Module 7: Introduction to Gibbs Sampling

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Agenda

- ► Background knowledge (inverse CDF method)
- Gibbs sampling (two-stage sampler)
- Exponential example
- Normal example
- Pareto example
- Diagnostics

What will you learn in this lecture

- What is a Gibbs sampler?
- Some important properties of a Gibbs sampler
- What is needed in order to run a Gibbs sampler (the conditional distributions)
- ▶ How to find the conditional distributions for some examples
- Diagnostics used for monitoring "convergence" of the Gibbs sampler
- By the end of the lecture, you should know how to derive conditional distributions, run a Gibbs sampler, analyze diagnostics, and interpret summary statistics from the Gibbs sampler!

Background knowledge

The inverse CDF technique for generating a random sample uses the fact that a continuous CDF, F, is a one-to-one mapping of the domain of the CDF into the interval (0,1).

Lemma

If U is a uniform random variable on (0,1), then $X = F^{-1}(U)$ has the distribution F.

Formal Proof: https://www.youtube.com/watch?v=irheiVXJRm8

Gibbs sampler

- Suppose p(x, y) is a p.d.f. or p.m.f. that is difficult to sample from directly.
- Suppose, though, that we can easily sample from the conditional distributions p(x|y) and p(y|x).
- The Gibbs sampler proceeds as follows:
 - 1. set x and y to some initial starting values
 - 2. then sample x|y, then sample y|x, then x|y, and so on.

Gibbs sampler

- 0. Set (x_0, y_0) to some starting value.
- 1. Sample $x_1 \sim p(x|y_0)$, that is, from the conditional distribution $X \mid Y = y_0$.

Current state: (x_1, y_0) Sample $y_1 \sim p(y|x_1)$, that is, from the conditional distribution $Y \mid X = x_1$.

Current state: (x_1, y_1)

2. Sample $x_2 \sim p(x|y_1)$, that is, from the conditional distribution $X \mid Y = y_1$.

Current state: (x_2, y_1) Sample $y_2 \sim p(y|x_2)$, that is, from the conditional distribution $Y \mid X = x_2$.

Current state: (x_2, y_2)

Repeat iterations 1 and 2, M times.

Gibbs sampler

This procedure defines a sequence of pairs of random variables

$$(X_0, Y_0), (X_1, Y_1), (X_2, Y_2), (X_3, Y_3), \dots$$

Markov chain and dependence

$$(X_0, Y_0), (X_1, Y_1), (X_2, Y_2), (X_3, Y_3), \dots$$

satisfies the property of being a Markov chain.

The conditional distribution of (X_{i+1}, Y_{i+1}) given all of the previous pairs depends only on (X_i, Y_i)

Example: The conditional distribution of (X_5, Y_5) given all of the previous pairs depends only on (X_4, Y_4)

 $(X_0, Y_0), (X_1, Y_1), (X_2, Y_2), (X_3, Y_3), \dots$ are not iid samples (Think about why).

Ideal Properties of MCMC

- (x_0, y_0) chosen to be in a region of high probability under p(x, y), but often this is not so easy.
- We run the chain for M iterations and discard the first B samples $(X_1, Y_1), \ldots, (X_B, Y_B)$. This is called *burn-in*.
- Typically: if you run the chain long enough, the choice of B doesn't matter.
- ▶ Roughly speaking, the performance of an MCMC algorithm—that is, how quickly the sample averages $\frac{1}{N}\sum_{i=1}^{N} h(X_i, Y_i)$ converge—is referred to as the *mixing rate*.
- ► An algorithm with good performance is said to "have good mixing", or "mix well".

Gibbs is a type of MCMC

Under some conditions, assume that $E|(X,Y)| < \infty$. Assume that

$$(X,Y) \sim p(x,y)$$

Then

$$\frac{1}{M}\sum_{i=1}^{M}(X_i,Y_i)\to E[(X,Y)]$$

as $M \to \infty$.

Thus, we have an approximation of E[(X, Y)], which is referred to MCMC in this setting (the pairs are not i.i.d.)

Exponential Example

Consider the following Exponential model for observation(s) $x = (x_1, ..., x_n)^{1}$:

$$p(x|a,b) = ab \exp(-abx)I(x > 0)$$

and suppose the prior is

$$p(a, b) = \exp(-a - b)I(a, b > 0).$$

You want to sample from the posterior p(a, b|x).

