Module 9: The Multivariate Normal Distribution

Rebecca C. Steorts

Announcements

- 1. The last day of classes with be April 16, 2019
- 2. There will be a special lecture on April 18, 2019 by one of my PhD students on mixture models (abstract/title forthcoming).
- 3. OH will be regularly scheduled until the final exam, April 29, 2019.
- 4. Your lab sections will serve as extra OH by your TAs until April 29, 2019.
- 5. The final exam will be April 29, 2019, 9 AM noon (Old Chem 116).

Agenda

- Moving from univariate to multivariate distributions.
- ► The multivariate normal (MVN) distribution.
- Conjugate for the MVN distribution.
- ▶ The inverse Wishart distribution.
- Conjugate for the MVN distribution (but on the covariance matrix).
- Combining the MVN with inverse Wishart.
- See Chapter 7 (Hoff) for a review of the standard Normal density.

Notation

Assume a matrix of covariates

$$m{X}_{p imes n} = \left(egin{array}{cccc} x_{11} & x_{12} & \dots & x_{1n} \\ x_{21} & x_{22} & \dots & x_{2n} \\ x_{i1} & x_{i2} & \dots & x_{in} \\ dots & dots & \ddots & dots \\ x_{p1} & x_{p2} & \dots & x_{pn} \end{array}
ight).$$

- ▶ A column of $X_{p \times n}$ represents a particular covariate we might be interested in, such as age of a person.
- ▶ Denote x_i as the ith column vector of the $X_{p \times n}$ matrix.

$$x_i = \begin{pmatrix} x_{i1} \\ x_{i2} \\ \vdots \\ x_{ip} \end{pmatrix}$$

where it's dimension is $p \times 1$.

Distribution of MVN

We assume that the population mean is $\mu_{p\times 1} = E(x_i)$ and $\Sigma_{p\times p} = \text{Var}(x_i) = E[(x_i - \mu_{p\times 1})(x_i - \mu_{p\times 1})^T]$, where

$$\boldsymbol{\mu}_{p\times 1} = \begin{pmatrix} \mu_1 \\ \mu_2 \\ \vdots \\ \mu_p \end{pmatrix}$$

and

$$\Sigma_{p\times p} = \begin{pmatrix} \sigma_1^2 & \sigma_{12} & \dots & \sigma_{1p} \\ \sigma_{21} & \sigma_2^2 & \dots & \sigma_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ \sigma_{p1} & \sigma_{p2} & \dots & \sigma_p^2 \end{pmatrix}.$$

Notation

Suppose matrix A is invertible. The

$$\det(A) = \sum_{i=1}^{j=n} a_{ij} A_{ij}.$$

I recommend using the det() commend in R.

Suppose now we have a square matrix $H_{p \times p}$.

$$\mathsf{trace}(H) = \sum_{i} h_{ii},$$

where h_{ii} are the diagonal elements of H.

Useful Tricks

Suppose that A is $n \times n$ matrix and suppose that B is a $n \times n$ matrix.

Lemma 1:

$$tr(AB) = tr(BA)$$

Proof: Exercise.

Lemma 2:

$$x^{T}Ax = tr(x^{T}Ax) = tr(xx^{T}A) = tr(Axx^{T})$$

Proof: Exercise.

Why are these useful? We'll get to this later in this module.

Notation

- MVN is generalization of univariate normal.
- ▶ For the MVN, we write $\mathbf{X} \sim \mathcal{MVN}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$.
- ► The $(i,j)^{\text{th}}$ component of Σ is the covariance between X_i and X_j (so the diagonal of Σ gives the component variances).

Example: $Cov(X_1, X_2)$ is just one element of the matrix Σ .

Multivariate Normal

Just as the probability density of a scalar normal is

$$p(x) = (2\pi\sigma^2)^{-1/2} \exp\left\{-\frac{1}{2}\frac{(x-\mu)^2}{\sigma^2}\right\},$$
 (1)

the probability density of the multivariate normal is

$$p(\vec{\mathbf{x}}) = (2\pi)^{-\rho/2} (\det \Sigma)^{-1/2} \exp\left\{-\frac{1}{2} (\mathbf{X} - \boldsymbol{\mu})^T \Sigma^{-1} (\mathbf{X} - \boldsymbol{\mu})\right\}.$$
(2)

Univariate normal is special case of the multivariate normal with a one-dimensional mean "vector" and a one-by-one variance "matrix."

