STAT 206B Chapter 6: Bayesian Calculations

Winter 2022

† Bayesian Inference

- So far we have discussed the selection of adequate loss function and prior.
- e.g. Consider the problem of estimating $g(\theta)$ under the squared error loss function,

$$\mathsf{E}^{\pi}(g(\theta)\mid x) = \int_{\Theta} g(\theta)\pi(\theta\mid x)d\theta = \frac{\int_{\Theta} g(\theta)f(x\mid \theta)\pi(\theta)d\theta}{\int_{\Theta} f(x\mid \theta)\pi(\theta)d\theta}$$

- $\star\star$ Evaluating the integrals can be quite difficult especially when Θ is high dimensional.
- ** Adapting a different loss function usually makes calculation even more difficult.
- CR Chapter 6 and JB Sections 4.9 & 4.10

• **Example 6.1.1** Consider x_1, \ldots, x_n a i.i.d. sample from $C(\theta, 1)$, a Cauchy distribution with location parameter θ , and $\theta \sim N(\mu, \sigma^2)$ with known hyperparameters μ and σ^2 . The posterior distribution of θ is then

$$\pi(\theta \mid \mathbf{x}) \propto e^{-(\theta-\mu)^2/(2\sigma^2)} \prod_{i=1}^n \{1 + (x_i - \theta)^2\}^{-1}.$$

** How to make an inference about $g(\theta)$, e.g., point estimates, testing or interval estimates?

• **Example 6.1.1**(contd) Under the squared error loss function, the Bayes estimator δ^{π} of θ is the posterior mean,

$$\delta^{\pi}(\mathbf{x}) = \frac{\int_{-\infty}^{\infty} \theta e^{-(\theta-\mu)^2/(2\sigma^2)} \prod_{i=1}^{n} \{1 + (x_i - \theta)^2\}^{-1} d\theta}{\int_{-\infty}^{\infty} e^{-(\theta-\mu)^2/(2\sigma^2)} \prod_{i=1}^{n} \{1 + (x_i - \theta)^2\}^{-1} d\theta}.$$

- ** Observe that closed form integrals are not available.
- ** Observe the calculation requires two numerical integrations.
- ** If we want to compute the posterior variance, it requires an additional integration, $\mathsf{E}^\pi(\theta^2\mid \mathbf{x}) = \int_{-\infty}^\infty \theta^2 \mathrm{e}^{-(\theta-\mu)^2/(2\sigma^2)} \prod_{i=1}^n \{1+(x_i-\theta)^2\}^{-1}d\theta$.

- † We will focus on approximations to $\pi(\theta \mid x)$ and integrals involving $\pi(\theta \mid x)$.
 - Classical approximation methods (CR 6.2)
 Laplace analytic approximation, Monte Carlo integration
 - Markov chain Monte Carlo methods (CR 6.3)
 Metropolis-Hastings algorithms, the Gibbs sampler.
- *Note 1:* Similar techniques can be used to predictive distributions, $f(y \mid x)$.
- *Note 2:* Read Robert and Casella (1999) "Monte Carlo Statistical Methods" for more.

† Classical Approximation Methods (CR 6.2)

Recall we consider the posterior inference problem,

$$\mathsf{E}^{\pi}(g(\theta)\mid x) = \int_{\Theta} g(\theta)\pi(\theta\mid x)d\theta = \frac{\int_{\Theta} g(\theta)f(x\mid \theta)\pi(\theta)d\theta}{\int_{\Theta} f(x\mid \theta)\pi(\theta)d\theta}$$

- Laplace Approximation: attempt to analytically approximate the integral (does not require simulation)
- Monte Carlo methods
- Also see PH Chapter 4 (many examples with R code!) and/or Robert and Casella Chapter 3.

- † Normal Approx. to Posterior (1)
 - General Idea: find a Gaussian approximation to $\pi(\theta \mid \mathbf{x})$.
 - Consider a univariate case;

$$\pi(\theta \mid \mathbf{x}) = \frac{f(\mathbf{x} \mid \theta)\pi(\theta)}{m(\mathbf{x})} \propto q(\theta)$$

** We find θ_0 and A such that $\pi(\theta \mid \mathbf{x}) \approx N(\theta_0, A^{-1})$.

- † Normal Approx. to Posterior (2)
 - θ_0 : a mode of $\pi(\theta \mid \mathbf{x})$, i.e., a mode of $q(\theta)$.

$$\Rightarrow$$
 find θ_0 st $\frac{dq(\theta)}{d\theta} = 0$.

** We can use any algorithms including numerical solution (e.g, Newton-Raphson method, R function optim).

- † Normal Approx. to Posterior (3)
 - Compute a truncated Taylor expansion of $\log\{q(\theta)\}$ at mode θ_0 ,

$$\log \left\{ q(\theta) \right\} \;\; \approx \;\; \log \left\{ q(\theta_0) \right\} + \frac{d \log \left\{ q(\theta) \right\}}{d \theta} \Big|_{\theta = \theta_0} (\theta - \theta_0)$$
$$+ \frac{1}{2} \frac{d^2 \log \left\{ q(\theta) \right\}}{d \theta^2} \Big|_{\theta = \theta_0} (\theta - \theta_0)^2.$$

** Let
$$A = -(d^2 \log \{q(\theta)\}/d\theta^2)\Big|_{\theta=\theta_0}$$
 and we have

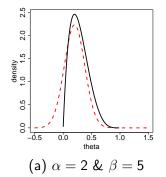
$$\log \{q(\theta)\} \approx \log \{q(\theta_0)\} - \frac{A}{2}(\theta - \theta_0)^2$$

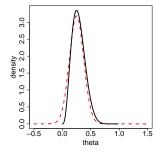
$$\Rightarrow$$
 $q(\theta) \approx q(\theta_0) \exp\left\{-\frac{A}{2}(\theta - \theta_0)^2\right\}$

$$\Rightarrow \pi(\theta \mid \mathbf{x}) \approx N(\theta_0, 1/A).$$

• **Example:** Suppose $\pi(\theta \mid \mathbf{x})$ is Be (α, β) . The Laplace approximation gives us

$$N\left(\frac{\alpha-1}{\alpha+\beta-2},\frac{(\alpha-1)(\beta-1)}{(\alpha+\beta-2)^3}\right),\alpha,\beta>1.$$

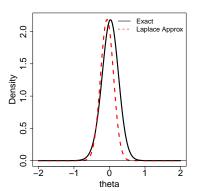




(b)
$$\alpha = 4 \& \beta = 10$$

• **Example:** Simulate a dataset of size n = 15, $x_i \stackrel{iid}{\sim} C(0, 1)$, i = 1, ..., n.

