An Introduction to Bayesian Statistics
Day 2

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March 18, 2019

A Motivating Example for Generalized Linear Models

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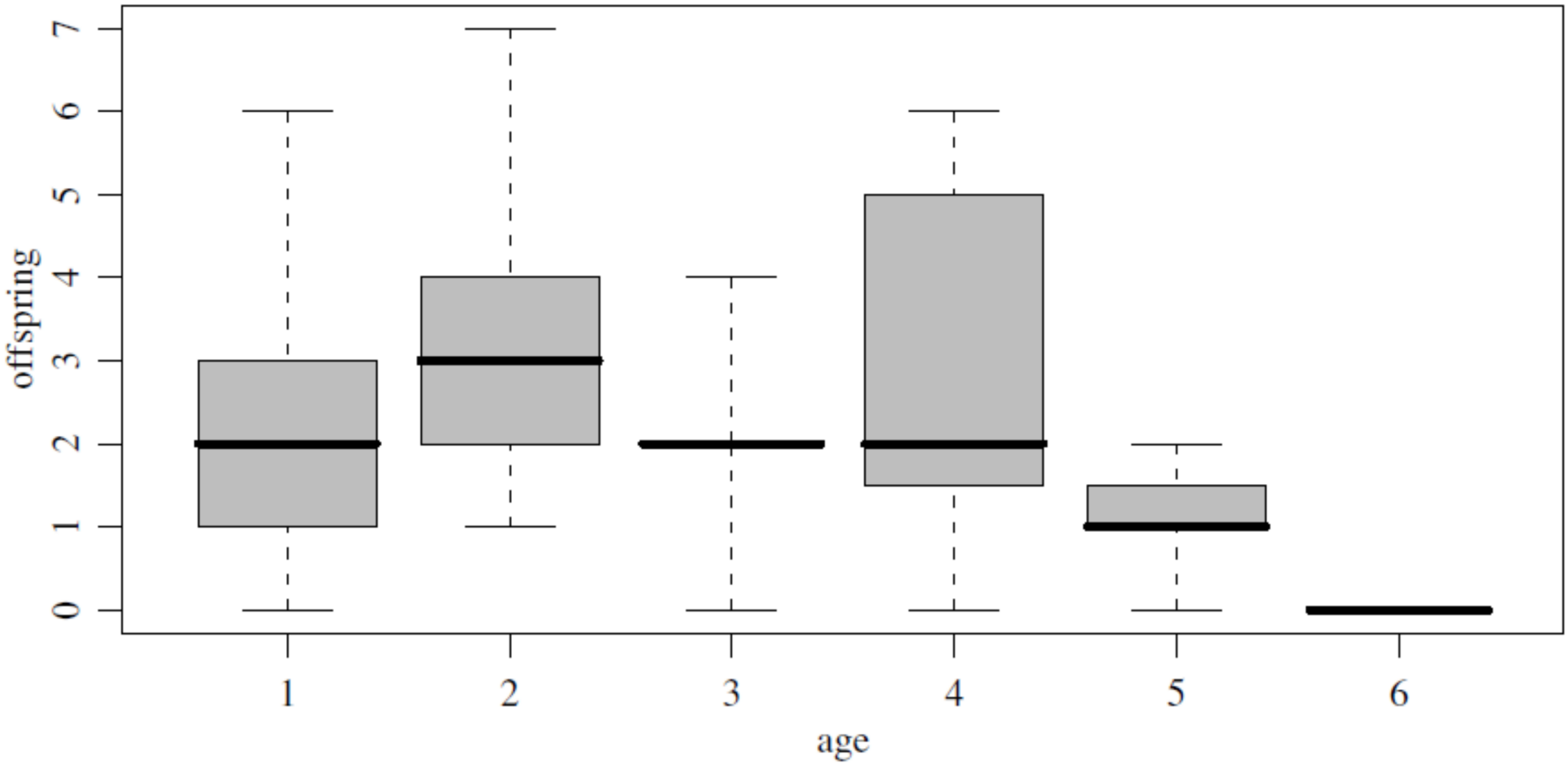
- Goal
  - Understand the relationship between age and reproductive success
  - Make population forecasts for this group of birds

The Data



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- Poisson regression: $y|x \sim Poisson(\exp(\boldsymbol{\beta}^T \boldsymbol{x}))$

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- No conjugate prior for GLM except identity link $\rightarrow$ we need a more general MCMC algorithm than Gibbs sampling

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  - Should we include θ^* into the collection?

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- We can always calculate this ratio easily

$$r = \frac{p(\theta^*|y)}{p(\theta^{(S)}|y)} = \frac{p(y|\theta^*)p(\theta^*)}{p(y)} \frac{p(y)}{p(y|\theta^{(S)})p(\theta^{(S)})} = \frac{p(y|\theta^*)p(\theta^*)}{p(y|\theta^{(S)})p(\theta^{(S)})}$$

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  - Example: $\theta^*|\theta^{(S)} \sim U(\theta^{(S)} - \delta, \theta^{(S)} + \delta)$ or $\theta^*|\theta^{(S)} \sim \mathcal{N}(\theta^{(S)}, \delta^2)$

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- Output: A Markov chain $\{\theta^{(1)}, \ldots, \theta^{(S)}\}$

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- From what we learned before, we can show that $\theta | y \sim \mathcal{N}(10.03, 0.44)$
- Let's sample from the posterior distribution using Metropolis algorithm and compare to exact solution

Example: Normal Model with Known Variance (cont.)