 $^{^{1}\}mbox{Please}$ note that in the attached data there are 40 observations, which can be found in data-exponential.csv.

Conditional distributions

$$p(\mathbf{x}|a,b) = \prod_{i=1}^{n} p(x_i|a,b)$$

$$= \prod_{i=1}^{n} ab \exp(-abx_i)$$

$$= (ab)^n \exp\left(-ab\sum_{i=1}^{n} x_i\right).$$

The function is symmetric for a and b, so we only need to derive $p(a|\mathbf{x},b)$.

Conditional distributions

This conditional distribution satisfies

$$p(a|\mathbf{x},b) \propto_a p(a,b,\mathbf{x})$$

= $p(\mathbf{x}|a,b)p(a,b)$
= fill in full details for lab this week

Gibbs sampling code

```
knitr::opts_chunk$set(cache=TRUE)
library(MASS)
data <- read.csv("data-exponential.csv", header = FALSE)</pre>
```

Gibbs sampling code

```
# This function is a Gibbs sampler
#
# Args
   start.a: initial value for a
# start.b: initial value for b
# n.sims: number of iterations to run
# data: observed data, should be in a
         # data frame with one column
#
# Returns:
# A two column matrix with samples
    # for a in first column and
# samples for b in second column
```

Gibbs sampling code

```
sampleGibbs <- function(start.a, start.b, n.sims, data){</pre>
  # get sum, which is sufficient statistic
 x <- sum(data)
  # qet n
 n <- nrow(data)
  # create empty matrix, allocate memory for efficiency
 res <- matrix(NA, nrow = n.sims, ncol = 2)
 res[1,] <- c(start.a, start.b)
 for (i in 2:n.sims){
    # sample the values
    res[i,1] \leftarrow rgamma(1, shape = n+1,
                        rate = res[i-1,2]*x+1)
    res[i,2] \leftarrow rgamma(1, shape = n+1,
                        rate = res[i,1]*x+1)
 return(res)
```

Gibbs sampler code

```
# run Gibbs sampler
n.sims < -10000
# return the result (res)
res <- sampleGibbs(0.25,0.25,n.sims,data)
head(res)
##
             \lceil .1 \rceil \qquad \lceil .2 \rceil
## [1.] 0.250000 0.2500000
   [2,] 1.859753 0.1732889
   [3,] 1.998903 0.2278472
## [4.] 1.990581 0.2137003
## [5,] 2.558853 0.1887937
## [6,] 2.116031 0.1844649
```

Exponential Example

You will explore this problem more in lab this week and in your homework.

$$p(x,y) \propto e^{-xy} \mathbb{1}(x,y \in (0,c))$$

$$p(x|y) \underset{x}{\propto} p(x,y) \underset{x}{\propto} e^{-xy} \mathbb{1}(0 < x < c) \underset{x}{\propto} \operatorname{Exp}(x|y) \mathbb{1}(x < c).^2$$

- \triangleright p(x|y) is a truncated version of the Exp(y) distribution
- ▶ It is the same as taking $X \sim \text{Exp}(y)$ and conditioning on it being less than c, i.e., $X \mid X < c$.
- Let's refer to this as the TExp(y, (0, c)) distribution.

²Under \propto , we write the random variable (x) for clarity.

- ► The Gibbs sampling approach is to alternately sample from p(x|y) and p(y|x).
- Note p(x, y) is symmetric with respect to x and y.
- ► Hence, only need to derive one of these and then we can get the other one by just swapping *x* and *y*.
- Let's look at p(x|y).

An easy way to generate a sample from $Z \sim \mathsf{TExp}(\theta, (0, c))$, is:

1. First, sample $U \sim \text{Uniform}(0, F(c|\theta))$ where

$$F(x|\theta) = 1 - e^{-\theta x}$$

is the $Exp(\theta)$ c.d.f.

2. Set $Z = F^{-1}(U|\theta)$ where

$$F^{-1}(u|\theta) = -(1/\theta)\log(1-u)$$

is the inverse c.d.f. for $u \in (0,1)$.

There is an exercise on the next slide to prove step 2.

