

Module 8: The Multivariate Normal Distribution

Rebecca C. Steorts

Hoff, Section 7.4

Exam II

- ▶ Coverage will be modules 5 – 7
- ▶ The exam will be during on Thursday, March 24
- ▶ The exam will be open note/open book (open resources)
- ▶ You may not talk to anyone during the exam except for myself or a TA
- ▶ All questions must be sent via private chat.
- ▶ Look over the ENTIRE exam during the first 15 minutes to see if you have clarifying questions to avoid a triage of questions at the end of the exam.
- ▶ You are to not talk/post/communicate with anyone about the exam until after grades are released (or this is an honor code violation), so DO NOT post anywhere (including piazza).

Exam II General Topics

- ▶ Module 5: Monte Carlo (naive, importance sampling, rejection sampling)
- ▶ Module 6: MCMC (MCMC, why MCMC, Markov property, advantages/disadvantages, ergodic theorem)
- ▶ Module 6: Example of MCMC: Metropolis Algorithm (original paper)
- ▶ Module 6: Metropolis Algorithm from a Bayesian perspective
- ▶ Module 6: Traceplots, Posterior Densities

Exam II General Topics

- ▶ Module 7: Gibbs sampling (two stage and multi-stage Gibbs sampler)
- ▶ Module 7: Latent variable models and data augmentation (censoring and gaussian mixture models)
- ▶ Module 7: Diagnostics: Traceplots, Running average plots, burn-in
- ▶ Module 7: Other topics: the label switching problem

Exam II

- ▶ Given the amount of material, I will not be able to test you on everything above. It's just not possible.
- ▶ So, use your time wisely, and make sure you have a firm knowledge of everything that we have covered.

What are the main topics for Exam II

1. Monte carlo (naive, importance sampling, rejection sampling)
2. General properties of MCMC (MCMC, why MCMC, Markov property, advantages/disadvantages, ergodic theorem)
3. Intro to the Metropolis algorithm (original 1959 paper)
4. The Metroplis Algorithm from a Bayesian perspective
5. Diagnostics (traceplots, running average plots, posterior densities, posterior credible intervals, burn-in)
6. Gibbs sampling (just the set up, deriving conditionals, and writing pseudo-code for the Gibbs sampler)
7. Censoring using latent variables
8. Gaussian mixture models using latent variables (data augmentation)

Agenda

- ▶ Motivational reading comprehension case study
- ▶ Introduction/Review of vectors, matrices
- ▶ Population means/covariance matrices
- ▶ General multivariate notation
- ▶ Background on linear algebra (with practice exercises)
- ▶ Determinants, traces, quadratic forms

Agenda

- ▶ The multivariate normal distribution (MVN)
- ▶ Exercise with the MVN
- ▶ MVN-MVN semi-conjugacy
- ▶ The inverse wishart distribution
- ▶ MVN-inverse wishart semi-conjugacy
- ▶ The MVN-MVN-inverse wishart model
- ▶ Applying a Gibbs sampler
- ▶ How to draw samples from the MVN and inverse wishart distributions
- ▶ Case study on reading comprehension

What you should learn

- ▶ You will learn background on linear algebra
- ▶ You will learn how to model multivariate data, where we consider an application to reading comprehension tests
- ▶ You will learn the notation for multivariate random variables
- ▶ You will learn about the multivariate density of the normal
- ▶ You will derive the posterior of the MVN-MVN
- ▶ You will derive the posterior of the MVN-inverseWishart
- ▶ You will consider a more complex model of the MVN-MVN-inverseWishart which will be covered in homework 7.
- ▶ Together we will look at the reading comprehension to understand how to make inferences and you will also finish this in lab and homework.

Goal

The goal of this module is to be able **to understand how to work with multivariate distributions**, such as the multivariate normal distribution.

We also want to understand how univariate models that we have used in the past translate to the multivariate setting.

Before we can delve in, we must review background on matrices, vectors, and **multivariate notation**. We also must review background on **linear algebra**.