- The acceptance ratio is

$$r = \frac{p(\theta^*|\boldsymbol{y})}{p(\theta^{(s)}|\boldsymbol{y}} = \left(\frac{\prod_{i=1}^n \Phi(y_i, \theta^*, \sigma)}{\prod_{i=1}^n \Phi(y_i, \theta^{(s)}, \sigma)}\right) \times \left(\frac{\Phi(\theta^*, \mu, \tau)}{\Phi(\theta^{(s)}, \mu, \tau)}\right)$$

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- Often, the above calculation is numerically unstable and may compute logarithm instead

$$\log r = \sum_{i=1}^n [\log \Phi(y_i, \theta^*, \sigma) - \log \Phi(y_i, \theta^{(s)}, \sigma)] + [\log \Phi(\theta^*, \mu, \tau) - \log \Phi(\theta^{(s)}, \mu, \tau)].$$

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- On the log scale, proposal is accepted if $\log U(0,1) < \log r$

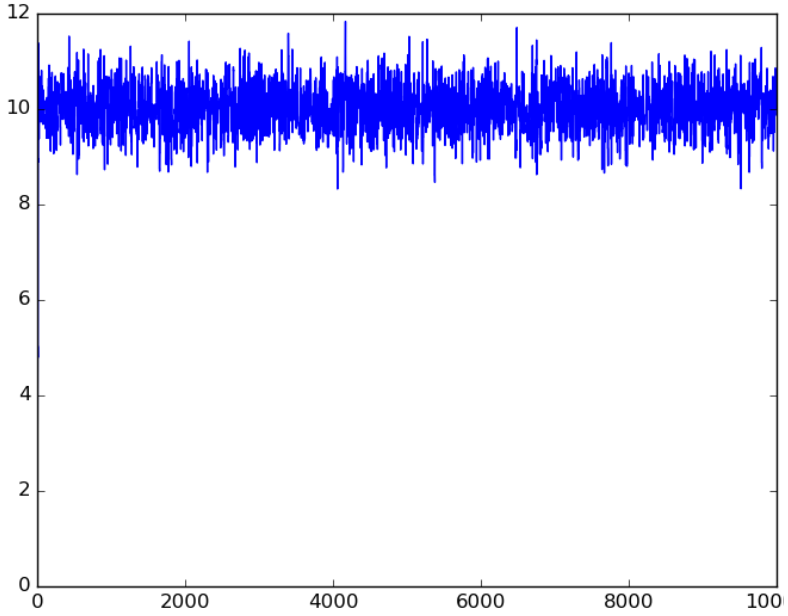
Python Code

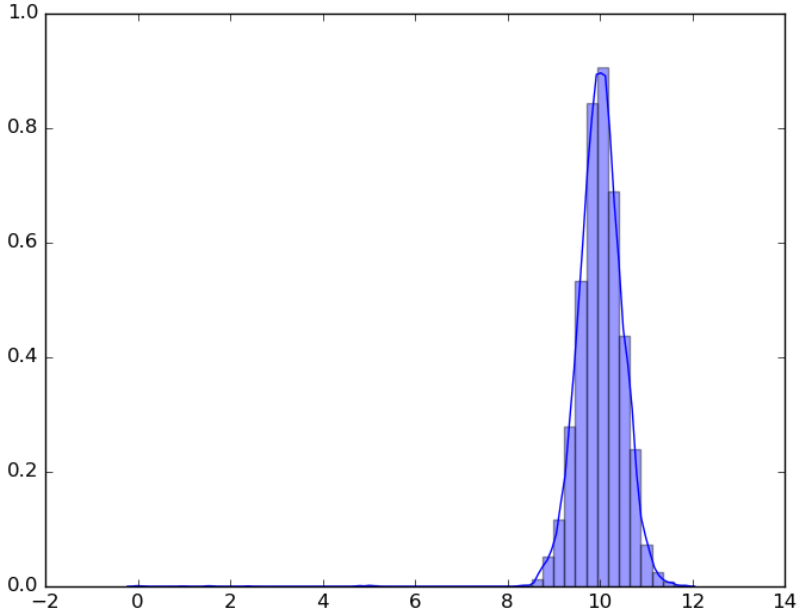
```
import numpy as np
import scipy.stats as stats
s2 = 1
t2 = 10
mu = 5
y = np.array([9.37, 10.18, 9.16, 11.60, 10.33])
theta = 0
delta2 = 2
S = 10000
THETA = []
```

Python Code (cont.)

```
for s in range(S):
    theta_star = np.random.normal(theta, np.sqrt(delta2), 1)
    log_r =
     (np.sum(np.log(stats.norm(theta_star, np.sqrt(s2)).pdf(y))) -
      np.sum(np.log(stats.norm(theta, np.sqrt(s2)).pdf(y)))) +
      (np.log(stats.norm(mu, np.sqrt(t2)).pdf(theta_star)) -
       np.log(stats.norm(mu, np.sqrt(t2)).pdf(theta)))
    if np.log(np.random.random(1)) < log_r:
        theta = theta_star

    THETA.append(theta)

import matplotlib as mpl
import matplotlib.pyplot as plt
plt.style.use('classic')
plt.plot(range(S), THETA)

import seaborn as sns
sns.distplot(THETA, hist = True)
```

Results


12
10
8
6
4
2
0
0
2000
4000
6000
8000
100


1.0
0.8
0.6
0.4
0.2
0.0
−2
0
2
4
6
8
10
12
14

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  - For any given value of θ_a,

$$\lim_{S\to\infty} \frac{\#\{\theta\text{'s in the sequence } < \theta_a\}}{S} = p(\theta < \theta_a|y)$$