Practice Exercise: Verify that

$$F^{-1}(u|\theta) = -(1/\theta)\log(1-u).$$

Solution:

To solve for F^{-1} , set u = F(x) for $u \in (0,1)$ and solve for x.

$$u = 1 - e^{-\theta x} \implies$$

$$e^{-\theta x} = 1 - u \implies$$

$$-\theta x = \log(1 - u) \implies$$

$$x = -\frac{1}{\theta}\log(1 - u).$$

This proves that $F^{-1}(u|\theta) = -(1/\theta)\log(1-u)$.

Let's apply Gibbs sampling, denoting S = (0, c).

- 0. Initialize $x_0, y_0 \in S$.
- 1. Sample $x_1 \sim \mathsf{TExp}(y_0, S)$, then sample $y_1 \sim \mathsf{TExp}(x_1, S)$.
- 2. Sample $x_2 \sim \mathsf{TExp}(y_1, S)$, then sample $y_2 \sim \mathsf{TExp}(x_2, S)$.
- N. Sample $x_N \sim \mathsf{TExp}(y_{N-1}, S)$, sample $y_N \sim \mathsf{TExp}(x_N, S)$.

Figure 1 demonstrates the algorithm, with c=2 and initial point $(x_0,y_0)=(1,1)$.

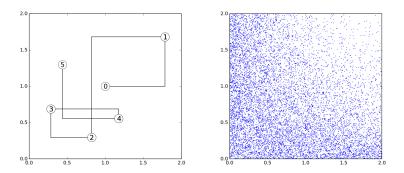


Figure 1: (Left) Schematic representation of the first 5 Gibbs sampling iterations/sweeps/scans. (Right) Scatterplot of samples from 10^4 Gibbs sampling iterations.

Example: Normal with semi-conjugate prior

Consider

$$X_1,\ldots,X_n|\mu,\lambda\stackrel{iid}{\sim}\mathcal{N}(\mu,\lambda^{-1}).$$

Then independently consider

$$oldsymbol{\mu} \sim \mathcal{N}(\mu_0, \lambda_0^{-1})$$
 $oldsymbol{\lambda} \sim \mathsf{Gamma}(a, b)$

We refer to this as a **semi-conjugate situation** for the following reasons:

- 1. The prior on μ is **conjugate** for each fixed value of λ since we get an updated Normal distribution.
- 2. The prior on λ is **conjugate** for each fixed value of μ since we get an updated Gamma distribution.

For ease of notation, denote the observed data points by $x_{1:n}$.

How does one derive $p(\mu, \lambda \mid x_{1:n})$?

Example

We know that for the Normal–Normal model, we know that for any fixed value of λ ,

$$\mu|\lambda, x_{1:n} \sim \mathcal{N}(M_{\lambda}, L_{\lambda}^{-1})$$

where

$$L_{\lambda} = \lambda_0 + n\lambda$$
 and $M_{\lambda} = \frac{\lambda_0 \mu_0 + \lambda \sum_{i=1}^n x_i}{\lambda_0 + n\lambda}$.

For any fixed value of μ , it is straightforward to derive³ that

$$\lambda | \mu, x_{1:n} \sim \mathsf{Gamma}(A_{\mu}, B_{\mu})$$
 (1)

where $A_{\mu} = a + n/2$ and

$$B_{\mu} = b + \frac{1}{2} \sum (x_i - \mu)^2 = n\hat{\sigma}^2 + n(\bar{x} - \mu)^2$$

where $\hat{\sigma}^2 = \frac{1}{n} \sum (x_i - \bar{x})^2$.

³derivation is found at the end of slides

Example

Goal: sample from $p(\mu, \lambda \mid x_{1:n})$

To implement Gibbs sampling in this example, each iteration consists of sampling:

$$\mu | \lambda, x_{1:n} \sim \mathcal{N}(M_{\lambda}, L_{\lambda}^{-1})$$

 $\lambda | \mu, x_{1:n} \sim \mathsf{Gamma}(A_{\mu}, B_{\mu}).$

This will give us samples

$$(\mu_0,\lambda_0),\ldots(\mu_S,\lambda_S)$$

Pareto example

Distributions of sizes and frequencies often tend to follow a "power law" distribution.

- wealth of individuals
- size of oil reserves
- size of cities
- word frequency
- returns on stocks

Power low distribution

The power law (also called the scaling law) states that a relative change in one quantity results in a proportional relative change in another.

Example: One simple example to think of is a square. If we double the length of one side, from 2 to 4 inches, then the area will quadruple (from 4 to 16 inches squared).