Standard Multivariate Normal Distribution

Consider

$$Z_1,\ldots,Z_n\stackrel{iid}{\sim}MVN(0,I)$$

$$f_z(z) = \prod_{i=1}^n \frac{1}{2\pi} e^{-z_i^2/2}$$
 (3)

$$= (2\pi)^{-n} e^{\sum_{i} -z_{i}^{2}/2} \tag{4}$$

$$= (2\pi)^{-n} e^{z^T z/2} \tag{5}$$

Exercise: Why does $\sum_{i} -z_{i}^{2} = z^{T}z$?

- ▶ E[Z] = 0
- Var[Z] = I

Conjugate to MVN

Suppose that

$$X_1 \dots X_n \mid \theta \stackrel{iid}{\sim} MVN(\theta, \Sigma).$$

Let

$$\pi(\boldsymbol{\theta}) \sim MVN(\boldsymbol{\mu}, \Omega).$$

What is the full conditional distribution of $\theta \mid \mathbf{X}, \Sigma$?

Prior

$$\pi(\theta) = (2\pi)^{-p/2} \det \Omega^{-1/2} \exp \left\{ -\frac{1}{2} (\theta - \mu)^T \Omega^{-1} (\theta - \mu) \right\}$$
(6)

$$\propto \exp \left\{ -\frac{1}{2} (\theta - \mu)^T \Omega^{-1} (\theta - \mu) \right\}$$
(7)

$$\propto \exp \left\{ -\frac{1}{2} \left\{ \theta^T \Omega^{-1} \theta - 2\theta^T \Omega^{-1} \mu + \mu^T \Omega^{-1} \mu \right\}$$
(8)

$$\propto \exp \left\{ -\frac{1}{2} \left\{ \theta^T \Omega^{-1} \theta - 2\theta^T \Omega^{-1} \mu \right\}$$
(9)

$$= \exp \left\{ -\frac{1}{2} \left\{ \theta^T A_o \theta - 2\theta^T b_o \right\}$$
(10)

 $\pi(\theta) \sim MVN(\mu, \Omega)$ implies that $A_0 = \Omega^{-1}$ and $b_0 = \Omega^{-1}\mu$.

(10)

Likelihood

$$\rho(\mathbf{X} \mid \boldsymbol{\theta}, \boldsymbol{\Sigma}) = \prod_{i=1}^{n} (2\pi)^{-p/2} \det \boldsymbol{\Sigma}^{-1/2} \exp \left\{ -\frac{1}{2} (x_i - \boldsymbol{\theta})^T \boldsymbol{\Sigma}^{-1} (x_i - \boldsymbol{\theta}) \right\}$$

$$\propto \exp -\frac{1}{2} \left\{ \sum_{i} x_i^T \boldsymbol{\Sigma}^{-1} x_i - 2 \sum_{i} \boldsymbol{\theta}^T \boldsymbol{\Sigma}^{-1} x_i + \sum_{i} \boldsymbol{\theta}^T \boldsymbol{\Sigma}^{-1} \boldsymbol{\theta} \right\}$$

$$\propto \exp -\frac{1}{2} \left\{ -2\boldsymbol{\theta}^T \boldsymbol{\Sigma}^{-1} n \bar{x} + n \boldsymbol{\theta}^T \boldsymbol{\Sigma}^{-1} \boldsymbol{\theta} \right\}$$

$$\propto \exp -\frac{1}{2} \left\{ -2\boldsymbol{\theta}^T b_1 + \boldsymbol{\theta}^T A_1 \boldsymbol{\theta} \right\},$$

$$(14)$$

where

$$b_1 = \Sigma^{-1} n \bar{x}, \quad A_1 = n \Sigma^{-1}$$

and

$$\bar{x} := \left(\frac{1}{n}\sum_{i}x_{i1},\ldots,\frac{1}{n}\sum_{i}x_{ip}\right)^{T}.$$

Full conditional

$$\rho(\theta \mid \mathbf{X}, \Sigma) \propto \rho(\mathbf{X} \mid \theta, \Sigma) \times \rho(\theta) \tag{15}$$

$$\propto \exp{-\frac{1}{2} \left\{ -2\theta^{T} b_{1} + \theta^{T} A_{1} \theta \right\}} \tag{16}$$

$$\times \exp{-\frac{1}{2} \left\{ \theta^{T} A_{o} \theta - 2\theta^{T} b_{o} \right\}} \tag{17}$$

$$\propto \exp{\theta^{T} b_{1} - \frac{1}{2} \theta^{T} A_{1} \theta - \frac{1}{2} \theta^{T} A_{o} \theta + \theta^{T} b_{o}} \tag{18}$$

$$\propto \exp{\theta^{T} (b_{o} + b_{1}) - \frac{1}{2} \theta^{T} (A_{o} + A_{1}) \theta} \tag{19}$$

