## Gibbs sampler and MCMC

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MATH 347 Bayesian Statistics

#### Outline

- Example: Expenditures in the Consumer Expenditure Surveys
- Prior and posterior distributions for mean AND standard deviation
- 3 Use JAGS (Just Another Gibbs Sampler) and Bayesian inferences
- MCMC diagnostics
- 6 Recap

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- 1 Example: Expenditures in the Consumer Expenditure Surveys
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- 5 Recap

## The TOTEXPPQ variable in the CE sample

```
CEsample <- read_csv("CEsample1.csv")

summary(CEsample$TotalExpLastQ)

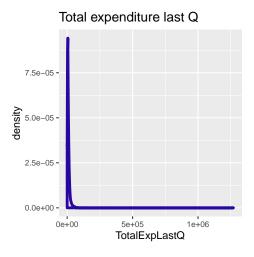
## Min. 1st Qu. Median Mean 3rd Qu. Max.

## 30 3522 6417 9513 11450 1270598

sd(CEsample$TotalExpLastQ)

## [1] 19341.25
```

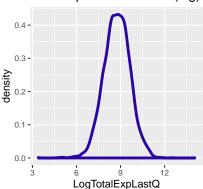
## The TOTEXPPQ variable in the CE sample cont'd



## Log transformation of the TOTEXPPQ variable

```
CEsample$LogTotalExpLastQ <- log(CEsample$TotalExpLastQ)
ggplot(data = CEsample, aes(LogTotalExpLastQ)) +
  geom_density(color = crcblue, size = 1) +
  labs(title = "Total expenditure last Q (log)") +
  theme_grey(base_size = 8, base_family = "")</pre>
```

#### Total expenditure last Q (log)

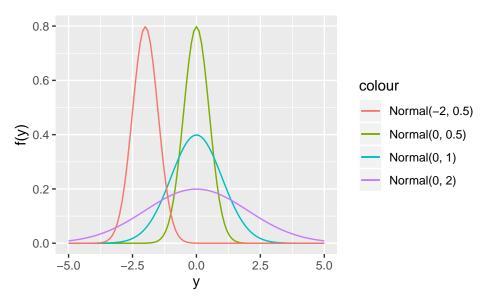


#### The Normal distribution

- The Normal distribution is a symmetric, bell-shaped distribution.
- ullet It has two parameters: mean  $\mu$  and standard deviation  $\sigma$ .
- The probability density function (pdf) of  $Normal(\mu, \sigma)$  is:

$$f(y) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(\frac{-(y-\mu)^2}{2\sigma^2}\right), -\infty < y < \infty.$$

#### The Normal distribution cont'd



#### i.i.d. Normals

- Suppose there are a sequence of n responses:  $Y_1, Y_2, \cdots, Y_n$ .
- Further suppose each response independently and identically follows a Normal distribution:

$$Y_i \stackrel{i.i.d.}{\sim} \text{Normal}(\mu, \sigma).$$

• Then the joint probability density function (joint pdf) of  $y_1, \dots, y_n$  is:

$$f(y_1, \dots, y_n) = \prod_{i=1}^n \frac{1}{\sqrt{2\pi}\sigma} \exp\left(\frac{-(y_i - \mu)^2}{2\sigma^2}\right), -\infty < y_i < \infty. \quad (1)$$

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### Step 1: Prior distributions

• The data model/sampling density for *n* observations:

$$Y_i \stackrel{i.i.d.}{\sim} \text{Normal}(\mu, \sigma).$$

- ullet There are two parameters  $\mu$  and  $\sigma$  in the Normal model.
- Therefore, the likelihood is in terms of both unknown parameters:

$$f(y_1, \cdots, y_n) = L(\mu, \sigma). \tag{2}$$

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- Therefore, the likelihood is in terms of both unknown parameters:

$$f(y_1, \cdots, y_n) = L(\mu, \sigma). \tag{2}$$

• Need a joint prior distribution:

$$\pi(\mu,\sigma)$$
. (3)