Consider the estimation of the location of x and assume that $x_i \mid \theta \sim C(\theta,1)$ and $\theta \sim N(\mu,\sigma^2)$, with fixed $\mu=0$ and $\sigma^2=25$. We then approximate the posterior distribution of θ using the Laplace approximation.



- † Normal Approx. to Posterior (4)
 - Consider a multivariate case with $\theta = (\theta_1, \dots, \theta_p)$;

$$\pi(\theta \mid \mathbf{x}) \approx \mathsf{N}(\boldsymbol{\theta}_0, A^{-1}),$$

where

** Find
$$\theta_0 = (\theta_{0j}, j = 1, \dots, p)$$
 such that $\frac{\partial q(\theta)}{\partial \theta_{0j}} = 0$.

****** Find A, Hessian matrix evaluated at θ_0 ,

$$A_{ij} = -rac{\partial^2 \log(q(m{ heta}))}{\partial heta_i \partial heta_j}igg|_{m{ heta} = heta_0}$$

- The Laplace approximation is only justified asymptotically Smith et al (1985).
- The Laplace approximation seems to perform quite well in most cases (e.g.: the prior is smooth and the sample size is large) and can be useful as a guide to the solution of the problem.
- Normal approximations are not be useful if the posterior distributions are skewed or multimodal.

† Bayesian CLT

- Suppose $x_i \stackrel{iid}{\sim} f(x \mid \theta)$ where θ is a p-dim parameter and that the prior on θ is $\pi(\theta)$.
- Under some regularity conditions, the posterior probability distribution is approximately a normal distribution as sample size grows.

$$\pi(\theta \mid x) \to \mathsf{N}_p(\theta_0, A^{-1}), \text{ as } n \to \infty,$$

where

- $\star\star$ θ_0 : posterior mode and A: Hassian matrix evaluated at θ_0 .
- The prior can be improper, but assume that the posterior is proper.

** Robert and Casella Example 3.16 (Gamma approximation)

As a simple illustration of the Laplace approximation for an integral, consider estimating a ${\sf Gamma}(\alpha,1/\beta)$ integral,

$$\int_{a}^{b} f(x)dx = \int_{a}^{b} \frac{x^{\alpha-1}}{\Gamma(\alpha)\beta^{\alpha}} e^{-x/\beta} dx.$$

- * check $x_0 = (\alpha 1)\beta$ and $A = 1/(\alpha 1)/\beta^2$.
- * Laplace approx. says

$$f(x) \approx f(x_0) \sqrt{2\pi 1/A} \phi(x_0, 1/A),$$

where $\phi(a, b)$ is the density function of $N(x_0, 1/A)$.

$$\Rightarrow \int_a^b f(x)dx \approx f(x_0)\sqrt{2\pi 1/A} \left\{ \Phi(\sqrt{A}(b-x_0)) - \Phi(\sqrt{A}(a-x_0)) \right\}.$$

**** Robert and Casella Example 3.16** (Gamma approximation – contd) Laplace approx. of a Gamma integral for $\alpha = 5$ and $\beta = 2$.

Interval	Approximation	Exact
(7,9)	0.193351	0.193341
(6, 10)	0.375046	0.37477
(2, 14)	0.848559	0.823349
$(15.987, \infty)$	0.0224544	0.100005

- † Laplace Analytic Approximation (CR 6.2.3)
 - Use the Laplace expansion to directly find

$$E^{\pi}(g(\theta) \mid x) = \frac{\int_{\Theta} g(\theta) f(x \mid \theta) \pi(\theta) d\theta}{\int_{\Theta} f(x \mid \theta) \pi(\theta) d\theta}$$
$$= \frac{\int_{\Theta} \exp{\{\tilde{q}^{\star}(\theta)\} d\theta}}{\int_{\Theta} \exp{\{\tilde{q}(\theta)\} d\theta}},$$

where $\tilde{q}^{\star}(\theta) = \log\{g(\theta)f(x \mid \theta)\pi(\theta)\}\$ and $\tilde{q}(\theta) = \log\{f(x \mid \theta)\pi(\theta)\}\$.

- Suppose $\tilde{q}^{\star}(\theta)$ and $\tilde{q}(\theta)$ have unique maxima, θ_0^{\star} and θ_0 , respectively.
 - ** Let $A^* = -(d^2\tilde{q}^*(\theta)/d\theta^2)\Big|_{\theta=\theta_0^*}$ and $A = -(d^2\tilde{q}(\theta)/d\theta^2)\Big|_{\theta=\theta_0}$

17 / 81

Then expand each in a second order Taylor expansion.

$$\mathsf{E}^{\pi}(g(\theta) \mid x) = \exp\{\tilde{q}^{\star}(\theta_0^{\star}) - \tilde{q}(\theta_0)\} \frac{\sqrt{A}}{\sqrt{A^{\star}}}.$$

- Can be extended for a multivariate θ .
- Lemma 6.2.4 and Corollary 6.2.5 discuss the Laplace approximation for $\mathsf{E}^\pi(g(\theta)\mid x)$. We skip them.

- † Monte Carlo Method (PH 4)
 - Suppose that we have $\theta^{(1)}, \dots, \theta^{(M)}$ iid samples from $\pi(\theta \mid \mathbf{x})$.
 - The law of large numbers implies that as $M \to \infty$,
 - ** Posterior mean

$$ar{ heta} = rac{1}{M} \sum_{m=1}^{M} heta^{(m)}
ightarrow \mathsf{E}(heta \mid oldsymbol{x}).$$

** Posterior variance

$$rac{1}{M-1}\sum_{m=1}^{M}(heta^{(m)}-ar{ heta})^2 o \mathsf{Var}(heta\mid oldsymbol{x}).$$

** Posterior probabilities

$$\frac{1}{M}\#(\theta^{(m)}\leq c)\to \mathsf{P}(\theta\leq c\mid \mathbf{x}).$$

** Posterior distribution function

the empirical distribution of $\{\theta^{(1)}, \dots, \theta^{(M)}\} \to \pi(\theta \mid \mathbf{x})$.

** Posterior percentile

the
$$\alpha$$
-percentile of $\{\theta^{(1)}, \dots, \theta^{(M)}\} \to \theta_{\alpha}$.