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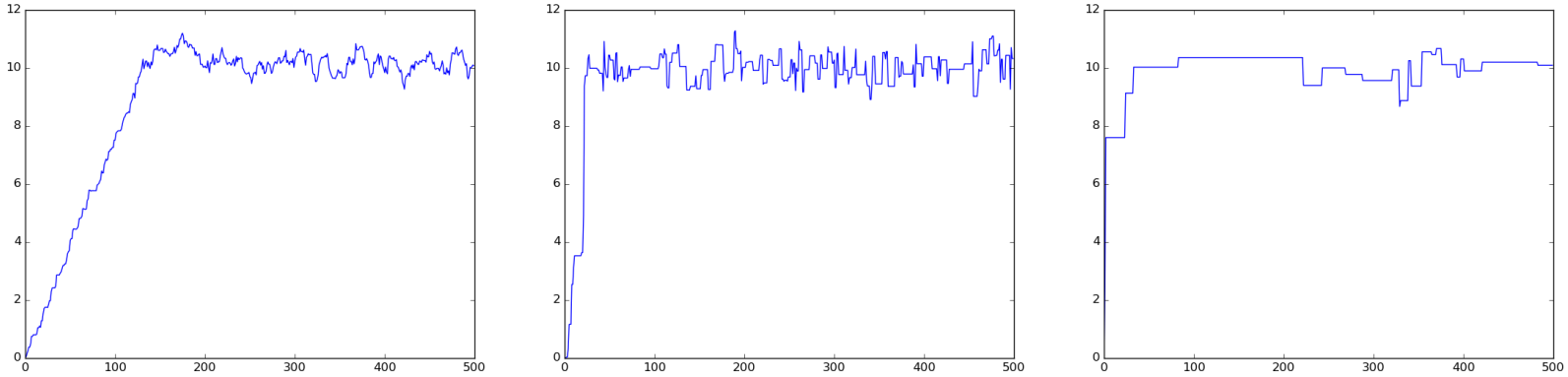
  - Large δ^2: If $\theta^{(s)}$ is close to posterior mode, θ^* is often very far from $\theta^{(s)}$ and leads to rejection. Then the chain gets stuck, because in most iterations $\theta^{(s+1)} = \theta^{(s)}$

Different Proposal Variances

- $\delta^2 = \left\{ \frac{1}{32}, \frac{1}{2}, 2, 32, 64 \right\}$

Different Proposal Variances

- $\delta^2 = \left\{\frac{1}{32}, \frac{1}{2}, 2, 32, 64\right\}$
- Corresponding autocorrelation: $(0.98, 0.77, \mathbf{0.69}, 0.84, 0.86)$



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- Acceptance rate:

$$
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- Proposal distribution: Multivariate normal

Metropolis Algorithm for Poisson Regression

- Model: $\log E(y_i|x_i) - \beta_1 + \beta_2 x_i + \beta_3 x_i^2$
- Let $\boldsymbol{x}_i = (1, x_i, x_i^2)$, then $\log E(y_i|x_i) = \boldsymbol{\beta}'\boldsymbol{x}_i$
- Prior distribution: $\boldsymbol{\beta} \sim \mathcal{N}(0, 100\boldsymbol{I})$
- Acceptance rate:

$$
\begin{aligned}
r &= \frac{p(\boldsymbol{\beta}^*|\boldsymbol{X}, \boldsymbol{y})}{p(\boldsymbol{\beta}^{(s)}|\boldsymbol{X}, \boldsymbol{y})} \\
&= \frac{\prod_{i=1}^n \mathcal{P}(y_i, \boldsymbol{x}_i'\boldsymbol{\beta}^*)}{\prod_{i=1}^n \mathcal{P}(y_i, \boldsymbol{x}_i'\boldsymbol{\beta}^{(s)})} \times \frac{\prod_{j=1}^3 \Phi(\beta_j^*, 0, 10)}{\prod_{j=1}^3 \Phi(\beta_j^{(s)}, 0, 10)}
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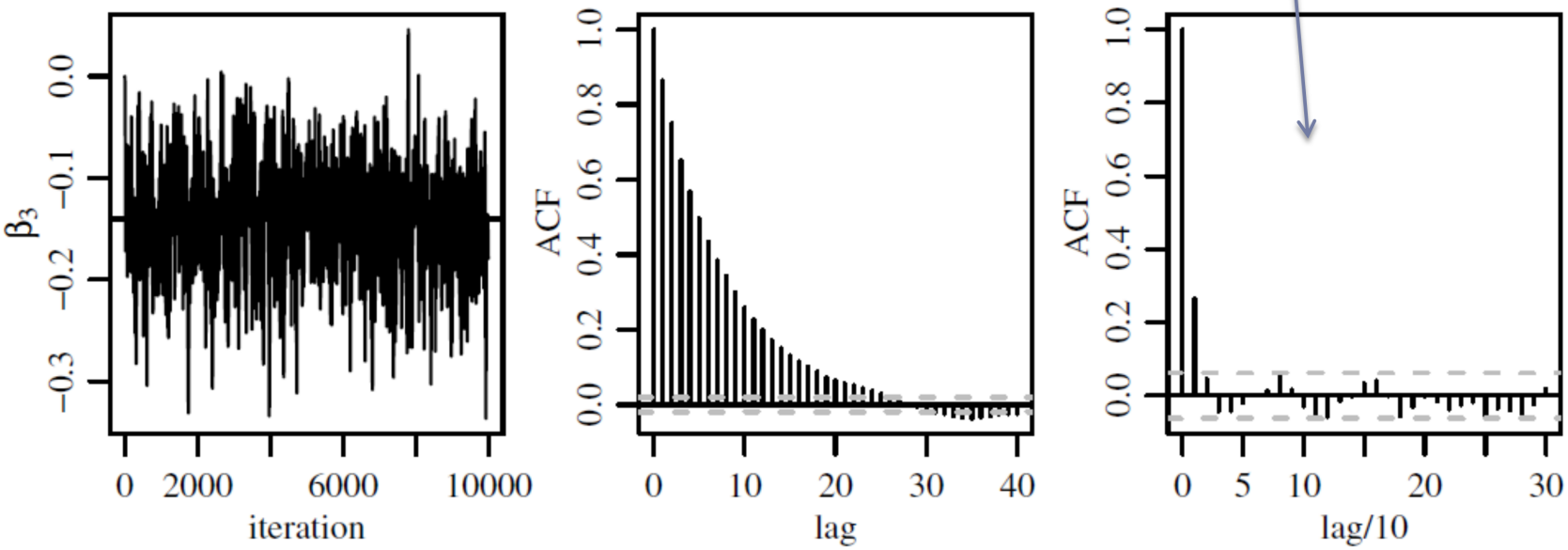
  - Construct $\hat{\sigma}^2$ using the sample variance of $\{\log(y_1 + \frac{1}{2}, \ldots, \log(y_n + \frac{1}{2})\}$

