \beta}\right). \qquad (2)$$

# Gamma-gamma conjugate relationship

The conjugate prior distribution for the $\beta$ parameter (rate) in a gamma likelihood gamma$(y_i|\alpha,\beta)$ is a gamma distribution gamma$\{\beta \mid \alpha_0,\beta_0)$. Given $n$ observations $y_i$ of new data, the posterior distribution of $\beta$ (assuming that $\alpha$ (shape) is known) is given by:

$$[\beta|\mathbf{y}] = \text{gamma}\left(\underbrace{\overbrace{\alpha_0}^{\text{The prior } \alpha} + n\alpha}_{\text{The new } \alpha}, \underbrace{\overbrace{\beta_o}^{\text{The prior } \beta} + \sum_{i=1}^{n} y_i}_{\text{The new } \beta}\right). \quad (3)$$

We can substitute any "known" quantity for $\mathbf{y}$, e.g., $\boldsymbol{\lambda}$.

# Gibbs updates exploit conjugates.

We see conjugates for the $\lambda_i$ and $\beta$:
Full conditionals:

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

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

$$[\alpha|.] \propto \prod_{i=1}^{n} \underbrace{\text{gamma}\left(\lambda_i|\alpha,\beta\right)\text{gamma}\left(\alpha|.001,.001\right)}_{\text{conjugate for } \alpha \text{ doesn't exist}}$$

# MCMC algorithm

1. Iterate over $i = 1...197$
2. At each $i$, make a draw from

$$\lambda_i^k \sim \underbrace{\text{gamma}\left(\alpha^{k-1} + y_i, \beta^{k-1} + 1\right)}_{\text{Gibbs update using gamma - Poisson conjugate for } each \lambda_i} \tag{4}$$

$$\beta^k \sim \underbrace{\text{gamma}\left(.001 + \alpha^{k-1} n, .001 + \sum_{i=1}^{n} \lambda_i^k\right)}_{\text{Gibbs update using gamma - gamma conjugate for } \beta} \tag{5}$$

$$\alpha^k \propto \underbrace{\prod_{i=1}^{n} \text{gamma}\left(\lambda_i^k | \alpha^{k-1}, \beta^k\right) \text{gamma}\left(\alpha^{k-1} | .001, .001\right)}_{\text{No conguate for } \alpha\text{. Use Metropolis - Hastings update}} \tag{6}$$

3. Repeat for $k = 1...K$ iterations, storing $\lambda_i^k, \alpha^k$ and $\beta^k$. Store the value of each parameter at each iteration in a vector.

# Inference from MCMC

Make inference on each unobserved quantity using the elements of their vectors stored after convergence. These post-convergence vectors, (i.e., the "rug" described above) approximate the marginal posterior distributions of unobserved quantities.

# Why use Gibbs updates?

We exploit conjugate relationships to sample from the posterior because they are easier to code and because they are faster than accept-reject methods like like Metropolis or Metropolis-Hastings. However, accept-reject methods will produce the same result.