****** Suppose $g(\theta) = \log(\theta/(1-\theta))$ for $0 < \theta < 1$

$$\frac{1}{M} \sum_{m=1}^{M} \log \left(\frac{\theta^{(m)}}{1 - \theta^{(m)}} \right) \to \mathsf{E} \left(\log \left(\frac{\theta}{1 - \theta} \right) \mid \mathbf{x} \right).$$

Similarly,

the empirical distribution of $\{g(\theta^{(1)}), \ldots, g(\theta^{(M)})\} \to \pi(g(\theta) \mid \mathbf{x}).$

Posterior predictive distribution

sample
$$x_m^{new} \sim f(x \mid \theta^{(m)})$$

The sequence of $\{x_m^{new}, \dots, x_M^{new}\}$ constitutes M independent samples from the *marginal* posterior distribution of x.

****** Go over Chapter 4 of PH for your practice.

- † An illustration of Monte Carlo approximation: simulation study
 - Suppose we have a dataset of size n=10 with $x_i \in \mathbb{R}$, $i=1,\ldots,n$.
 - ** We consider the estimation problem of the mean of x. For the inference, we use a model that assumes

$$x_i \mid \theta \stackrel{iid}{\sim} N(\theta, \sigma^2)$$
 with fixed $\sigma^2 = 9$,

and consider

$$heta \sim N(\mu, au^2)$$
 with $\mu = 0$ and $au^2 = 2$

for unknown θ .

- † An illustration of Monte Carlo approximation: (contd)
 - We can analytically obtain the posterior distributions of θ and x^{new}

$$\theta \mid \mathbf{x} \sim N(\mu_1, \tau_1^2), \quad \text{and} \quad \mathbf{x}^{\text{new}} \mid \mathbf{x} \sim N(\mu_1, \tau_1^2 + \sigma^2),$$
 where $\tau_1^2 = (n/\sigma^2 + 1/\tau^2)^{-1}$ and $\mu_1 = \tau_1^2 (n\bar{\mathbf{x}}/\sigma^2 + \mu/\tau^2).$

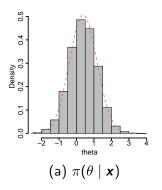
** For our dataset, we obtained

```
> c(post_m, post_var)
[1] 0.3834903 0.6206897
> c(pred_m, pred_var)
[1] 0.3834903 9.6206897
>
```

** Let's numerically approximate posterior quantities using the Monte Carlo method.

Simulate $\theta^{(m)}$ from $N(\mu_1, \tau_1^2)$ and x_m^{new} from $N(\theta^{(m)}, \sigma^2)$, $m = 1, \ldots, M$.

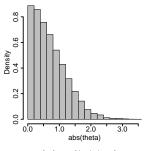
† An illustration of Monte Carlo approximation: (contd)



```
> mean(th_sam); post_m
[1] 0.3863699
[1] 0.3834903
> quantile(th_sam, prob=c(0.025, 0.5, 0.975))
2.5% 50% 97.5%
n-1.1696378 0.3880421 1.9103658
,> qnorm(c(0.025, 0.5, 0.975), post_m. sqrt(post_var))
[1] -1.1606450 0.3834903 1.9276256
> var(th_sam); post_var
[1] 0.6253918
[1] 0.6206897
```

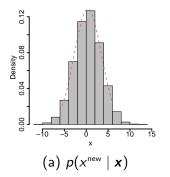
† An illustration of Monte Carlo approximation: (contd)

$$\star\star$$
 Let $g(\theta) = |\theta|$



(a)
$$\pi(|\theta| | \mathbf{x})$$

† An illustration of Monte Carlo approximation: (contd)



† Simulating Samples from Distributions

 Most statistical packages provide random number generators to simulate from common families of distributions, e.g.,

```
> runif(1, 0, 1)
[1] 0.985409
```

- † Simulating Samples from Distributions (contd)
 - Starting with samples from the uniform distribution Unif(0,1), we can generate samples from various distributions through transformations. e.g.,
 - ** If $U \sim \text{Unif}(0,1)$, then $W = -\log(U) \sim \text{Exp}(1)$ and $V = \lambda W \sim \text{Gamma}(1,\lambda)$.
 - ** If $U_1, U_2 \stackrel{iid}{\sim}$ Unif(0,1), we obtain a pair of indep. standard normal random variables $(Z_1, Z_2) = (\sqrt{-2\log(U_1)}\cos(2\pi U_2), \sqrt{-2\log(U_1)}\sin(2\pi U_2))$ by the Box-Muller transformation.

- † Simulating Samples from Distributions (contd)
 - Inverse CDF Method: Use the probability integral transform $U = F(X) = \int_{-\infty}^{x} f(s)ds$.
 - ** We can easily see U have a Unif(0,1) distribution.
 - ** So generate X having cdf F via $X = F^{-1}(U)$ (works nicely when F^{-1} has a simple analytic form).
 - e.g., let X have $\text{Exp}(\lambda)$, i.e., $F(x) = 1 e^{-\lambda x}$.
 - $\star\star$ Generate $U \sim \text{Unif}(0,1)$ and let $X = -\log(1-u)/\lambda$.
 - Also, check rejection sampling, adaptive rejection sampling...

29 / 81

- † Monte Carlo Integration Importance Sampling
 - We can actually generate $(\theta^{(1)}, \dots, \theta^{(M)})$ from a density other than the distribution function of interest and approximate the integral.
 - Suppose h is a probability density function with supp(h) including the support of $g(\theta)f(x \mid \theta)\pi(\theta)$.
 - Recall that we have a problem of approximating

$$\mathsf{E}(g(\theta) \mid \mathbf{x}) = \frac{\int_{\Theta} g(\theta) f(\mathbf{x} \mid \theta) \pi(\theta) d\theta}{\int_{\Theta} f(\mathbf{x} \mid \theta) \pi(\theta) d\theta}$$

We have

$$\mathsf{E}(g(\theta) \mid \mathbf{x}) = \frac{\int_{\Theta} g(\theta) f(\mathbf{x} \mid \theta) \pi(\theta) d\theta}{\int_{\Theta} f(\mathbf{x} \mid \theta) \pi(\theta) d\theta}$$

We express

$$\int_{\Theta} g(\theta) f(x \mid \theta) \pi(\theta) d\theta = \int_{\Theta} \frac{g(\theta) f(x \mid \theta) \pi(\theta)}{h(\theta)} h(\theta) d\theta$$
$$\int_{\Theta} f(x \mid \theta) \pi(\theta) d\theta = \int_{\Theta} \frac{f(x \mid \theta) \pi(\theta)}{h(\theta)} h(\theta) d\theta.$$