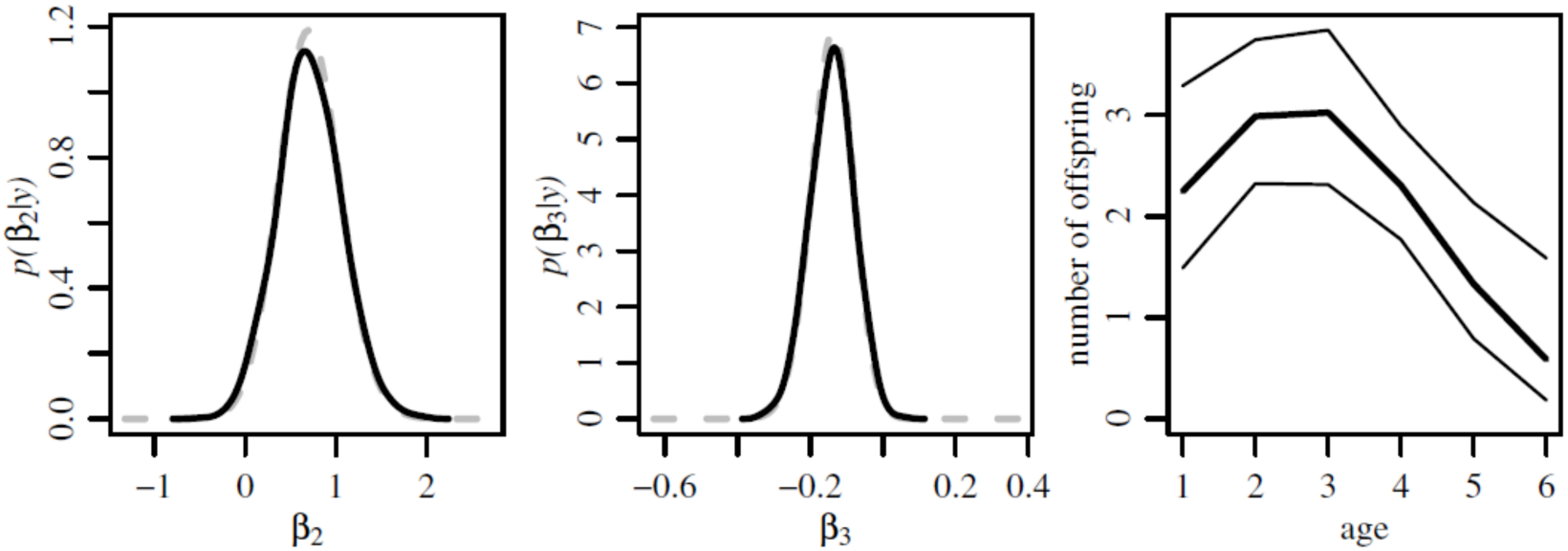
Result

- Acceptance rate: 43%

After thinning (every 10th observation)



Result


p(β2|y)
0.0
0.4
0.8
1.2
−1
0
1
2
β2
p(β3|y)
0
1
2
3
4
5
6
7
−0.6
−0.2
0.2
0.4
β3
number of offspring
0
1
2
3
1
2
3
4
5
6
age

The Metropolis-Hastings (M-H) Algorithm

- Consider to sample from a bivariate distribution $p_0(u, v)$
- Gibbs sampler

1. update U: sample $u^{(s+1)} \sim p_0(u|v^{(s)})$;
2. update V: sample $v^{(s+1)} \sim p_0(v|u^{(s+1)})$.

1. Proposal: full conditional distribution
2. Always accept

- The Metropolis algorithm

1. update U:
   a) sample $u^* \sim J_u(u|u^{(s)})$;
   b) compute $r = p_0(u^*, v^{(s)})/p_0(u^{(s)}, v^{(s)})$;
   c) set $u^{(s+1)}$ to u^* or $u^{(s)}$ with probability $\min(1, r)$ and $\max(0, 1 - r)$.
2. update V:
   a) sample $v^* \sim J_v(v|v^{(s)})$;
   b) compute $r = p_0(u^{(s+1)}, v^*)/p_0(u^{(s+1)}, v^{(s)})$;
   c) set $v^{(s+1)}$ to v^* or $v^{(s)}$ with probability $\min(1, r)$ and $\max(0, 1 - r)$.

Symmetric proposal distribution

The Metropolis-Hastings (M-H) Algorithm (cont.)

- Arbitrary proposal

1. update U:
   a) sample $u^* \sim J_u(u|u^{(s)}, v^{(s)})$;
   b) compute the acceptance ratio

$$r = \frac{p_0(u^*, v^{(s)})}{p_0(u^{(s)}, v^{(s)})} \times \frac{J_u(u^{(s)}|u^*, v^{(s)})}{J_u(u^*|u^{(s)}, v^{(s)})};$$

   c) set $u^{(s+1)}$ to u^* or $u^{(s)}$ with probability $\min(1, r)$ and $\max(0, 1-r)$.
2. update V:
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$$r = \frac{p_0(u^{(s+1)}, v^*)}{p_0(u^{(s+1)}, v^{(s)})} \times \frac{J_v(v^{(s)}|u^{(s+1)}, v^*)}{J_v(v^*|u^{(s+1)}, v^{(s)})};$$

   c) set $v^{(s+1)}$ to v^* or $v^{(s)}$ with probability $\min(1, r)$ and $\max(0, 1-r)$.