Full conditional

From the previous slide, recall that

$$p(\boldsymbol{\theta} \mid \mathbf{X}, \boldsymbol{\Sigma}) \propto \exp\{\boldsymbol{\theta}^{T}(b_{o} + b_{1}) - \frac{1}{2}\boldsymbol{\theta}^{T}(A_{o} + A_{1})\boldsymbol{\theta}\}$$

Using the kernel of the multivariate normal, we can now find the posterior mean and the posterior covariance:

Then

$$A_n = A_o + A_1 = \Omega^{-1} + n\Sigma^{-1}$$

and

$$b_n = b_o + b_1 = \Omega^{-1}\mu + \Sigma^{-1}nar{x}$$

 $m{ heta} \mid \mathbf{X}, \Sigma \sim MVN(A_n^{-1}b_n, A_n^{-1}) = MVN(\mu_n, \Sigma_n).$

Interpretations

$$\theta \mid \mathbf{X}, \Sigma \sim MVN(A_n^{-1}b_n, A_n^{-1}) = MVN(\mu_n, \Sigma_n)$$

$$\mu_n = A_n^{-1} b_n = [\Omega^{-1} + n\Sigma^{-1}]^{-1} (b_o + b_1)$$

$$= [\Omega^{-1} + n\Sigma^{-1}]^{-1} (\Omega^{-1} \mu + \Sigma^{-1} n\bar{x})$$
(20)

$$\Sigma_n = A_n^{-1} = [\Omega^{-1} + n\Sigma^{-1}]^{-1}$$
 (22)

inverse Wishart distribution

Suppose $\Sigma \sim \text{inverseWishart}(\nu_o, S_o^{-1})$ where ν_o is a scalar and S_o^{-1} is a matrix.

Then

$$p(\Sigma) \propto \det(\Sigma)^{-(\nu_o + p + 1)/2} \times \exp\{-\operatorname{tr}(S_o \Sigma^{-1})/2\}$$

For the full distribution, see Hoff, Chapter 7 (p. 110).

inverse Wishart distribution

- The inverse Wishart distribution is the multivariate version of the Gamma distribution.
- ► The full hierarchy we're interested in is

$$m{X} \mid m{ heta}, \Sigma \sim extit{MVN}(m{ heta}, \Sigma).$$
 $m{ heta} \sim extit{MVN}(\mu, \Omega)$ $m{\Sigma} \sim ext{inverseWishart}(
u_o, S_o^{-1}).$

We first consider the conjugacy of the MVN and the inverse Wishart, i.e.

$$m{X} \mid m{ heta}, \Sigma \sim extit{MVN}(m{ heta}, \Sigma).$$
 $\Sigma \sim ext{inverseWishart}(
u_o, S_o^{-1}).$

Continued

What about $p(\Sigma \mid \boldsymbol{X}, \boldsymbol{\theta}) \propto p(\Sigma) \times p(\boldsymbol{X} \mid \boldsymbol{\theta}, \Sigma)$. Let's first look at

$$p(\mathbf{X} \mid \boldsymbol{\theta}, \boldsymbol{\Sigma}) \tag{23}$$

$$\propto \det(\mathbf{\Sigma})^{-n/2} \exp\{-\sum_{i} (\mathbf{X}_{i} - \boldsymbol{\theta})^{T} \mathbf{\Sigma}^{-1} (\mathbf{X}_{i} - \boldsymbol{\theta})/2\}$$
 (24)

$$\propto \det(\Sigma)^{-n/2} \exp\{-tr(\sum_{i} (\mathbf{X}_{i} - \boldsymbol{\theta})(\mathbf{X}_{i} - \boldsymbol{\theta})^{T} \Sigma^{-1}/2)\}$$
 (25)

$$\propto \det(\Sigma)^{-n/2} \exp\{-\operatorname{tr}(S_{\theta}\Sigma^{-1}/2)\} \tag{26}$$

where
$$S_{\theta} = \sum_{i} (\mathbf{X}_{i} - \boldsymbol{\theta}) (\mathbf{X}_{i} - \boldsymbol{\theta})^{T}$$
.

Note that

$$\sum_{k} b_{k}^{T} A b_{k} = tr(BB^{T} A),$$

where B is the matrix whose kth row is b_k . (Here we are applying Lemma 2.)