• The method of *importance sampling* is an evaluation of the integral based on generating a sample $\theta^{(1)}, \ldots, \theta^{(M)}$ from a given distribution h and approximating

$$\begin{split} \int_{\Theta} g(\theta) f(\mathbf{x} \mid \theta) \pi(\theta) d\theta & \approx & \frac{1}{M} \sum_{m=1}^{M} g(\theta^{(m)}) \frac{f(\mathbf{x} \mid \theta^{(m)}) \pi(\theta^{(m)})}{h(\theta^{(m)})} \\ & = & \frac{1}{M} \sum_{m=1}^{M} g(\theta^{(m)}) w_{m}, \\ & \int_{\Theta} f(\mathbf{x} \mid \theta) \pi(\theta) d\theta & \approx & \frac{1}{M} \sum_{m=1}^{M} w_{m}. \end{split}$$

$$\star\star$$
 $h(\theta)$: importance function

**
$$w_m = w(\theta^{(m)}) = \frac{f(\mathbf{X}|\theta^{(m)})\pi(\theta^{(m)})}{h(\theta^{(m)})}$$
: weights

$$\Rightarrow \mathsf{E}(g(\theta) \mid \mathbf{x}) = \frac{\int_{\Theta} g(\theta) f(\mathbf{x} \mid \theta) \pi(\theta) d\theta}{\int_{\Theta} f(\mathbf{x} \mid \theta) \pi(\theta) d\theta} \approx \frac{\frac{1}{M} \sum_{m=1}^{M} g(\theta^{(m)}) w_{m}}{\frac{1}{M} \sum_{m=1}^{M} w_{m}}.$$

- Example (Example 6.1.1 with some changes)
 - ** Consider a dataset $\mathbf{x} = (x_1, \dots, x_n)$ with n = 10, where x_i 's simulated from N(0, 9).
 - $\star\star$ We consider the estimation problem of the mean of x. For the inference, we use a model that assumes

$$x_i \mid \theta \stackrel{iid}{\sim} N(\theta, \sigma^2)$$
 with fixed $\sigma^2 = 9$,

and consider

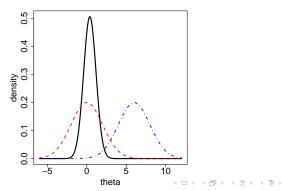
$$\theta \sim N(\mu, \tau^2)$$
 with $\mu = 0$ and $\tau^2 = 2$

for unknown θ .

** Suppose we use the Bayes estimator under the squared error loss (the posterior mean)

$$\delta^{\pi}(\mathbf{x}) = \mathsf{E}(\theta \mid \mathbf{x}) = \left(\frac{1}{\sigma^2/n} + \frac{1}{\tau^2}\right)^{-1} \left(\frac{\bar{\mathbf{x}}}{\sigma^2/n} + \frac{\mu}{\tau^2}\right).$$

- Example (contd)
 - For my simulated dataset, the exact value of $\delta^{\pi}(\mathbf{x}) = 0.38349$
 - Let's use the importance sampling method to numerically approximate $\delta^{\pi}(\mathbf{x})$;
 - ** Case 1: $h(\theta) = N(0, 2^2)$
 - ** Case 2: $h(\theta) = N(6, 2^2)$



- Generate $\theta^{(m)}$, $m=1,\ldots,M$ from $N(a,v^2)$ for large enough M.
- Compute

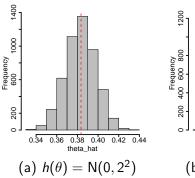
$$\hat{\delta}^{\pi}(\mathbf{x}) = \frac{\sum_{m=1}^{M} \theta^{(m)} w_m}{\sum_{m=1}^{M} w_m},$$

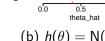
where
$$w_m = w(\theta^{(m)}) = \frac{f(\mathbf{X}|\theta^{(m)})\pi(\theta^{(m)})}{h(\theta^{(m)})}$$
 .

```
>
> c(post_mean_0, post_mean_1, post_mean_2)
[1]_0.3834903 0.3885833 0.2876347
```

• Example (contd)

* Repeat 5000 times and make histograms of approximated $\delta^{\pi}(\mathbf{x})$ for the same dataset.





$$0.0 0.5 1.0$$
(b) $h(\theta) = N(6, 2^2)$

- **Example** Case 1: $h(\theta) = N(0, 2^2)$
- > summary(imp_v)
 Min. 1st Qu. Median Mean 3rd Qu. Max.
 0.000e+00 7.821e-14 9.000e-13 1.343e-12 2.580e-12 3.594e-12
- Case 2: $h(\theta) = N(6, 2^2)$
- > summary(imp_v)
 Min. 1st Qu. Median Mean 3rd Qu. Max.
 0.000e+00 0.000e+00 0.000e+00 1.592e-12 0.000e+00 3.743e-10
- ** Recall: $w_m = w(\theta^{(m)}) = \frac{f(x|\theta^{(m)})\pi(\theta^{(m)})}{h(\theta^{(m)})}$: weights.

Remarks

- ** Simulation according to *h* must be easily implemented, requiring a fast and reliable pseudo-random generator.
- $\star\star$ h can be almost any density but the choice of the importance function h is crucial.
- ** The function $h(\theta)$ must be close enough to $g(\theta)\pi(\theta)$ to reduce the variability of $\hat{E}(g(\theta) \mid x)$.
- ** Obviously there are some choices that are better than others, and it is natural to try to compare different distinctions h for the evaluation of $\mathsf{E}(g(\theta) \mid x)$.

- † Markov chain Monte Carlo (MCMC) methods (CR 6.3)
 - A more general Monte Carlo method that approximates the generation of random variables from $\pi(\theta \mid x)$.
 - A Markov chain is a sequence of random variables $\theta^{(1)}, \theta^{(2)}, \ldots$, where for any t, the distribution of $\theta^{(t)}$ given all previous θ 's depends only on the most recent value, $\theta^{(t-1)}$.
 - i.e., draw $\theta^{(t)}$ from a transition distribution, $T(\theta^{(t)} \mid \theta^{(t-1)})$.
 - If $T(\cdot \mid \cdot)$ satisfies certain conditions, the distribution of $\theta^{(t)}$ converges to a unique stationary distribution that is the posterior distribution as t grows, regardless of where the chain was initiated.

- The working principle of MCMC algorithms
 - For an arbitrary starting value $\theta^{(0)}$, a chain $(\theta^{(t)})$ is generated using a transition kernel with stationary distribution $\pi(\theta \mid \mathbf{x})$.

Note: we will discuss schemes to produce valid transition kernels associated with arbitrary stationary distributions.