A power law distribution has the form

$$Y = kX^{\alpha}$$

, where:

X,Y are random variables, k is a constant and α is a fixed exponent.

Power law distribution

The Pareto distribution with shape $\alpha > 0$ and scale c > 0 has p.d.f.

$$\mathsf{Pareto}(x|\alpha,c) = \frac{\alpha c^\alpha}{x^{\alpha+1}} \mathbb{1}(x>c) \propto \frac{1}{x^{\alpha+1}} \mathbb{1}(x>c).$$

- ► This is referred to as a power law distribution, because the p.d.f. is proportional to x raised to a power.
- c is a lower bound on the observed values.
- \blacktriangleright We will use Gibbs sampling to perform inference for α and c.
- ► Let *X* be the population of a city.

Pareto example Population

Rank	City	Population
1	Charlotte	731424
2	Raleigh	403892
3	Greensboro	269666
4	Durham	228330
5	Winston-Salem	229618
6	Fayetteville	200564
7	Cary	135234
8	Wilmington	106476
9	High Point	104371
10	Greenville	84554
11	Asheville	85712
12	Concord	79066
:	:	:
44	Havelock	20735
45	Carrboro	19582
46	Shelby	20323
47	Clemmons	18627
48	Lexington	18931
49	Elizabeth City	18683

Parameter intepretations

- ightharpoonup lpha tells us the scaling relationship between the size of cities and their probability of occurring.
 - $\blacktriangleright \ \ \mathsf{Let} \ \alpha = 1.$
 - ▶ Density looks like $1/x^{\alpha+1} = 1/x^2$.
 - Cities with 10,000-20,000 inhabitants occur roughly $10^{\alpha+1}=100$ times as frequently as cities with 100,000-110,000 inhabitants (or $10^{\alpha+1}/10=10$ times as frequently as cities with 100,000-200,000 inhabitants)
- c represents the cutoff point—any cities smaller than this were not included in the dataset.

Prior selection

For simplicity, let's use an (improper) default prior:

$$p(\alpha, c) \propto \mathbb{1}(\alpha, c > 0).$$

Recall:

- ► An *improper/default prior* is a non-negative function of the parameters which integrates to infinity.
- Often (but not always!) the resulting "posterior" will be proper.
- ▶ It is important that the "posterior" be proper, since otherwise the whole Bayesian framework breaks down.

Pareto example

Recall

$$p(x|\alpha,c) = \frac{\alpha c^{\alpha}}{x^{\alpha+1}} \mathbb{1}(x > c)$$

$$\mathbb{1}(\alpha,c > 0)$$
(2)

Let's derive the posterior:

$$p(\alpha, c|x_{1:n}) \overset{\text{def}}{\underset{\alpha,c}{\propto}} p(x_{1:n}|\alpha, c)p(\alpha, c)$$

$$\underset{\alpha,c}{\propto} \mathbb{1}(\alpha, c > 0) \prod_{i=1}^{n} \frac{\alpha c^{\alpha}}{x_{i}^{\alpha+1}} \mathbb{1}(x_{i} > c)$$

$$= \frac{\alpha^{n} c^{n\alpha}}{(\prod x_{i})^{\alpha+1}} \mathbb{1}(c < x_{*}) \mathbb{1}(\alpha, c > 0)$$
(4)

where $x_* = \min\{x_1, \dots, x_n\}$.

Pareto example

As a joint distribution on (α, c) ,

- ▶ this does not seem to have a recognizable form,
- and it is not clear how we might sample from it directly.

Gibbs sampling

Let's try Gibbs sampling! To use Gibbs, we need to be able to sample $\alpha|c, x_{1:n}$ and $c|\alpha, x_{1:n}$.

By Equation 4, we find that

$$p(\alpha|c, x_{1:n}) \underset{\alpha}{\propto} p(\alpha, c|x_{1:n}) \underset{\alpha}{\propto} \frac{\alpha^n c^{n\alpha}}{(\prod x_i)^{\alpha}} \mathbb{1}(\alpha > 0)$$

$$= \alpha^n \exp(-\alpha(\sum \log x_i - n \log c)) \mathbb{1}(\alpha > 0)$$

$$\underset{\alpha}{\propto} \mathsf{Gamma}(\alpha \mid n+1, \sum \log x_i - n \log c),$$

and

$$p(c|\alpha, x_{1:n}) \underset{c}{\propto} p(\alpha, c|x_{1:n}) \underset{c}{\propto} c^{n\alpha} \mathbb{1}(0 < c < x_*),$$

which we will define to be $Mono(n\alpha + 1, x_*)$, and we define generally on the next slide.