• Bayes' rule will help us derive a joint posterior:

$$\pi(\mu,\sigma\mid y_1,\cdots,y_n). \tag{4}$$

### If only mean $\mu$ is unknown: Normal conjugate prior

- ullet For this special case, Normal prior for  $\mu$  is a conjugate prior:
  - ► The prior distribution:

$$\mu \mid \sigma \sim \text{Normal}(\mu_0, \sigma_0).$$
 (5)

► The sampling density:

$$y_1, \dots, y_n \mid \mu, \sigma \stackrel{i.i.d.}{\sim} \text{Normal}(\mu, \sigma).$$
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The sampling density:

$$y_1, \dots, y_n \mid \mu, \sigma \stackrel{i.i.d.}{\sim} \text{Normal}(\mu, \sigma).$$
 (6)

The posterior distribution:

$$\mu \mid y_1, \cdots, y_n, \frac{\phi}{\phi} \sim \text{Normal}\left(\frac{\phi_0 \mu_0 + n\phi \bar{y}}{\phi_0 + n\phi}, \sqrt{\frac{1}{\phi_0 + n\phi}}\right),$$
 (7)

where  $\phi = \frac{1}{\sigma^2}$  (and  $\phi_0 = \frac{1}{\sigma_0^2}$ ), the precision. Since  $\sigma$  (and  $\sigma_0$ ) is known,  $\phi$  (and  $\phi_0$ ) is known too.

• We can then use the rnorm() R function to sample posterior draws of  $\mu$  from Equation (7). Known quantities:  $\phi_0, \mu_0, n, \bar{y}, \phi$ 

# If only standard deviation $\sigma$ is unknown: Gamma conjugate prior for $1/\sigma^2$

- For this special case, Gamma prior for  $1/\sigma^2$  is a conjugate prior:
  - ► The prior distribution:

$$1/\sigma^2 \mid \mu \sim \text{Gamma}(\alpha, \beta).$$
 (8)

► The sampling density:

$$y_1, \dots, y_n \mid \mu, \sigma \stackrel{i.i.d.}{\sim} \text{Normal}(\mu, \sigma).$$
 (9)

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► The sampling density:

$$y_1, \dots, y_n \mid \mu, \sigma \stackrel{i.i.d.}{\sim} \text{Normal}(\mu, \sigma).$$
 (9)

► The posterior distribution:

$$1/\sigma^2 \mid y_1, \dots, y_n, \mu \sim \text{Gamma}\left(\alpha + \frac{n}{2}, \beta + \frac{1}{2} \sum_{i=1}^n (y_i - \mu)^2\right)$$
 (10)

• We can then use rgamma() R function to sample posterior draws of  $\sigma$  from Equation (10). Known quantities:  $\alpha$ , n,  $\beta$ ,  $\{y_i\}$ ,  $\mu$ 

### Go back to: both $\mu$ and $\sigma$ are unknown

• Given what we have seen, how about a joint prior distribution as:

$$\pi(\mu,\sigma) = \pi_1(\mu)\pi_2(\sigma), \tag{11}$$

and let priors be

$$\mu \sim \text{Normal}(\mu_0, \sigma_0),$$
 (12)

$$1/\sigma^2 \sim \text{Gamma}(\alpha, \beta).$$
 (13)

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 (12)

$$1/\sigma^2 \sim \text{Gamma}(\alpha, \beta).$$
 (13)

Bayes' rule will produce two full conditional posterior distributions:

$$\mu \mid y_1, \cdots, y_n, \frac{\phi}{\phi} \sim \operatorname{Normal}\left(\frac{\phi_0 \mu_0 + n \phi \bar{y}}{\phi_0 + n \phi}, \sqrt{\frac{1}{\phi_0 + n \phi}}\right), \quad (14)$$

$$1/\sigma^2 = \phi \mid y_1, \cdots, y_n, \mu \quad \sim \quad \operatorname{Gamma}\left(\alpha + \frac{n}{2}, \beta + \frac{1}{2} \sum_{i=1}^{n} (y_i - \mu)^2\right). \tag{15}$$