- Markov chain theory asserts that we will eventually sample from the target distribution π .
- Given that the chain is ergodic, the starting value $\theta^{(0)}$ is, in principle, unimportant.
- Draws from the chain are slightly dependent, but independence of $(\theta^{(1)},\ldots,\theta^{(T)})$ is not critical for an approximation of the form $\mathsf{E}(g(\theta)\mid x) \approx \frac{1}{T}\sum_{t=1}^T g(\theta^{(t)})$ (Ergodic Theorem).

- † How to build a transition kernel such that the Markov chain converges to a unique stationary distribution that is our posterior distribution $\pi(\theta \mid \mathbf{x})$.
 - Metropolis-Hastings algorithms (CR 6.3.2, PH Chapter 10, BDA Chapter 11.2)
 - The Gibbs sampler (CR 6.3.3, PH Chapter 6, BDA Chapter 11.1)
 - Building Markov chain algorithms using the Gibbs sampler and Metropolis algorithm

† Metropolis-Hastings algorithms

- 1. Start with an arbitrary initial value $\theta^{(0)}$.
- 2. Update from $\theta^{(t-1)}$ to $\theta^{(t)}$ (t=1,2,...) by
 - 2.1 Generate $\xi \sim q(\xi \mid \theta^{(t-1)})$
 - 2.2 Define

$$\rho(\theta^{(t-1)}, \xi) = \min \left\{ \frac{\pi(\xi) q(\theta^{(t-1)} \mid \xi)}{\pi(\theta^{(t-1)}) q(\xi \mid \theta^{(t-1)})}, 1 \right\}.$$

2.3 Take

$$\theta^{(t)} = \begin{cases} \xi & \text{with probability } \rho(\theta^{(t-1)}, \xi), \\ \theta^{(t-1)} & \text{otherwise.} \end{cases}$$

- † Metropolis-Hastings algorithms contd
 - The distribution with density $\pi(\theta)$ (can be known upto a normalizing factor) is called the *target* or *objective distribution*.
 - The distribution with density $q(\cdot \mid \theta)$ (a conditional density) is the *proposal distribution* (candidate generating, or instrumental distribution).
 - Conditions for the proposal distribution
 - ** The support of $q(\cdot \mid \theta)$ contain the support of π for every θ .
 - ** $q(\cdot \mid \theta)$ is positive in a neighborhood of θ of fixed radius.
 - The probability $\rho(\theta, \xi)$ is called the *Metropolis-Hastings acceptance probability.*

† Proposal distributions

- A good proposal density q has the following properties:
 - ****** For any $\xi \in \Theta$, it is easy to sample from $q(\xi \mid \theta^{(t-1)})$.
 - ****** It is easy to compute ρ
 - ** Each move goes a reasonable distance in the parameter space (otherwise the chain moves too slowly)
 - ** The jumps are not rejected too frequently (otherwise the chain wastes too much time standing still)
- The infinite number of proposed distributions yield a Markov chain that converges to the distribution of interest.
 - ** Random-walk proposal: $q(\xi \mid \theta)$ is of the form $f(||\theta \xi||)$.
 - ** Independence proposal: $q(\xi \mid \theta) = h(\xi)$.

- M-H with Random-walk Proposal
 - ** Recall $q(\xi \mid \theta)$ is of the form $f(||\theta \xi||)$.
 - ** \Rightarrow The proposed value ξ is of the form $\xi = \theta^{(t-1)} + \epsilon$, where ϵ is distributed as a symmetric random variable.
 - $\star\star$ The standard choices for f are uniform, normal or Cauchy.
 - ** Idea: Perturb the current value of the chain at random, while staying in a neibhborhood of this value and then see if the new value ξ is likely for the distribution of interest.

- M-H with Random-walk Proposal (contd)
- Since $q(\theta^{(t-1)} \mid \xi) = q(\xi \mid \theta^{(t-1)})$, the acceptance probability is

$$ho = \min \left\{ rac{\pi(\xi)}{\pi(heta^{(t)})}, 1
ight\}.$$

- ** Appears to be the "gold standard" of MCMC techniques.
- M-H with Independent Proposal: density $q(\cdot \mid \theta)$ does not depend on θ , $q(\xi \mid \theta) = h(\theta)$.
 - $\star\star$ For good performance, h should fit the target distribution.
 - ⇒ limited applicability.
- Read BDA Section 12.2 for Efficient Metropolis jumping rules.

- † Checking Convergence BDA Section 11.4
 - <u>Possible problem 1:</u> If the iterations have not proceeded long enough, the simulations may be grossly unrepresentative of the target distribution.
 - <u>Possible problem 2:</u> Even when the simulations have reached approximate convergence, the early iterations still are influenced by the starting approximation rather than the target distribution.
 - <u>Possible problem 3:</u> Iterative simulation draws have within-sequence correlations which may cause some convergence issues.

† Checking Convergence - contd.

• Burn-in:

To diminish the effect of the starting distribution, discard early iterations of the simulation runs.

• Thin:

To diminish the dependence of the iterations in a sequence, thin the sequence by keeping every kth simulation draw and discard the rest.

- Run multiple sequences with overdispersed starting points:
 Run multiple sequences with different starting points and compare them.
- May check the sample autocorrelation, the effective sample size....

- **Example 4:** Let $\pi(\theta)$ be IG(a, b) with a = 3 and b = 3 (that is, mean=1.5 and sd=1.5). Simulate θ using a M-H algorithm.
 - **** Strategy 1:** Use with random-walk proposal on $\theta \in \mathbb{R}^+$
 - **Strategy 2:** Use with random-walk proposal on $\eta = \log(\theta) \in \mathbb{R}$

$$\pi_1(\eta) = rac{b^a}{\Gamma(a)} \left(e^{\eta}
ight)^{-a} \exp\left(-rac{b}{e^{\eta}}
ight).$$

 \Rightarrow draw a sample of η and let $\theta = \log(\eta)$.