Continued

Now we can calculate $p(\Sigma \mid \boldsymbol{X}, \boldsymbol{\theta})$

$$\rho(\Sigma \mid \mathbf{X}, \boldsymbol{\theta}) \qquad (27)$$

$$= \rho(\Sigma) \times \rho(\mathbf{X} \mid \boldsymbol{\theta}, \Sigma) \qquad (28)$$

$$\propto \det(\Sigma)^{-(\nu_o + p + 1)/2} \times \exp\{-\operatorname{tr}(S_o \Sigma^{-1})/2\} \qquad (29)$$

$$\times \det(\Sigma)^{-n/2} \exp\{-\operatorname{tr}(S_\theta \Sigma^{-1})/2\} \qquad (30)$$

This implies that

$$\Sigma \mid \mathbf{X}, \mathbf{\theta} \sim \text{inverseWishart}(\nu_o + n, [S_o + S_{\theta}]^{-1} =: S_n)$$

 $\propto \det(\Sigma)^{-(\nu_o+n+p+1)/2} \exp\{-\operatorname{tr}((S_o+S_\theta)\Sigma^{-1})/2\}$

(31)

Continued

Suppose that we wish now to take

$$\boldsymbol{\theta} \mid \boldsymbol{X}, \boldsymbol{\Sigma} \sim MVN(\mu_n, \boldsymbol{\Sigma}_n)$$

(which we finished an example on earlier). Now let

$$\Sigma \mid \mathbf{X}, \mathbf{ heta} \sim \mathsf{inverseWishart}(
u_n, S_n^{-1})$$

There is no closed form expression for this posterior. Solution?

Gibbs sampler

Suppose the Gibbs sampler is at iteration s.

- 1. Sample $\theta^{(s+1)}$ from it's full conditional:
 - a) Compute μ_n and Σ_n from \boldsymbol{X} and $\Sigma^{(s)}$
 - b) Sample $\theta^{(s+1)} \sim MVN(\mu_n, \Sigma_n)$
- 2. Sample $\Sigma^{(s+1)}$ from its full conditional:
 - a) Compute S_n from **X** and $\theta^{(s+1)}$
 - b) Sample $\Sigma^{(s+1)} \sim \text{inverseWishart}(\nu_n, S_n^{-1})$

Working with Multivariate Normal Distribution

The R package, mvtnorm, contains functions for evaluating and simulating from a multivariate normal density.

```
library(mvtnorm)
```

Warning: package 'mvtnorm' was built under R version 3.

Simulating Data

Simulate a single multivariate normal random vector using the rmvnorm function.

```
# Each row corresponds to a sample

# Here we have one sample (one row)

rmvnorm(n = 1, mean = rep(0, 2), sigma = diag(2))

## [,1] [,2]

## [1,] -1.424615 -0.1691306
```

Evaluation

Evaluate the multivariate normal density at a single value using the dmynorm function.

```
dmvnorm(rep(0, 2), mean = rep(0, 2), sigma = diag(2))
## [1] 0.1591549
```

Working with the Multivariate Normal

- Now let's simulate many multivariate normals.
- Each row is a different sample from this multivariate normal distribution.

```
rmvnorm(n = 3, mean = rep(0, 2), sigma = diag(2))
```

```
## [,1] [,2]
## [1,] -0.6306398 0.1543993
## [2,] 1.9442503 1.7630681
## [3,] 0.2131082 -1.1553461
```

Work with the Wishart density

- The R package, stats, contains functions for evaluating and simulating from a Wishart density.
- ► We can simulate a single Wishart distributed matrix using the rWishart function.
- Each row is a different sample from the Wishart distribution.

```
nu0 <- 2
Sigma0 <- diag(2)
rWishart(1, df = nu0, Sigma = Sigma0)[, , 1]</pre>
```

```
## [,1] [,2]
## [1,] 4.362454 -2.332523
## [2,] -2.332523 1.412829
```

An Application to Reading Comprehension

We will follow an example from Hoff (Section 7.4, p. 112).

A sample of 22 children are given reading comprehension tests before and after receiving a particular instructional method.

Each student i will then have two scores, $Y_{i,1}$ and $Y_{i,2}$ denoting the pre- and post-instructional scores respectively.