#### Go back to: both $\mu$ and $\sigma$ are unknown

• Given what we have seen, how about a joint prior distribution as:

$$\pi(\mu, \sigma) = \pi_1(\mu)\pi_2(\sigma)$$
, requires independence (11)

and let priors be

$$\mu \sim \text{Normal}(\mu_0, \sigma_0),$$
 (12)

$$1/\sigma^2 \sim \text{Gamma}(\alpha, \beta).$$
 (13)

Bayes' rule will produce two full conditional posterior distributions:

$$\mu \mid y_1, \cdots, y_n, \frac{\phi}{\phi} \sim \operatorname{Normal}\left(\frac{\phi_0 \mu_0 + n\phi \bar{y}}{\phi_0 + n\phi}, \sqrt{\frac{1}{\phi_0 + n\phi}}\right), \quad (14)$$

$$1/\sigma^2 = \phi \mid y_1, \dots, y_n, \mu \sim \text{Gamma}\left(\alpha + \frac{n}{2}, \beta + \frac{1}{2} \sum_{i=1}^{n} (y_i - \mu)^2\right).$$
 (15)

• Why and how to derive them? Key: independent priors.

## Sampling scheme: A Gibbs sampler

$$\mu \mid y_1, \dots, y_n, \frac{\phi}{\phi} \sim \operatorname{Normal}\left(\frac{\phi_0 \mu_0 + n \phi \overline{y}}{\phi_0 + n \phi}, \sqrt{\frac{1}{\phi_0 + n \phi}}\right),$$

$$1/\sigma^2 = \phi \mid y_1, \dots, y_n, \frac{\mu}{\phi} \sim \operatorname{Gamma}\left(\alpha + \frac{n}{2}, \beta + \frac{1}{2} \sum_{i=1}^n (y_i - \mu)^2\right).$$

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$$1/\sigma^2 = \phi \mid y_1, \cdots, y_n, \stackrel{\mu}{\mu} \sim \operatorname{Gamma}\left(\alpha + \frac{n}{2}, \beta + \frac{1}{2} \sum_{i=1}^{n} (y_i - \mu)^2\right).$$

Start with initial values for parameters,  $(\mu^{(0)}, \phi^{(0)})$ . For  $s=1,\ldots,S$ , generate from the following sequence of full conditional posterior distributions:

$$-\mu^{(s)} \sim p(\mu \mid \phi^{(s-1)}, Y)$$

$$-\phi^{(s)}\sim p(\phi\mid \mu^{(s)}, Y)$$

essentially Markov Chain

you can find that mu\_0 is never used!

- Set  $\theta^{(s)} = (\mu^{(s)}, \phi^{(s)})$ 

The sequence  $\{\theta^{(s)}: s=1,\ldots,S\}$  may be viewed (but is not necessarily...yet) as a dependent sample from the joint posterior distribution of  $(\mu,\phi)$ .

```
gibbs_normal <- function(input, S, seed){
  set.seed(seed)
  ybar <- mean(input$y)</pre>
  n <- length(input$y)</pre>
  para \leftarrow matrix(0, S, 2)
  phi <- input$phi_init</pre>
  for(s in 1:S){
    mu1 <- (input$mu_0/input$sigma_0^2 + n*phi*ybar)/</pre>
    (1/input$sigma_0^2 + n*phi)
    sigma1 <- sqrt(1/(1/input$sigma_0^2 + n*phi))</pre>
    mu <- rnorm(1, mean = mu1, sd = sigma1)
    alpha1 <- input$alpha + n/2
    beta1 <- input$beta + sum((input$y - mu)^2)/2
    phi <- rgamma(1, shape = alpha1, rate = beta1)</pre>
    para[s, ] <- c(mu, phi)</pre>
  }
  para }
```