- Strategy 1: Use with Random-walk Proposal
 - 1. Specify a proposal distribution, $q(\xi \mid \theta) = N(\theta, 0.8^2)$.
 - 2. Let $\theta^{(0)} = 1.0$ for a starting value.
 - 3. Iterate for t = 1, ..., T (= 10000)
 - 3.1 Generate $\xi \sim N(\theta^{(t-1)}, 0.8^2)$
 - 3.2 Compute the acceptance probability

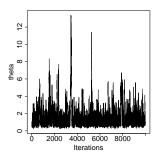
$$\rho = \min \left\{ \frac{\xi^{-\mathsf{a}-1} \exp(-b/\xi)}{\left(\theta^{(t-1)}\right)^{-\mathsf{a}-1} \exp(-b/\theta^{(t-1)})}, 1 \right\}$$

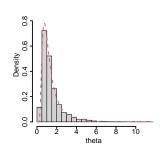
3.3 Generate $r \sim \text{Unif}(0,1)$ and take

$$\theta^{(t)} = \begin{cases} \xi & \text{if } r < \rho, \\ \theta^{(t-1)} & \text{otherwise.} \end{cases}$$

4. Discard the first 4000 iterations and keep every other iteration from the remaining.

• Example 4: - Strategy 1 (contd)





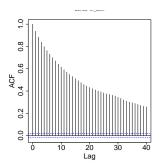
> mean(th_sam)

[1] 1.443216

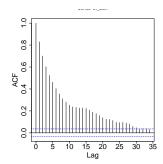
> sd(th_sam)

[1] 1.057938

• Example 4: - Strategy 1 (contd)



(a) Including Burn-in before thinning



(b) Discard burn-in after thinning

• Example 4: - Strategy 1 (contd) Autocorrelation plots

```
> library(coda)
> effectiveSize(th_sam)
    var1
238.1634
```

* The precision of the MCMC approximation to $E(\theta \mid x)$ is as good as the precision that would have been obtained by about 238 independent samples of θ .

- **Strategy 2:** Use with Random-walk Proposal for $\eta = \log(\theta)$
 - 1. Specify a proposal distribution, $q(\xi \mid \eta) = N(\eta, 0.5^2)$.
 - 2. Let $\eta^{(0)} = \log(1.0)$ for a starting value.
 - 3. Iterate for t = 1, ..., T (= 10000)
 - 3.1 Generate $\xi \sim N(\eta^{(t-1)}, 0.5^2)$
 - 3.2 Compute the acceptance probability

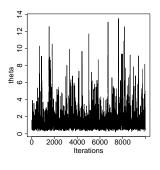
$$\rho = \min \left\{ \frac{(e^{\xi})^{-a} \exp(-b/e^{\xi})}{(e^{\eta^{(t-1)}})^{-a} \exp(-b/e^{\eta^{(t-1)}})}, 1 \right\}$$

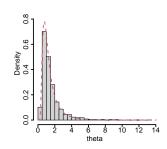
3.3 Generate $r \sim \text{Unif}(0,1)$ and take

$$\eta^{(t)} = \begin{cases} \xi & \text{if } r < \rho, \\ \theta^{(t-1)} & \text{otherwise.} \end{cases}$$

- 4. Let $\theta^{(t)} = e^{\eta^{(t)}}$
- 5. Discard the first 4000 iterations and keep every other iteration from the remaining.

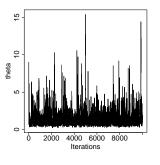
• Example 4: - Strategy 2 (contd)

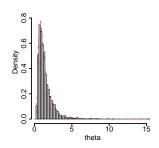




```
> mean(exp(eta_sam))
[1] 1.537653
> sd(exp(eta_sam))
[1] 1.250824
> effectiveSize(exp(eta_sam))
    var1
474.8557
```

- Example 4: Strategy 2 (contd)
- * different initial value, $\eta^{(0)} = 10$.





```
> mean(exp(eta_sam))
[1] 1.450118
> sd(exp(eta_sam))
[1] 1.141774
> effectiveSize(exp(eta_sam))
    var1
505.196
```

• Example 6.3.2: Weibull distributions are used extensively in reliability and other engineering applications, partly for their ability to describe different hazard rate behaviors, and partly for historic reasons. Suppose x_i is a random sample of size n from the Weibull distribution

$$f(x \mid \alpha, \eta) \propto \alpha \eta x^{\alpha - 1} e^{-x^{\alpha} \eta}$$
.

For $\theta = (\alpha, \eta) \in (\mathbb{R}^+, \mathbb{R}^+)$, consider the prior

$$\pi(\theta) \propto \underbrace{e^{-\alpha}}_{=\pi_1(\alpha)} \underbrace{\eta^{\beta-1} e^{-\xi\eta}}_{\pi_2(\eta)}.$$

That is, assume a priori independence and place E(1) and Gamma(β, ξ) (with mean β/ξ) for α and η , respectively. Let $\beta=1$ and $\xi=0.01$.

Simulate θ from $\pi(\theta \mid \mathbf{x})$ using a Metropolis-Hastings algorithm.

****** Find the posterior distribution of θ .

$$\pi(\alpha, \eta \mid \mathbf{x}) \propto f(\mathbf{x} \mid \alpha, \eta) \pi(\alpha, \eta)$$

$$\propto \prod_{i=1}^{n} \left\{ \alpha \eta x_{i}^{\alpha-1} e^{-x_{i}^{\alpha} \eta} \right\} e^{-\alpha} \eta^{\beta-1} e^{-\xi \eta}$$

$$\propto \alpha^{n} \eta^{n+\beta-1} \prod_{i=1}^{n} x_{i}^{\alpha-1} \exp \left\{ -\eta \sum_{i=1}^{n} x_{i}^{\alpha} - \alpha - \xi \eta \right\}.$$

 $\star\!\star$ Let $z_1 = \log(\alpha) \in \mathbb{R}$ and $z_2 = \log(\eta) \in \mathbb{R}$ and find

$$\pi_{1}(\mathbf{z} \mid \mathbf{x}) \propto (e^{z_{1}})^{(n+1)}(e^{z_{2}})^{(n+\beta)}$$

$$\prod_{i=1}^{n} x_{i}^{e^{z_{1}}-1} \exp \left\{-e^{z_{1}} \sum_{i=1}^{n} x_{i}^{e^{z_{1}}} - e^{z_{1}} - \xi e^{z_{1}}\right\},$$

where $z = (z_1, z_2)$

- Example 6.3.2: (contd) Use MH with Random-walk Proposal
 - 1. Specify a proposal distribution, $q(\xi \mid \mathbf{z}) = N(z_1, 0.05)N(z_2, 0.1)$.
 - 2. Let $z^{(0)} = (1.0, 1.0)$ for a starting value.
 - 3. Iterate for $t = 1, \ldots, T$
 - 3.1 Generate $\xi_1 \sim N(z_1^{(t-1)}, 0.05)$ and $\xi_2 \sim N(z_2^{(t-1)}, 0.1)$ and let $\boldsymbol{\xi} = (\xi_1, \xi_2)$.
 - 3.2 Compute the acceptance probability