Denote each student's pair of scores Y_i

$$\mathbf{Y}_i = \left(\begin{array}{c} Y_{i,1} \\ Y_{i,2} \end{array}\right) = \left(\begin{array}{c} \text{score on first test} \\ \text{score on second test} \end{array}\right)$$

Model set up

$$oldsymbol{Y}_i \mid oldsymbol{ heta}, \Sigma \sim extit{MVN}(oldsymbol{ heta}_j, \Sigma). \ oldsymbol{ heta}_j \sim extit{MVN}(oldsymbol{\mu_0}, oldsymbol{\Lambda}_0) \ \Sigma \sim ext{inverseWishart}(
u_o, S_o^{-1}).$$

Let
$$\theta = (\theta_1, \theta_2)$$
. $i = 1, \dots, n$ and $j = 1, 2$

Prior settings

$$oldsymbol{Y}_i \mid oldsymbol{ heta}, \Sigma \sim extit{MVN}(oldsymbol{ heta}_j, \Sigma).$$
 $oldsymbol{ heta}_j \sim extit{MVN}(oldsymbol{\mu}_0, \Lambda_0)$ $\Sigma \sim ext{inverseWishart}(
u_o, S_o^{-1}).$

The exam was designed to give average scores of around 50 out of 100, so $\mu_0 = (50, 50)^T$ would be a good choice for our prior mean.

Prior settings

$$oldsymbol{Y}_i \mid oldsymbol{ heta}, \Sigma \sim extit{MVN}(oldsymbol{ heta}_j, \Sigma).$$
 $oldsymbol{ heta}_j \sim extit{MVN}(oldsymbol{\mu}_0, oldsymbol{\Lambda}_0)$ $\Sigma \sim ext{inverseWishart}(
u_o, S_o^{-1}).$

Since the true mean cannot be below 0 or above 100, we will use a prior variance that puts little probability outside of this range.

We'll take the prior variances on θ_1 and θ_2 to be

$$\lambda_{0,1}^2 = \lambda_{0,2}^2 = (50/2)^2 = 625$$

so that the prior probability that $P(\theta_j \neq [0, 100]) = 0.05$.

The two exams are measuring similar things, so we will take the prior correlation of 0.5 or rather $\lambda_{1,2}=625/2=312.5$

Prior settings (continued)

$$oldsymbol{Y}_i \mid oldsymbol{ heta}, \Sigma \sim extit{MVN}(oldsymbol{ heta}_j, \Sigma).$$
 $oldsymbol{ heta}_j \sim extit{MVN}(oldsymbol{\mu}_0, \Lambda_0)$ $\Sigma \sim ext{inverseWishart}(
u_o, S_o^{-1}).$

What about the prior settings for Σ ?

We take S_o to be about the same as Λ_o .

We will center Σ around S_o by setting $\nu_0 = p + 2 = 4$.

Load in data

Quick calculations

```
(n <- dim(Y)[1])

## [1] 22

(ybar <- apply(Y,2,mean))
```

Application to reading comprehension

```
# set hyper-parameters
mu0 <- c(50,50)
L0 <- matrix(c(625,312.5,312.5,625),nrow=2)
nu0 <- 4
S0 <- L0</pre>
```

Gibbs sampler

```
## Loading required package: coda
## Loading required package: MASS
## ##
## ## Markov Chain Monte Carlo Package (MCMCpack)
## ## Copyright (C) 2003-2019 Andrew D. Martin, Kevin M. Q
## ##
## ## Support provided by the U.S. National Science Foundar
## ## (Grants SES-0350646 and SES-0350613)
## ##
```

Gibbs sampler (review)

Suppose the Gibbs sampler is at iteration s.

- 1. Sample $\theta^{(s+1)}$ from it's full conditional:
 - a) Compute μ_n and Σ_n from \boldsymbol{X} and $\Sigma^{(s)}$
 - b) Sample $\theta^{(s+1)} \sim MVN(\mu_n, \Sigma_n)$
- 2. Sample $\Sigma^{(s+1)}$ from its full conditional:
 - a) Compute S_n from **X** and $\theta^{(s+1)}$
 - b) Sample $\Sigma^{(s+1)} \sim \text{inverseWishart}(\nu_n, S_n^{-1})$

Gibbs sampler

```
THETA <- STGMA <- NULL.
set.seed(1)
for (s in 1:5000) {
 ## update theta
 Ln <- solve(solve(L0) + n*solve(Sigma))</pre>
  mun <- Ln %*% (solve(L0) %*% mu0 +
                    n*solve(Sigma) %*% ybar)
  theta <- rmvnorm(1, mun, Ln)
  ## update Sigma
  Sn \leftarrow SO + (t(Y) - c(theta)) %*% t(t(Y)-c(theta))
  Sigma <- solve(rwish(nu0 + n, solve(Sn)))
  ## save results
  THETA <- rbind(THETA, theta)
  SIGMA <- rbind(SIGMA, c(Sigma))</pre>
```

Posterior inference

Using the samples from the Gibbs sampler, we have generated 5,000 samples

$$(\theta^{(1)}, \Sigma^{(1)}, \dots, \theta^{(5000)}, \Sigma^{(5000)})$$

that approxmiates $p(\theta, \Sigma \mid y_1, \dots, y_n)$.