Gibbs Sampler as the M-H Algorithm

- If the proposal distribution is $J_u(u^*|u^{(s)}, v^{(s)}) = p_0(u^*|v^{(s)})$ in the M-H algorithm, the acceptance ratio is

$$
\begin{aligned}
r &= \frac{p_0(u^*, v^{(s)})}{p_0 u^{(s)}, v^{(s)}} \times \frac{J_u(u^{(s)}|u^*, v^{(s)})}{J_u(u^*|u^{(s)}, v^{(s)})} \\
&= \frac{p_0(u^*, v^{(s)})}{p_0 u^{(s)}, v^{(s)}} \frac{p_0(u^{(s)}|v^{(s)})}{p_0(u^*|v^{(s)})} \\
&= \frac{p_0(u^*|v^{(s)}) p_0(v^{(s)})}{p_0(u^{(s)}|v^{(s)}) p_0(v^{(s)})} \frac{p_0(u^{(s)}|v^{(s)})}{p_0(u^*|v^{(s)})} \\
&= \frac{p_0(v^{(s)})}{p_0(v^{(s)})} = 1
\end{aligned}
$$

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  - A value x is periodic with period $k > 1$ in a Markov chain if it can only be visited every kth iteration
- Recurrent: A value x is said to be recurrent if, when we continue to run the Markov chain from x, we are guaranteed to eventually return to x. And we want all of the possible values of x to be recurrent in our Markov chain

Ergodic Theorem

- If $\{x^{(1)}, x^{(2)}, \ldots\}$ is an irreducible, aperiodic, and recurrent Markov chain, then there is a unique probability distribution π such that as $s \to \infty$,

$$Pr(x^{(s)} \in A) \to \pi(A) \text{ for any set } A;$$
$$\frac{1}{S}\sum g(x^{(s)}) \to \int g(x)\pi(x)dx.$$

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- $\to$ Once you are sampling from the stationary distribution, you are always sampling from the stationary distribution

Combining the Metropolis and Gibbs Algorithms

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Combining the Metropolis and Gibbs Algorithms

- In complex models it is often the case that conditional distributions are available for some parameters but not others
- In these situations we can combine Gibbs and Metropolis-type proposal distributions to generate a Markov chain to approximate the joint posterior distribution of all the parameters

A Regression Model with Correlated Errors

- Ordinary linear regression

$$\boldsymbol{Y} = \begin{pmatrix} Y_1 \\ \vdots \\ Y_n \end{pmatrix} \sim \text{multivariate normal}(\mathbf{X}\boldsymbol{\beta}, \sigma^2\mathbf{I}).$$

- Introducing AR(1) structure

$$\Sigma = \sigma^2\mathbf{C}_\rho = \sigma^2 \begin{pmatrix} 1 & \rho & \rho^2 & \cdots & \rho^{n-1} \\ \rho & 1 & \rho & \cdots & \rho^{n-2} \\ \rho^2 & \rho & 1 & & \\ \vdots & \vdots & & \ddots & \\ \rho^{n-1} & \rho^{n-2} & & & 1 \end{pmatrix}$$

MCMC

- Prior: $\beta \sim N(\beta_0, \Sigma_0)$ and $\sigma^{-2} \sim gamma(\frac{\nu_0}{2}, \frac{\nu_0 \sigma_0^2}{2})$
- If ρ is known, a Gibbs sampler is available

$$\{\boldsymbol{\beta}|\mathbf{X}, \boldsymbol{y}, \sigma^2, \rho\} \sim \text{multivariate normal}(\boldsymbol{\beta}_n, \Sigma_n) \ , \ \text{where}$$
$$\Sigma_n = (\mathbf{X}^T \mathbf{C}_\rho^{-1} \mathbf{X}/\sigma^2 + \Sigma_0^{-1})^{-1}$$
$$\boldsymbol{\beta}_n = \Sigma_n (\mathbf{X}^T \mathbf{C}_\rho^{-1} \boldsymbol{y}/\sigma^2 + \Sigma_0^{-1} \boldsymbol{\beta}_0) \ , \ \text{and}$$

$$\{\sigma^2|\mathbf{X}, \boldsymbol{y}, \boldsymbol{\beta}, \rho\} \sim \text{inverse-gamma}([\nu_0 + n]/2, [\nu_0 \sigma_0^2 + \text{SSR}_\rho]/2) \ , \ \text{where}$$
$$\text{SSR}_\rho = (\boldsymbol{y} - \mathbf{X}\boldsymbol{\beta})^T \mathbf{C}_\rho^{-1} (\boldsymbol{y} - \mathbf{X}\boldsymbol{\beta}).$$

- But ρ is unknown and the full conditional distribution of ρ is not so simple

MCMC (cont.)

1. Update $\boldsymbol{\beta}$: Sample $\boldsymbol{\beta}^{(s+1)} \sim$ multivariate normal$(\boldsymbol{\beta}_n, \Sigma_n)$, where $\boldsymbol{\beta}_n$ and Σ_n depend on $\sigma^{2(s)}$ and $\rho^{(s)}$.
2. Update σ^2: Sample $\sigma^{2(s+1)} \sim$ inverse-gamma$([\nu_0+n]/2, [\nu_0\sigma_0^2+\mathrm{SSR}_\rho]/2)$, where SSR_ρ depends on $\boldsymbol{\beta}^{(s+1)}$ and $\rho^{(s)}$.
3. Update ρ:
   a) Propose $\rho^* \sim$ uniform$(\rho^{(s)} - \delta, \rho^{(s)} + \delta)$. If $\rho^* < 0$ then reassign it to be $|\rho^*|$. If $\rho^* > 1$ reassign it to be $2 - \rho^*$.
   b) Compute the acceptance ratio

$$r = \frac{p(\boldsymbol{y}|\mathbf{X}, \boldsymbol{\beta}^{(s+1)}, \sigma^{2(s+1)}, \rho^*)p(\rho^*)}{p(\boldsymbol{y}|\mathbf{X}, \boldsymbol{\beta}^{(s+1)}, \sigma^{2(s+1)}, \rho^{(s)})p(\rho^{(s)})}$$

   and sample $u \sim$ uniform(0,1). If $u < r$ set $\rho^{(s+1)} = \rho^*$, otherwise set $\rho^{(s+1)} = \rho^{(s)}$.