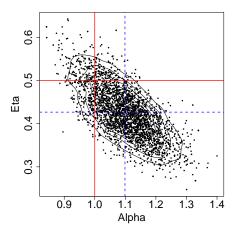
$$\rho = \min \left\{ \frac{\pi(\boldsymbol{\xi} \mid \boldsymbol{x})}{\pi(\boldsymbol{z}^{(t-1)} \mid \boldsymbol{x}))}, 1 \right\}$$

3.3 Generate $r \sim \text{Unif}(0,1)$ and take

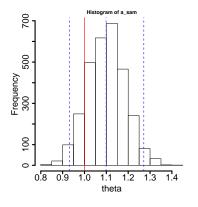
$$\mathbf{z}^{(t)} = egin{cases} \mathbf{\xi} & \text{if } r < \rho, \\ \mathbf{z}^{(t-1)} & \text{otherwise}. \end{cases}$$

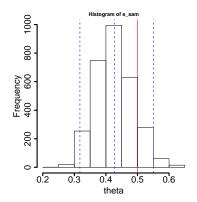
- 4. Let $\alpha^{(t)} = \exp(z_1^{(t)})$ and $\eta^{(t)} = \exp(z_2^{(t)})$
- 5. Discard the first 4000 iterations and keep every other iteration from the remaining.

- **Example 6.3.2:** (contd)
- * Joint posterior distribution $\pi(\alpha, \eta \mid \mathbf{x})$



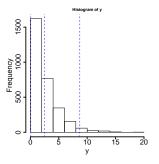
* Marginal posterior distributions $\pi(\alpha \mid \mathbf{x}) \& \pi(\eta \mid \mathbf{x})$





• **Example 6.3.2:** (contd) Predictive distribution $f(y \mid x)$

** obtain a sample from the posterior predictive distribution by simulating $y^{(t)} \sim \text{Weibull}(\alpha^{(t)}, \eta^{(t)})$.



Let's consider the following,

$$\pi(\theta \mid x) = \int \pi_1(\theta \mid x, \lambda) \pi_2(\lambda \mid x) d\lambda.$$

Generating a sample of θ from $\pi(\theta \mid x)$ is equivalent to

- ****** Generating $\lambda^{(t)}$ from $\pi_2(\lambda \mid x)$.
- ****** Generating $\theta^{(t)}$ from $\pi_1(\theta \mid x, \lambda^{(t)})$

• **Example 6.3.4:** Consider $(\theta, \lambda) \in \mathbb{N} \times [0, 1]$ and

$$\pi(\theta, \lambda \mid x) \propto \binom{n}{\theta} \lambda^{\theta + \alpha - 1} (1 - \lambda)^{n - \theta + \beta - 1}$$

- ****** Suppose we want to simulate θ from $\pi(\theta \mid x)$.
- ** We can find that the marginal distribution of θ is a beta-binomial distribution (n, α, β) ,

$$\pi(\theta \mid x) = \binom{n}{\theta} \frac{B(\alpha + \theta, \beta + n - \theta)}{B(\alpha, \beta)}.$$

It is not easy to simulate θ from $\pi(\theta \mid x)$.

• **Example 6.3.4:** (contd) Consider $(\theta, \lambda) \in \mathbb{N} \times [0, 1]$ and

$$\pi(\theta, \lambda \mid x) \propto \binom{n}{\theta} \lambda^{\theta + \alpha - 1} (1 - \lambda)^{n - \theta + \beta - 1}$$

- ** Alternatively, we utilize the hierarchical structure,
 - 1. Simulate $\lambda^{(t)}$ from $\pi_2(\lambda \mid x) = \text{Be}(\alpha, \beta)$.
 - 2. Simulate $\theta^{(t)}$ from $\pi_1(\theta \mid x, \lambda^{(t)}) = \text{Binom}(n, \lambda^{(t)})$.
- ****** We obtain a sample of (θ, λ) from $\pi(\theta, \lambda \mid x)$.
- ** A sample of $\{\theta^{(t)}\}$ can be used to infer $\pi(\theta \mid x)$.

† Let's reconsider

$$\pi(\theta \mid x) = \int \pi_1(\theta \mid x, \lambda) \pi_2(\lambda \mid x) d\lambda.$$

- How can we simulate θ from $\pi(\theta \mid x)$ if $\pi_2(\lambda \mid x)$ is not available?
- Often both $\pi_1(\theta \mid x, \lambda)$ and $\pi_2(\lambda \mid x, \theta)$ can be simulated.
- Possible to simulate θ using the conditionals, $\pi_1(\theta \mid x, \lambda)$ and $\pi_2(\lambda \mid x, \theta)$.

† The Gibbs sampler (CR 6.3.3, BDA Section 11.1 and PH Chapter 6)

- 1. Start with an arbitrary value $\lambda^{(0)}$.
- 2. Given $\lambda^{(t-1)}$, $t=1,\ldots,T$, generate 2.1 $\theta^{(t)}$ from $\pi_1(\theta \mid x, \lambda^{(t-1)})$.
 - 2.2 $\lambda^{(t)}$ from $\pi_2(\lambda \mid x, \theta^{(t)})$.
- \Rightarrow { $(\theta^{(t)}, \lambda^{(t)}), t = 1, ..., T$ } is a sample of (θ, λ) from their joint distribution.
- \Rightarrow $\{\theta^{(t)}, t = 1, ..., T\}$ is a sample of θ from its marginal distribution.
- \Rightarrow $\{\lambda^{(t)}, t = 1, ..., T\}$ is a sample of λ from its marginal distribution.

• **Example 6.3.4:** Consider $(\theta, \lambda) \in \mathbb{N} \times [0, 1]$ and

$$\pi(\theta, \lambda \mid x) \propto \binom{n}{\theta} \lambda^{\theta + \alpha - 1} (1 - \lambda)^{n - \theta + \beta - 1}$$

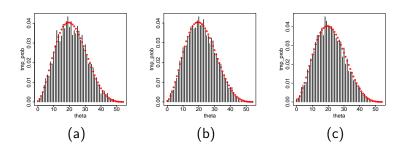
We can simulate θ and λ using Gibbs sampling as follows;

** Recognize

$$\theta \mid x, \lambda \sim \mathsf{Binom}(n, \lambda), \ \lambda \mid x, \theta \sim \mathsf{Be}(\alpha + \theta, \beta + n - \theta).$$

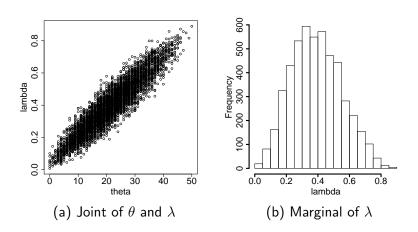
** Iteratively sample $\theta^{(t)}$ and $\lambda^{(t)}$ from their full conditionals.