Example: Reading Comprehension

A sample of 22 children are given reading comprehension tests before and after receiving a particular instructional method.¹

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 by the vector \mathbf{Y}_i

$$\mathbf{Y}_i = \begin{pmatrix} Y_{i,1} \\ Y_{i,2} \end{pmatrix} = \begin{pmatrix} \text{score on first test} \\ \text{score on second test} \end{pmatrix}$$

where $i = 1, \dots, n$ and $p = 2$.

¹This example follows Hoff (Section 7.4, p. 112).

Example: Reading Comprehension

$$\mathbf{X}_{n \times p} = \begin{pmatrix} x_{11} & \color{red}{x_{12}} & \dots & x_{1p} \\ x_{21} & \color{red}{x_{22}} & \dots & x_{2p} \\ x_{31} & \color{red}{x_{32}} & \dots & x_{3p} \\ x_{i1} & \color{red}{x_{i2}} & \dots & x_{ip} \\ \vdots & \vdots & \ddots & \vdots \\ x_{n1} & \color{red}{x_{n2}} & \dots & x_{np} \end{pmatrix}.$$

- ▶ A row of $\mathbf{X}_{n \times p}$ represents a covariate we might be interested in, such as age of a person.
- ▶ Denote x_i ($p \times 1$) as the i th **row vector** of the $\mathbf{X}_{n \times p}$ matrix.

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

Example: Reading Comprehension

We may be interested in the population mean $\mu_{p \times 1}$.

$$E[\mathbf{Y}] =: E[\mathbf{Y}_i] = \begin{pmatrix} Y_{i,1} \\ Y_{i,2} \end{pmatrix} = \begin{pmatrix} \mu_1 \\ \mu_2 \end{pmatrix} = \boldsymbol{\mu}$$

Example: Reading Comprehension

We also may be interested in the population covariance matrix, $\Sigma_{p \times p}$.

By definition:

$$\Sigma = \text{Cov}(\mathbf{Y}) \quad (1)$$

$$= \begin{pmatrix} E[Y_1^2] - E[Y_1]^2 & E[Y_1 Y_2] - E[Y_1]E[Y_2] \\ E[Y_1 Y_2] - E[Y_1]E[Y_2] & E[Y_2^2] - E[Y_2]^2 \end{pmatrix} \quad (2)$$

$$= \begin{pmatrix} \sigma_1^2 & \sigma_{1,2} \\ \sigma_{1,2} & \sigma_2^2 \end{pmatrix} \quad (3)$$

Remark: $\text{Cov}(Y_1) = \text{Var}(Y_1) = \sigma_1^2$. $\text{Cov}(Y_1, Y_2) = \sigma_{1,2}$.

How do we expand this beyond our reading comprehension example

We introduced our notation based upon a specific example to reading comprehension.

How can we make this more general and applicable to general case studies and problems?

General Notation

Assume that $\mathbf{y}_{p \times 1} \sim (\mu_{p \times 1}, \Sigma_{p \times p})$.

$$\mathbf{y}_{p \times 1} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_p \end{pmatrix}.$$

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

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

Background

Before proceeding, we need to review some basic concepts from linear algebra:

1. Basic properties of matrices
2. Useful lemmas for working with matrices

The determinant of a matrix

Assume a matrix $A_{n \times n}$ is invertible. The

$$\det(A) = a_{i1}A_{i1} + a_{i2}A_{i2} + \cdots + a_{in}A_{in},$$

where A_{ij} are the co-factors and are computed from

$$A_{ij} = (-1)^{i+j} \det(M_{ij}).$$

M_{ij} is known as the minor matrix and is the matrix you get if you eliminate row i and column j from matrix A . You must apply this technique recursively.

We only use this technique when doing such calculations by hand or in proof-based approaches.

The determinant of a matrix

- ▶ How on earth do I use the complicated formula on the pervious slide.

Easy: Use the `det` command in R when faced with an application.

- ▶ You will also see a determinant in the definition of the multivariate normal distribution.

Important point: It's just a function and we typically do not need to evalute it in this course!

The trace of a matrix

Assume a matrix $H_{p \times p}$.

$$\text{trace}(H) = \sum_i h_{ii},$$

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

The trace of a matrix

$$H = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

What is $\text{tr}(H)$?