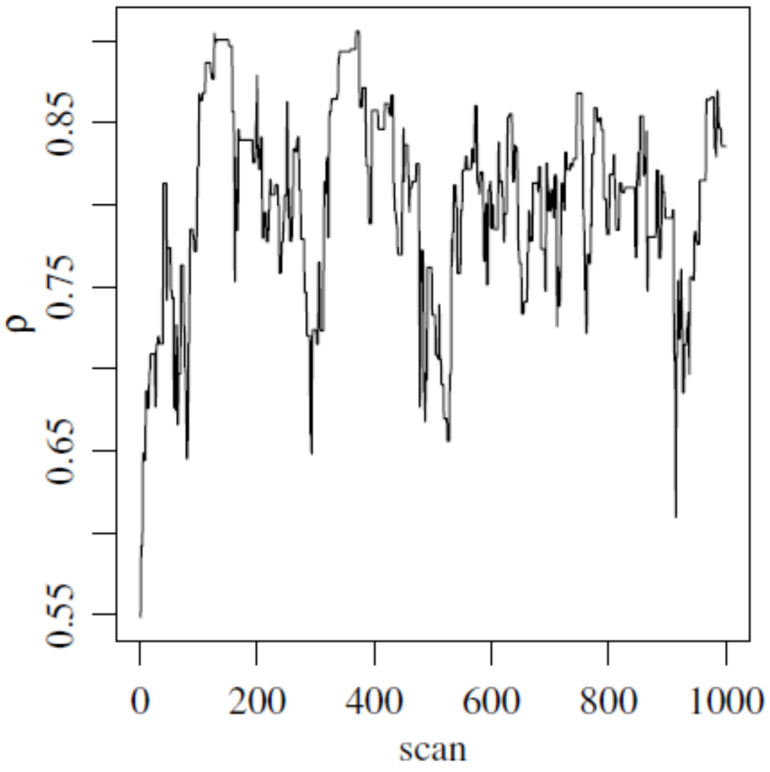
This proposal distribution is called reflecting random walk, which ensures $0 < \rho < 1$