Mono distribution

Here, we define the Mono distribution generally before returning to our example.

For a > 0 and b > 0, define the distribution Mono(a, b) (for monomial) with p.d.f.

Mono
$$(x|a, b) \propto x^{a-1} \mathbb{1}(0 < x < b).$$

Since $\int_0^b x^{a-1} dx = b^a/a$, we have

Mono
$$(x|a,b) = \frac{a}{b^a}x^{a-1}\mathbb{1}(0 < x < b),$$

and for 0 < x < b, the c.d.f. is

$$F(x|a,b) = \int_0^x \mathsf{Mono}(y|a,b) dy = \frac{a}{b^a} \frac{x^a}{a} = \frac{x^a}{b^a}.$$

Pareto example

To use the inverse c.d.f. technique, we solve for the inverse of F on 0 < x < b: Let $u = \frac{x^a}{b^a}$ and solve for x.

$$u = \frac{x^a}{b^a} \tag{5}$$

$$b^a u = x^a \tag{6}$$

$$bu^{1/a} = x (7)$$

Can sample from Mono(a,b) by drawing $U \sim \text{Uniform}(0,1)$ and setting $X = bU^{1/a}$.⁴

⁴It turns out that this is an inverse of the Pareto distribution, in the sense that if $X \sim \operatorname{Pareto}(\alpha,c)$ then $1/X \sim \operatorname{Mono}(\alpha,1/c)$.

Pareto example

So, in order to use the Gibbs sampling algorithm to sample from the posterior $p(\alpha, c|x_{1:n})$, we initialize α and c, and then alternately update them by sampling:

$$\alpha | c, x_{1:n} \sim \operatorname{Gamma}(n+1, \sum \log x_i - n \log c)$$

 $c | \alpha, x_{1:n} \sim \operatorname{Mono}(n\alpha + 1, x_*).$

Traceplots

Traceplots. A traceplot simply shows the sequence of samples, for instance $\alpha_1, \ldots, \alpha_N$, or c_1, \ldots, c_N . Traceplots are a simple but very useful way to visualize how the sampler is behaving.

Traceplots

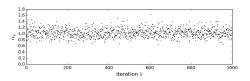


Figure 2: Traceplot of $\boldsymbol{\alpha}$

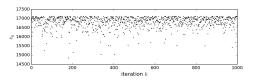


Figure 3: Traceplot of c.

Estimated density

Estimated density. We are primarily interested in the posterior on α , since it tells us the scaling relationship between the size of cities and their probability of occurring.

By making a histogram of the samples $\alpha_1, \ldots, \alpha_N$, we can estimate the posterior density $p(\alpha|x_{1:n})$.

The two vertical lines indicate the lower ℓ and upper u boundaries of an (approximate) 90% credible interval $[\ell, u]$ —that is, an interval that contains 90% of the posterior probability:

$$\mathbb{P}(\alpha \in [\ell, u] | x_{1:n}) = 0.9.$$

Estimated density

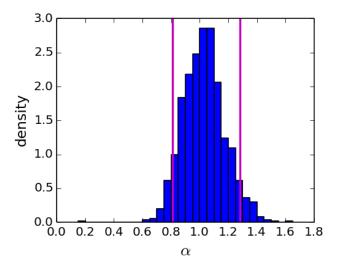


Figure 4: Estimated density of $\alpha | x_{1:n}$ with \approx 90 percent credible intervals.

Running averages

Running averages. Panel (d) shows the running average $\frac{1}{k} \sum_{i=1}^{k} \alpha_i$ for k = 1, ..., N.

In addition to traceplots, running averages such as this are a useful heuristic for visually assessing the convergence of the Markov chain.

The running average shown in this example still seems to be meandering about a bit, suggesting that the sampler needs to be run longer (but this would depend on the level of accuracy desired).

Running averages

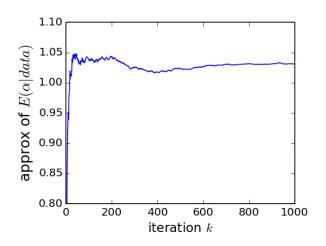


Figure 5: Running average plot

Survival functions

A survival function is defined to be

$$S(x) = \mathbb{P}(X > x) = 1 - \mathbb{P}(X \le x).$$

Power law distributions are often displayed by plotting their survival function S(x), on a log-log plot.