Glance at Gibbs sampler

head (THETA)

```
## [,1] [,2]

## [1,] 45.76871 53.64765

## [2,] 43.84243 51.80471

## [3,] 43.41651 51.30521

## [4,] 46.85067 50.64238

## [5,] 42.62048 53.71350

## [6,] 50.32035 58.93397
```

head(SIGMA)

```
## [,1] [,2] [,3] [,4]

## [1,] 270.7381 175.9276 175.9276 213.0155

## [2,] 237.3720 191.0999 191.0999 266.0570

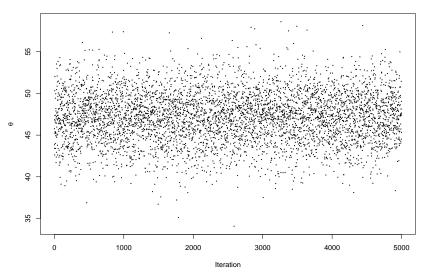
## [3,] 245.6029 183.9140 183.9140 248.4452

## [4,] 169.6788 114.1658 114.1658 200.8390

## [5,] 247.0899 197.0802 197.0802 295.1981
```

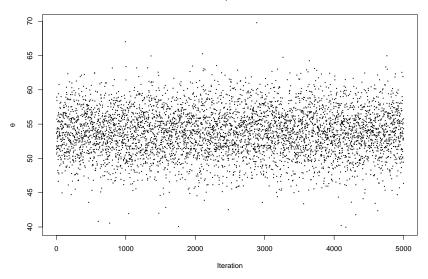
Traceplot of θ_1





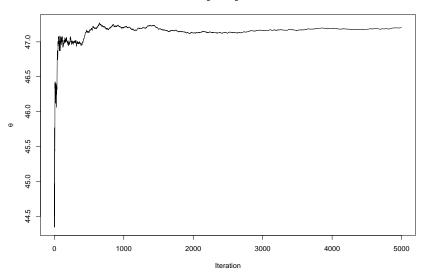
Traceplot of θ_2



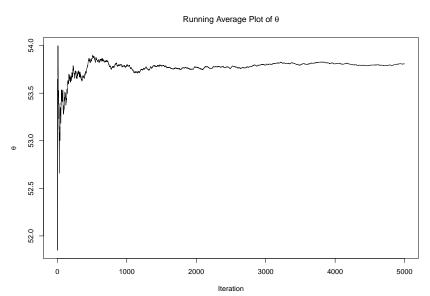


Running average plot of θ_1

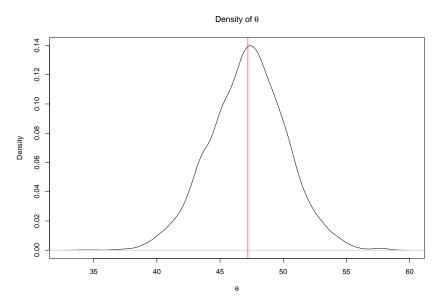




Running average plot of θ_2



Estimated density of θ_1



Estimated density of θ_2



Traceplots and running average plots

The traceplots don't tell us much of anything, so this is why we examine the running average plots. Specifically, the traceplots indicate that the chain has not failed to converged.

The running average plots indicate that the sampler appears to be mixing well by 5,000 iterations and that the chain has not failed to converged.

Traceplots and running average plots of σ

Examine the trace plots and running average plots of Σ on your own.

Return to posterior inference

Given our samples from our Gibbs sampler, we can approximate posterior probabilities and confidence regions.

Confidence regions

```
quantile(THETA[,2] - THETA[,1], prob=c(0.025,0.5,0.975))
## 2.5% 50% 97.5%
## 1.356260 6.614818 11.667128
```

Posterior inference

Suppose we were to give the exams/instruction to a large population, then would the average score on the second exam be higher than the first second?

We can quanify this by calculating

$$Pr(\theta_2 > \theta_1 \mid y_1, \dots y_n) = 0.99$$

[1] 0.9926