(Take 1 minute to complete this.)

Linear Algebra Tricks

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

Lemma 1:

$$\text{tr}(AB) = \text{tr}(BA)$$

Proof: Exercise. (You can find the proof at the end of the slides to check your work).

Linear Algebra Tricks

Lemma 2:

Suppose \mathbf{x} is a vector. $\mathbf{x}^T A \mathbf{x}$ is called a **quadratic form**.

$$\mathbf{x}^T A \mathbf{x} = \text{tr}(\mathbf{x}^T A \mathbf{x}) = \text{tr}(\mathbf{x} \mathbf{x}^T A) = \text{tr}(A \mathbf{x} \mathbf{x}^T)$$

Proof: Exercise.

Linear Algebra Tricks

Proof of Lemma 2:

$$\text{tr}(\mathbf{x}^T \mathbf{A} \mathbf{x}) = \sum_i (\mathbf{x}^T \mathbf{A} \mathbf{x})_{ii} \quad (4)$$

$$= (\mathbf{x}^T (\mathbf{A} \mathbf{x})) \quad (5)$$

$$= \text{tr}(\mathbf{A} \mathbf{x} \mathbf{x}^T) \text{ (by Lemma 1)} \quad (6)$$

$$\text{tr}(\mathbf{x}^T \mathbf{A} \mathbf{x}) = \sum_i (\mathbf{x}^T \mathbf{A} \mathbf{x})_{ii} \quad (7)$$

$$= ((\mathbf{x}^T \mathbf{A}) \mathbf{x}) \quad (8)$$

$$= \text{tr}(\mathbf{x} \mathbf{x}^T \mathbf{A}) \text{ (by Lemma 1)} \quad (9)$$

Notation

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

Example: $\text{Cov}(Y_1, Y_2)$ is just one element of the matrix Σ .

Multivariate Normal

Just as the probability density of a scalar normal is

$$p(x) = \left(2\pi\sigma^2\right)^{-1/2} \exp \left\{ -\frac{1}{2} \frac{(x - \mu)^2}{\sigma^2} \right\}, \quad (10)$$

the probability density of the multivariate normal is

$$p(\mathbf{x}) = (2\pi)^{-p/2} (\det \Sigma)^{-1/2} \exp \left\{ -\frac{1}{2} (\mathbf{x} - \boldsymbol{\mu})^T \Sigma^{-1} (\mathbf{x} - \boldsymbol{\mu}) \right\}. \quad (11)$$

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

Lemma 3.

Consider

$$Z_1, \dots, Z_n \stackrel{iid}{\sim} N(0, 1).$$

Show that

$$Z_1, \dots, Z_n \sim MVN(\mathbf{0}, I_{n \times n}).$$

Proof of Lemma 3

Proof:

$$f_z(z) = \prod_{i=1}^n (2\pi)^{-1/2} e^{-z_i^2/2} \quad (12)$$

$$= (2\pi)^{-n/2} e^{\sum_i -z_i^2/2} \quad (13)$$

$$= (2\pi)^{-n/2} e^{-z^T z/2}. \quad (14)$$

The last line follows since $\sum_i -z_i^2 = -z^T z$.

Thus, $Z_1, \dots, Z_n \sim \text{MVN}(\mathbf{0}, I)$.

Goals

1. We will derive the MVN-MVN.
2. We will derive the MVN-inverse Wishart
3. We will then consider a hierarchical model and use 1-2 in order to derive our full conditional distributions and construct a Gibbs sampler. (This will help you on Homework 7).