• Run the Gibbs sampler:

```
input <- list(y = CEsample$LogTotalExpLastQ, mu_0 = 5,sigma_0 = 1,
alpha = 1, beta = 1,phi_init = 1)
output <- gibbs_normal(input, S = 10000, seed = 123)</pre>
```

• Run the Gibbs sampler:

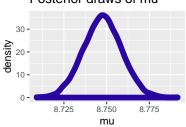
```
input <- list(y = CEsample$LogTotalExpLastQ, mu_0 = 5,sigma_0 = 1,
alpha = 1, beta = 1,phi_init = 1)
output <- gibbs_normal(input, S = 10000, seed = 123)</pre>
```

• Extract posterior draws of mu and phi from the Gibbs sampler output:

```
para_post <- as.data.frame(output)
names(para_post) <- c("mu", "phi")</pre>
```

```
ggplot(para_post, aes(mu)) +
  geom_density(size = 2, color = crcblue) +
  labs(title = "Posterior draws of mu") +
  theme_grey(base_size = 8,
  base_family = "")
```

#### Posterior draws of mu

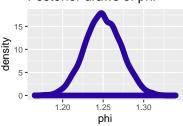


```
quantile(para_post$mu, c(0.025,0.975))
```

```
## 2.5% 97.5%
## 8.725482 8.769543
```

```
ggplot(para_post, aes(phi)) +
  geom_density(size = 2, color = crcblue) +
  labs(title = "Posterior draws of phi") +
  theme_grey(base_size = 8,
  base_family = "")
```

#### Posterior draws of phi



```
quantile(para_post$phi, c(0.025,0.975))
```

```
## 2.5% 97.5%
## 1.206482 1.294191
```

#### Exercise: Gibbs sampler

mu\_init. Compare your results to the existing results.

• Exercise 1: Update the following Gibbs sampler to initiate it with

 Exercise 2: Update the following Gibbs sampler to initiate it with mu\_init and phi\_init. Compare your results to the existing results.

### Extends to more than 2 parameters

Suppose the full conditional posterior distributions of  $\theta = (\theta_1, \theta_2, \dots, \theta_m)$  are all tractable.

- Start the Gibbs sampler at the initial value  $(\theta_1^{(0)}, \theta_2^{(0)}, \dots, \theta_m^{(0)})$ , or a subset of them.
- For the (s + 1)-th iteration: generate from the following full conditionals sequentially:

$$\begin{array}{l} \bullet \ \ \theta_{1}^{(s+1)} \sim p(\theta_{1} \mid \theta_{2}^{(s)}, \theta_{3}^{(s)}, \theta_{4}^{(s)}, \ldots, \theta_{m}^{(s)}, Y) \\ \bullet \ \ \theta_{2}^{(s+1)} \sim p(\theta_{2} \mid \theta_{1}^{(s+1)}, \theta_{3}^{(s)}, \theta_{4}^{(s)}, \ldots, \theta_{m}^{(s)}, Y) \\ \bullet \ \ \theta_{3}^{(s+1)} \sim p(\theta_{3} \mid \theta_{1}^{(s+1)}, \theta_{2}^{(s+1)}, \theta_{4}^{(s)}, \ldots, \theta_{m}^{(s)}, Y) \\ \bullet \ \ \vdots \\ \bullet \ \ \theta_{m}^{(s+1)} \sim p(\theta_{m} \mid \theta_{1}^{(s+1)}, \theta_{2}^{(s+1)}, \theta_{3}^{(s+1)}, \ldots, \theta_{m-1}^{(s+1)}, Y) \end{array}$$

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- R package runjags to run Markov chain Monte Carlo simulations.
- Descriptive of the sampling model and the prior.