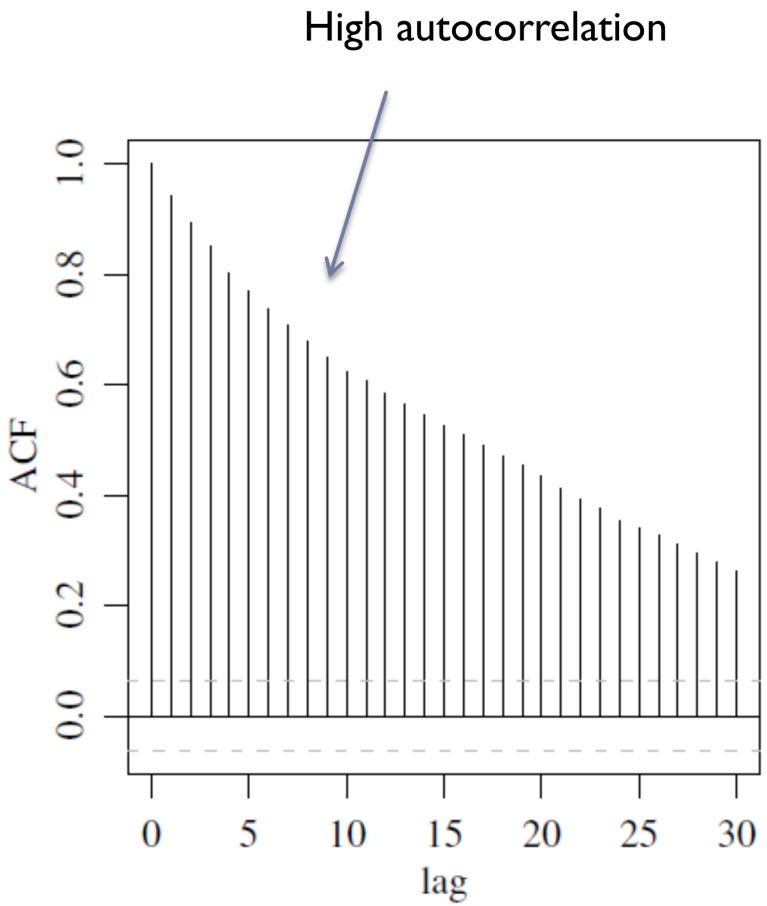
- It is symmetric

Example: Historical CO2 and Temperature Data

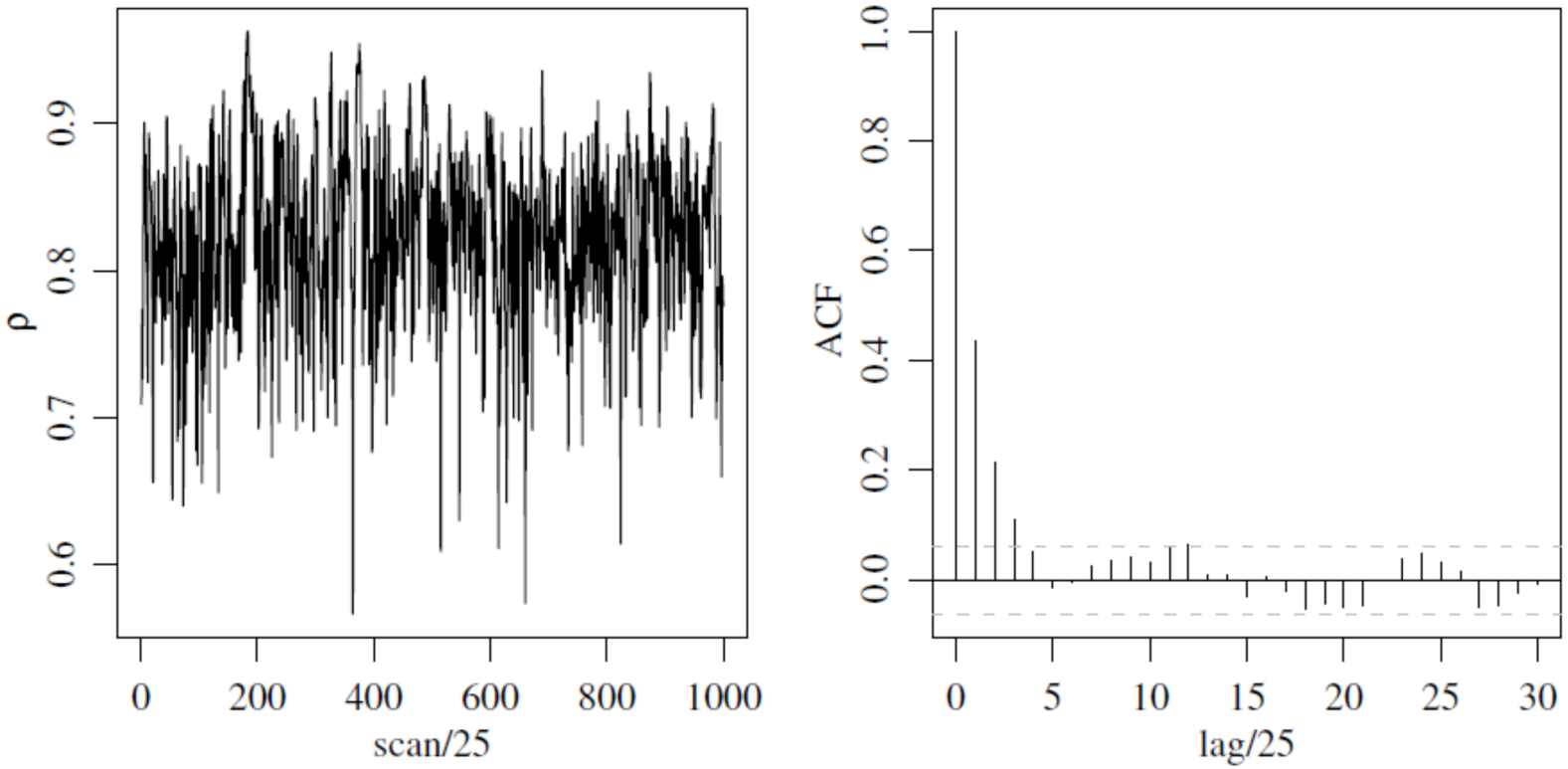
- "diffuse" prior:
  - $\beta \sim N(\beta_0, \Sigma_0)$ and $\sigma^{-2} \sim gamma(\frac{\nu_0}{2}, \frac{\nu_0 \sigma_0^2}{2})$ with $\beta_0 = 0, \Sigma_0 = diag(1000), \nu_0 = 1, \sigma_0^2 = 1$
  - $\rho \sim U(0,1)$