Why? $S(x) = (c/x)^{\alpha}$ for the Pareto (α, c) distribution and on a log-log plot this appears as a line with slope $-\alpha$.

The posterior survival function (or more precisely, the posterior predictive survival function), is $S(x|x_{1:n}) = \mathbb{P}(X_{n+1} > x \mid x_{1:n})$.

Survival functions

Figure 6(e) shows an empirical estimate of the survival function (based on the empirical c.d.f., $\hat{F}(x) = \frac{1}{n} \sum_{i=1}^{n} \mathbb{1}(x \ge x_i)$) along with the posterior survival function, approximated by

$$S(x|x_{1:n}) = \mathbb{P}(X_{n+1} > x \mid x_{1:n})$$

$$= \int \mathbb{P}(X_{n+1} > x \mid \alpha, c) p(\alpha, c \mid x_{1:n}) d\alpha dc$$

$$\approx \frac{1}{N} \sum_{i=1}^{N} \mathbb{P}(X_{n+1} > x \mid \alpha_i, c_i) = \frac{1}{N} \sum_{i=1}^{N} (c_i/x)^{\alpha_i}.$$
 (10)

This is computed for each x in a grid of values.

Survival functions

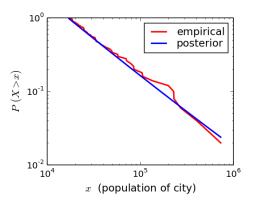


Figure 6: Empirical vs posterior survival function

Detailed Takeways

- inverse CDF method
- ► Two-stage Gibbs sampler
- Markov Chain
- properties of Markov chains
- Exponential Example
- Truncated Exponential
- ► Normal-Normal-Gamma
- Pareto Case Study
- Trace plots
- Estimated Densities
- ► Running Aveage Plots
- Survival Funtions

In class notes

Notes on burn-in can be found here:

 $https://github.com/resteorts/modern-bayes/blob/master/lectures\\ ModernBayes20/lecture-7/class-notes/gibbs-partI/burn-in.pdf$

Notes on Exponential example can be found here:

https://github.com/resteorts/modern-

bayes/blob/master/lectures Modern Bayes 20/lecture - 7/class-notes/gibbs-part I/gibbs-exponential-example.pdf

Notes on truncated exponential example can be found here:

https://github.com/resteorts/modern-

bayes/blob/master/lectures Modern Bayes 20/lecture-7/class-notes/gibbs-partI/gibbs-truncated-exponential-example.pdf

Notes on the two-stage Gibbs sampler set up can be found here: $https://github.com/resteorts/modern-bayes/blob/master/lectures \\ ModernBayes20/lecture-7/class-notes/gibbs-partl/intro-gibbs.pdf$

Exercise

Recall that

$$X_1, \dots, X_n \mid \lambda \stackrel{iid}{\sim} \text{Normal}(\mu, \lambda^{-1})$$
 (11)
 $\lambda \sim \text{Gamma}(a, b)$ (12)

Let's derive the posterior update of $\lambda \mid x_{1:n}$, which we utilized in an earlier derivation.

Exercise

$$p(\lambda \mid x_{1:n}) \propto p(x_{1:n} \mid \lambda)p(\lambda)$$

$$= \prod_{i=1}^{n} \left[\sqrt{\frac{\lambda}{2\pi}} \exp\left\{-\frac{\lambda}{2}(x_{i} - \mu)^{2}\right\} \right] \times \frac{b^{a}}{\Gamma(a)} \lambda^{a-1} e^{-b\lambda}$$

$$\propto (\lambda)^{n/2} \exp\left\{-\frac{\lambda}{2} \sum_{i=1}^{n} (x_{i} - \mu)^{2}\right\} \times \lambda^{a-1} e^{-b\lambda}$$

$$\propto (\lambda)^{a+n/2-1} \exp\left\{\lambda \left[b + \sum_{i=1}^{n} (x_{i} - \mu)^{2}\right]\right\}$$

$$(15)$$

This implies that

$$\lambda \mid x_{1:n} \sim \text{Gamma}(a + n/2, b + \sum_{i=1}^{n} (x_i - \mu)^2)$$
 (17)