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- Descriptive of the sampling model and the prior.
- Installing JAGS software and runjags R package
  - Download JAGS at this link
  - ▶ Install and load runjags R package

```
install.packages("runjags")
library(runjags)
```

- Example: Normal model with unknown mean and standard deviation.
  - ► The prior distributions:

$$\mu \sim \operatorname{Normal}(\mu_0, \sigma_0),$$
  
 $1/\sigma^2 = \phi \sim \operatorname{Gamma}(\alpha, \beta).$ 

► The sampling density:

$$y_1, \dots, y_n \mid \mu, \sigma \stackrel{i.i.d.}{\sim} \text{Normal}(\mu, \sigma).$$

► Bayes' rule will produce two full conditional posterior distributions:

$$\begin{split} \mu \mid y_1, \cdots, y_n, \phi &\sim \operatorname{Normal}\left(\frac{\phi_0 \mu_0 + n \bar{y} \phi}{\phi_0 + n \phi}, \sqrt{\frac{1}{\phi_0 + n \phi}}\right), \\ 1/\sigma^2 &= \phi \mid y_1, \cdots, y_n, \mu &\sim \operatorname{Gamma}\left(\alpha + \frac{n}{2}, \beta + \frac{1}{2} \sum_{i=1}^n (y_i - \mu)^2\right). \end{split}$$

- Only need to focus on the sampling density and the prior:
  - ► The sampling density:

$$y_1, \dots, y_n \mid \mu, \sigma \stackrel{i.i.d.}{\sim} \text{Normal}(\mu, \sigma).$$

► The prior distributions:

```
\mu \sim \text{Normal}(\mu_0, \sigma_0),

1/\sigma^2 = \phi \sim \text{Gamma}(\alpha, \beta).
```

```
modelString <- "
model{
for (i in 1:N) {
  y[i] ~ dnorm(mu, phi)
}
mu ~ dnorm(mu_0, phi_0)
phi ~ dgamma(alpha, beta)
}</pre>
```

• Pass the data and hyperparameter values to JAGS:

```
y <- CEsample$LogTotalExpLastQ
N <- length(y)
the_data <- list("y" = y, "N" = N, "mu_0" = 5, "phi_0" = 1/1^2,
"alpha" = 1,"beta" = 1)</pre>
```

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"alpha" = 1,"beta" = 1)</pre>
```

• Run the JAGS code for this model:

Obtain posterior summaries of mu and phi:

```
summary(posterior)
```

```
Lower95
                Median Upper95
                                  Mean
                                              SD Mode
                                                             MCerr MC%ofSD
      8.72529 8.747810 8.76868 8.747781 0.01111673 NA 0.0001572144
                                                                       1.4
## phi 1.20652 1.251015 1.29268 1.250759 0.02206280 NA 0.0003091955
                                                                       1.4
      SSeff
                   AC.10 psrf
      5000 0.030116334
## m11
                          NΑ
## phi 5092 -0.002062701
                          NΑ
```

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## MCMC Convergence to posterior distribution

Theory proves that if a Gibbs sampler iterates enough, the draws will be from the joint posterior distribution (called the target or stationary distribution).

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Theory proves that if a Gibbs sampler iterates enough, the draws will be from the joint posterior distribution (called the target or stationary distribution).

- Do initial values matter? Should they matter?
- "Markov chain" indicate dependence of draws. How to create independent parameter draws?
- How long do we need to run the MCMC to adequately explore the posterior distribution?
- How can we tell if the chain is not converging?

#### Discard initial steps: burn-in

- Do not want pre-convergence values to influence the summary of the posterior distribution (the draws of the parameters from the MCMC) too much.
- Ideal is to throw away all draws before convergence to target distribution, and use only draws after convergence.
- Hard to know exactly when convergence has happened. Thus, it is standard to throw out the first p% of draws (default is 50%) as burn-in after you are satisfied that convergence has been achieved.
- Inference done with remaining (100 p%) of draws.

#### Discard initial steps: burn-in cont'd

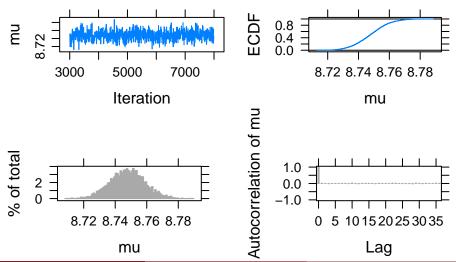
# Trace plots to check MCMC mixing

- Trace plots show the progress of the chain over time. The ideal trace plot has a lot of movement around the mode from iteration to iteration and not a lot of "stickiness."
- Trace plots with a clear trend are evidence that MCMC sampler has not yet converged, and it needs to run longer (or there is an error in your code).
- Trace plots with extreme stickiness suggest that the chain may not have explored the entire parameter space yet, and it needs to run longer.
- Hard to tell convergence from trace plots alone, because you might be stuck in one region of the parameter space in all of the iterations.

#### Trace plots example

plot(posterior, vars = "mu")

## Generating plots...



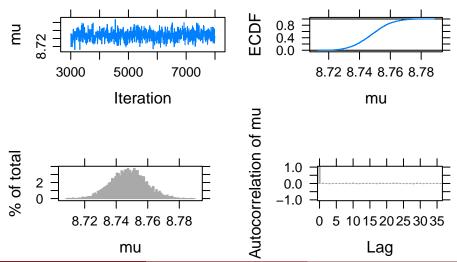
# ACF plots and effective sample size to check correlation diagnostics

- Independent (Monte Carlo) draws have zero autocorrelations.
   Dependent draws (MCMC) have non-zero, usually positive, autocorrelations.
- Large autocorrelations indicate that chain is not mixing well, i.e., the chain possibly has not explored the full space of the posterior distribution (has not converged).
- Large autocorrelations often arise in multi-parameter MCMC algorithms when the parameters are highly correlated.
- This usually means you need to run the chains longer to feel comfortable about convergence. It also implies a smaller effective sample size. . . .
- ACF plots (auto correlation function) & effective sample size.

#### ACF plots example

plot(posterior, vars = "mu")

## Generating plots...



# Effective sample size example

• The column of SSeff; recall sample is 5000.