Before Thinning

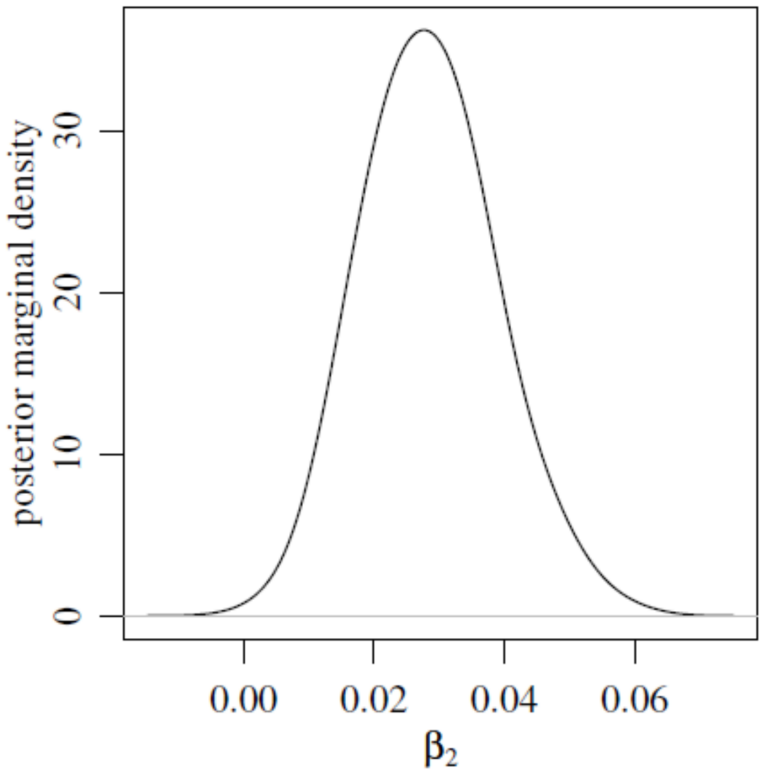


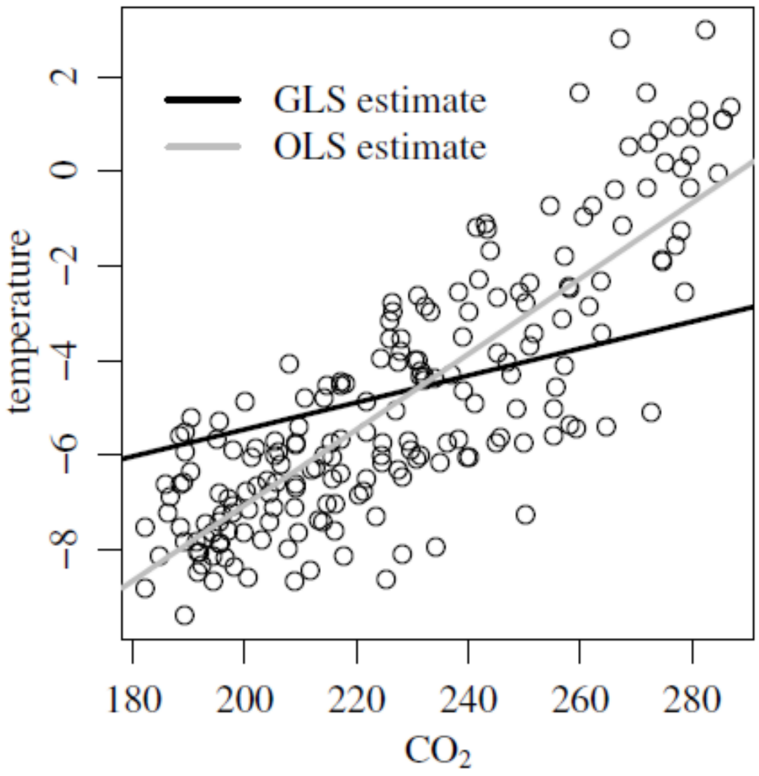


After Thinning (every 25th value)



Posterior


posterior marginal density
0
10
20
30
0.00
0.02
0.04
0.06
β_2


GLS estimate
OLS estimate
temperature
−8
−6
−4
−2
0
2
180
200
220
240
260
280
CO_2

Process the MCMC Output

- Burn-in

Process the MCMC Output

- Burn-in
- Thinning

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- Burn-in
- Thinning
- Monitoring convergence

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- Thinning
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- Tools

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- Monitoring convergence
- Tools
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  - ACF plot
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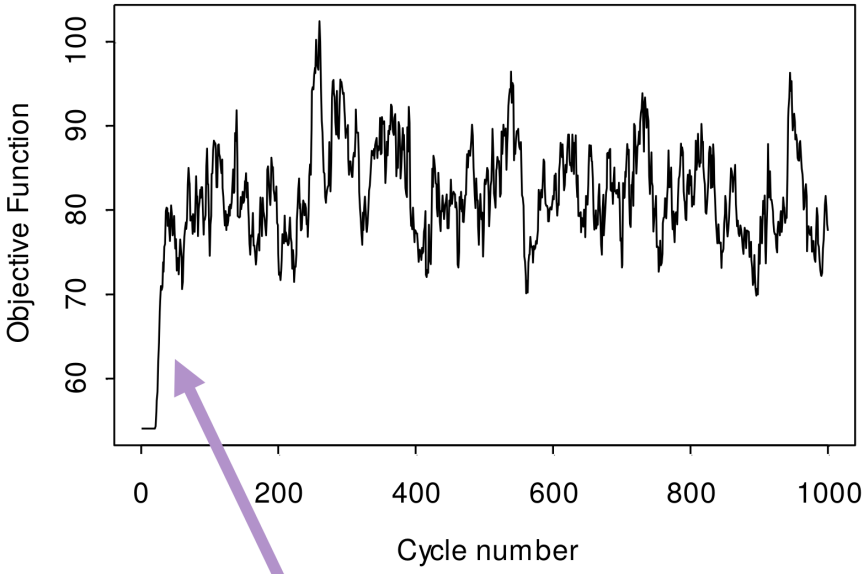
  - Quantitative procedures

Burn-In

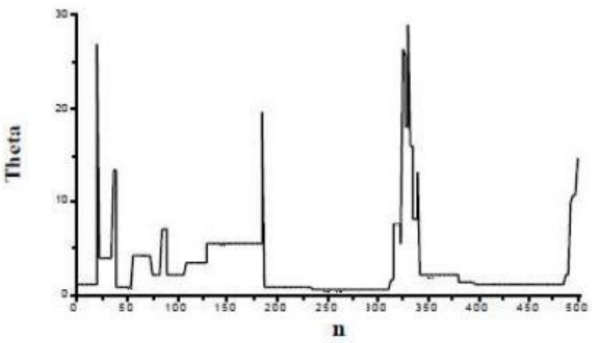


Need for a burn-in (the "pigtail")

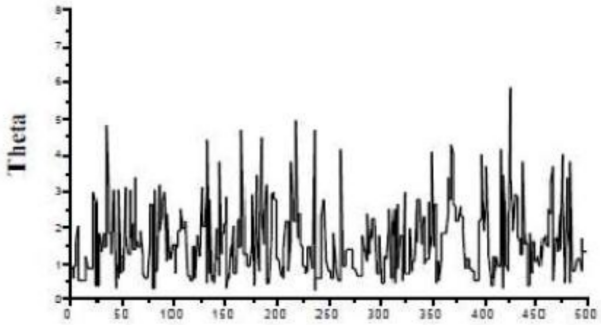
Mixing

- MCMC may have poor mixing when
  - autocorrelation is high
  - it takes a long time between jumps to different parts of the parameter space
  - Looking at the traceplot

- Poor mixing



- Well mixing



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- Based on normal theory approximation to exact Bayesian posterior inference

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- This is called $\hat{R}$

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- Be cautious when using these diagnostics
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- Learn as much as possible about the target density before applying the MCMC algorithm

Hamiltonian MC

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- Hamiltonian MC employs the trick developed by nature. Velocity v is added to the parameters describing the system. Energy of the system consists of potential and kinetic parts
- velocities v and positions x have independent canonical distributions
- So once we can sample from joint distribution $p(x, v)$, we also can sample x by ignoring computed velocities v

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- Hamiltonian MC in most cases accepts new states
- HMC has problems with sampling from distributions with isolated local minimums puck doesn't have enough energy to jump from the first minimum to the second over the energy barrier