• **Example 6.3.4:** (contd) Marginal distribution $\pi(\theta \mid x)$.



- ▶ (a) Directly from the marginal
- ▶ (b) Using the hierarchical structure
- ► (c) Using Gibbs sampling

• Example 6.3.4: (contd) More from Gibbs sampling



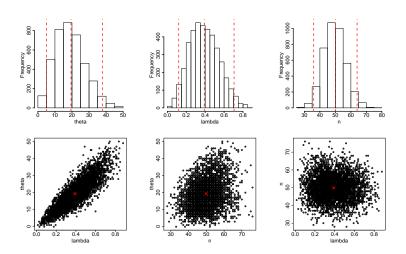
- † The General Gibbs Sampler (CR 6.3.5)
 - alternating conditional sampling: Each iterations of the Gibbs sampler cycles through the subvectors of θ , drawing each subset conditional on the value of all the others.
 - Suppose the parameter vector θ has been divided into d components, $\theta = (\theta_1, \dots, \theta_d)$. Let θ_{-j} all the components of θ except θ_j .
 - There are *d* steps in an iteration.
 - At each iteration m, an ordering of the d subvectors of θ is chosen and each θ_j is sampled from the conditional distributions given all the other components of θ , $\pi(\theta_j \mid \theta_{-j}, x)$.

• **Example 6.3.9:** (Example 6.3.4 contd) Consider $(\theta, \lambda, n) \in \mathbb{N} \times [0, 1] \times \mathbb{N}$, $n > \theta$ and

$$\pi(\theta, \lambda, n \mid x) \propto \binom{n}{\theta} \lambda^{\theta+\alpha-1} (1-\lambda)^{n-\theta+\beta-1} e^{-\xi} \frac{\xi^n}{n!}.$$

- $\star\star$ The marginal distribution of θ cannot be derived.
- ** To obtain an estimate of $\pi(\theta \mid x)$, we can simulate θ , λ and n using Gibbs sampling. The full conditionals are

$$\begin{array}{rcl} \theta \mid x, \lambda, \xi & \sim & \mathsf{Binom}(n, \lambda), \\ \lambda \mid x, \theta, \xi & \sim & \mathsf{Be}(\theta + \alpha, n - \theta + \beta), \\ n - \theta \mid x, \theta, \lambda & \sim & \mathsf{Poi}(\xi(1 - \lambda)). \end{array}$$



- † Building Markov chain algorithms using the Gibbs sampler and Metropolis algorithm
 - We use the Gibbs sampler and the Metropolis algorithms as building blocks for simulating from complicated distributions.
 - ** Use the Gibbs sampler for conditionally conjugate models.
 - ** Use the Metropolis algorithm for models that are not conditionally conjugate.
 - The Metropolis algorithm can be
 - ** performed in vector form moving in the multi-dimensional space
 - ** embedded within a Gibbs sampler structure, by alternately updating one parameter at a time.
 - When parameters are highly correlated in the target distribution, conditional sampling algorithms can be slow.

• **Example 6.3.2:** (cond) Suppose x_i is a random sample of size n from the Weibull distribution

$$f(x \mid \alpha, \eta) \propto \alpha \eta x^{\alpha - 1} e^{-x^{\alpha} \eta}$$
.

For $\theta = (\alpha, \eta)$, consider the prior

$$\pi(\theta) \propto e^{-\alpha} \eta^{\beta-1} e^{-\xi \eta}$$
.

That is, assume a priori independence and place E(1) and Gamma(β, ξ) (with mean β/ξ) for α and η , respectively.

 $\star\star$ Find the posterior distribution of θ .

$$\pi(\alpha, \eta \mid \mathbf{x}) \propto f(\mathbf{x} \mid \alpha, \eta) \pi(\alpha, \eta)$$

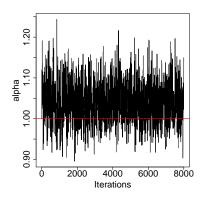
$$\propto \alpha^{n} \eta^{n+\beta-1} \prod_{i=1}^{n} x_{i}^{\alpha-1} \exp \left\{ -\eta \sum_{i=1}^{n} x_{i}^{\alpha} - \alpha - \xi \eta \right\}.$$

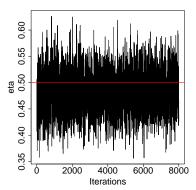
** Simulate θ from $\pi(\theta \mid \mathbf{x})$ using the Gibbs sampler. First, derive the full conditionals:

$$\begin{split} \pi(\alpha \mid \eta, \mathbf{x}) & \propto & \alpha^n \prod_{i=1}^n x_i^{\alpha-1} \exp\left\{-\eta \sum_{i=1}^n x_i^{\alpha} - \alpha\right\}, \\ \pi(\eta \mid \alpha, \mathbf{x}) & \propto & \eta^{n+\beta-1} \prod_{i=1}^n x_i^{\alpha-1} \exp\left\{-\eta \sum_{i=1}^n x_i^{\alpha} - \xi\eta\right\}. \end{split}$$

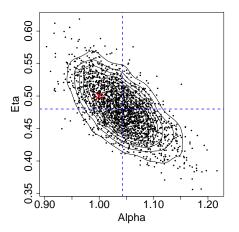
- **Example 6.3.2**: (contd)
 - 1. Start with an arbitrary value $\eta^{(0)}$.
 - 2. Iterate the following steps, t = 1, ..., T
 - 2.1 Given $\eta^{(t-1)}$, simulate $\alpha^{(t)}$ from $\pi_1(\alpha \mid x, \eta^{(t-1)})$: use a MH step
 - 2.2 Given $\alpha^{(t)}$, simulate $\eta^{(t)}$ from $\pi_2(\eta \mid x, \alpha^{(t)})$: use a MH step
 - 3. Do burn-in and thinning as needed.

- **Example 6.3.2**: (contd)
- * Trace plots to check the MCMC (mixing, convergence...)





- **Example 6.3.2**: (contd)
- * Joint posterior distribution $\pi(\alpha, \eta \mid x)$



** Report a posterior summary.

```
> post_m_a
[1] 1.04259
> post_sd_a
[1] 0.04684268
> ci_a
    2.5% 97.5%
0.9570524 1.1415434
>
> post_m_e
[1] 0.4800338
> post_sd_e
[1] 0.03730137
> ci_e
    2.5% 97.5%
0.4075282 0.5530123
>
```

* Marginal posterior distributions $\pi(\alpha \mid x) \& \pi(\eta \mid x)$