```
summary(posterior)
```

```
Lower95
                Median Upper95
                                   Mean
                                                SD Mode
                                                               MCerr MC%ofSD
      8.72529 8.747810 8.76868 8.747781 0.01111673 NA 0.0001572144
                                                                         1.4
## phi 1.20652 1.251015 1.29268 1.250759 0.02206280 NA 0.0003091955
                                                                         1.4
##
      SSeff
                   AC.10 psrf
      5000 0.030116334
## m11
                           NΑ
## phi 5092 -0.002062701
                           NA
```

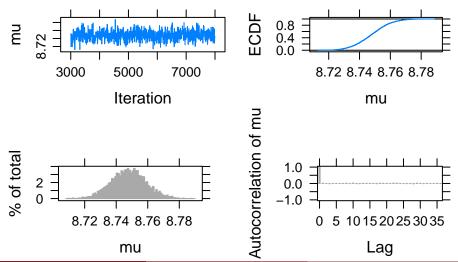
## Create independent samples: thin

- Monte Carlo samples come from independent parameter draws, thus they move around the parameter space freely.
- Markov chain properties could create dependence among adjacent parameter draws.
- Use thin to save every x draws.

#### MCMC diagnostics for the CE example

plot(posterior, vars = "mu")

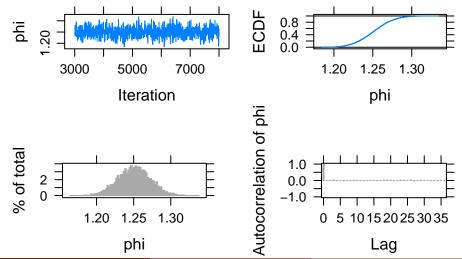
## Generating plots...



# MCMC diagnostics for the CE example cont'd

plot(posterior, vars = "phi")

## Generating plots...



# Gelman-Rubin diagnostics

- Gelman and Rubin (1992) propose running m>1 separate Markov chains each of length S. When convergence is reached, the draws from the chains are all from the target distribution. Hence, at convergence, the output from all chains is indistinguishable.
- Diagnostic based on the contrapositive: if output from chains is not indistinguishable, convergence has not been reached. Diagnostic applied to one variable at a time.
- Use different starting values that are overdispersed (really spread out) relative to the posterior distribution. This helps ensure all the chains are not stuck in the same region.
- Gelman-Rubin diagnostic based a comparison of within-chain and between-chain variances, which is similar to a classical analysis of variance.

## Gelman-Rubin diagnostics example

Create intinial values of mu and phi:

## Gelman-Rubin diagnostics example

• Create intinial values of mu and phi:

• Feed in inits1 and inits2, and let n.chains = 2:

# Gelman-Rubin diagnostics example cont'd

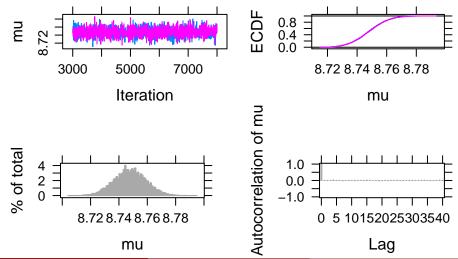
Return psrf from the output, as Gelman-Rubin diagnostic results:

## 1.05

## MCMC diagnostics for the CE example. 2 chains

plot(posterior\_2chains, vars = "mu")

## Generating plots...



# Useful diagnostics/functions in coda package

The coda R package provides many popular diagnostics for assessing convergence of MCMC output from self-coded Gibbs sampler.

- Trace plots: traceplot()
- Autocorrelation: autocorr.plot()
- Effective Sample Size: effectiveSize()
- Gelman-Rubin: gelman.diag()

# Useful diagnostics/functions in coda package

 One needs to convert parameter draws into an MCMC object. For example:

```
install.packages("coda")
library(coda)
out <- gibbs_normal(input, S = 10000, seed = 123)
para_post = as.data.frame(out)
names(para_post) = c("mu", "phi")</pre>
```

# Useful diagnostics/functions in coda package

 One needs to convert parameter draws into an MCMC object. For example:

```
install.packages("coda")
library(coda)
out <- gibbs_normal(input, S = 10000, seed = 123)
para_post = as.data.frame(out)
names(para_post) = c("mu", "phi")</pre>
```

• Then one can perform MCMC diagnostics. For example:

```
mu.mcmc = as.mcmc(para_post$mu)

traceplot(mu.mcmc)
autocorr.plot(mu.mcmc)
effectiveSize(mu.mcmc)
gelman.diag(mu.mcmc)
```

Note: gelman.diag() needs at least 2 chains.

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#### Recap

- Bayesian inference procedure:
  - Step 1: express an opinion about the location of mean  $\mu$  and standard deviation  $\sigma$  (or precision  $\phi$ ) before sampling (prior).
  - Step 2: take the sample (data/likelihood).
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- For Normal data/likelihood, Normal distributions are conjugate priors for  $\mu$ , and Gamma distributions are conjugate priors for  $\phi$ . The same goes for the full conditional posterior distributions.
- One can either write a loop function to run a Gibbs sampler, or use JAGS.

#### Recap cont'd

- MCMC diagnostics!
  - Diagnostics cannot guarantee that chain has converged.
  - Diagnostics can indicate that it has not converged.
  - Solutions: run longer, thinning, standardize variables in multi-parameter models (can reduce auto correlations).