Conjugate to MVN

Suppose that

$$\mathbf{y} = (y_1 \dots y_n)^T \mid \theta \sim MVN(\theta, \Sigma).$$

Let

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

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

Prior

$$\pi(\boldsymbol{\theta}) = (2\pi)^{-p/2} \det \Omega^{-1/2} \exp \left\{ -\frac{1}{2}(\boldsymbol{\theta} - \boldsymbol{\mu})^T \Omega^{-1}(\boldsymbol{\theta} - \boldsymbol{\mu}) \right\} \quad (15)$$

$$\propto \exp \left\{ -\frac{1}{2}(\boldsymbol{\theta} - \boldsymbol{\mu})^T \Omega^{-1}(\boldsymbol{\theta} - \boldsymbol{\mu}) \right\} \quad (16)$$

$$\propto \exp -\frac{1}{2} \left\{ \boldsymbol{\theta}^T \Omega^{-1} \boldsymbol{\theta} - 2\boldsymbol{\theta}^T \Omega^{-1} \boldsymbol{\mu} + \boldsymbol{\mu}^T \Omega^{-1} \boldsymbol{\mu} \right\} \quad (17)$$

$$\propto \exp -\frac{1}{2} \left\{ \boldsymbol{\theta}^T \Omega^{-1} \boldsymbol{\theta} - 2\boldsymbol{\theta}^T \Omega^{-1} \boldsymbol{\mu} \right\} \quad (18)$$

$$= \exp -\frac{1}{2} \left\{ \boldsymbol{\theta}^T A_o \boldsymbol{\theta} - 2\boldsymbol{\theta}^T b_o \right\} \quad (19)$$

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

Likelihood

$$p(\mathbf{y} \mid \boldsymbol{\theta}, \Sigma) = \prod_{i=1}^n (2\pi)^{-p/2} \det \Sigma^{-1/2} \exp \left\{ -\frac{1}{2} (y_i - \boldsymbol{\theta})^T \Sigma^{-1} (y_i - \boldsymbol{\theta}) \right\} \quad (20)$$

$$\propto \exp -\frac{1}{2} \left\{ \sum_i y_i^T \Sigma^{-1} y_i - 2 \sum_i \boldsymbol{\theta}^T \Sigma^{-1} y_i + \sum_i \boldsymbol{\theta}^T \Sigma^{-1} \boldsymbol{\theta} \right\} \quad (21)$$

$$\propto \exp -\frac{1}{2} \left\{ -2 \boldsymbol{\theta}^T \Sigma^{-1} n \bar{\mathbf{y}} + n \boldsymbol{\theta}^T \Sigma^{-1} \boldsymbol{\theta} \right\} \quad (22)$$

$$\propto \exp -\frac{1}{2} \left\{ -2 \boldsymbol{\theta}^T \mathbf{b}_1 + \boldsymbol{\theta}^T \mathbf{A}_1 \boldsymbol{\theta} \right\}, \quad (23)$$

where

$$\mathbf{b}_1 = \Sigma^{-1} n \bar{\mathbf{y}}, \quad \mathbf{A}_1 = n \Sigma^{-1}$$

and

$$\bar{\mathbf{y}} := \left(\frac{1}{n} \sum_i y_{i1}, \dots, \frac{1}{n} \sum_i y_{ip} \right)^T.$$

Full conditional

$$p(\boldsymbol{\theta} \mid \mathbf{y}, \Sigma) \propto p(\mathbf{y} \mid \boldsymbol{\theta}, \Sigma) \times p(\boldsymbol{\theta}) \quad (24)$$

$$\propto \exp - \frac{1}{2} \left\{ -2\boldsymbol{\theta}^T \mathbf{b}_1 + \boldsymbol{\theta}^T \mathbf{A}_1 \boldsymbol{\theta} \right\} \quad (25)$$

$$\times \exp - \frac{1}{2} \left\{ \boldsymbol{\theta}^T \mathbf{A}_o \boldsymbol{\theta} - 2\boldsymbol{\theta}^T \mathbf{b}_o \right\} \quad (26)$$

$$\propto \exp \left\{ \boldsymbol{\theta}^T \mathbf{b}_1 - \frac{1}{2} \boldsymbol{\theta}^T \mathbf{A}_1 \boldsymbol{\theta} - \frac{1}{2} \boldsymbol{\theta}^T \mathbf{A}_o \boldsymbol{\theta} + \boldsymbol{\theta}^T \mathbf{b}_o \right\} \quad (27)$$

$$\propto \exp \left\{ \boldsymbol{\theta}^T (\mathbf{b}_o + \mathbf{b}_1) - \frac{1}{2} \boldsymbol{\theta}^T (\mathbf{A}_o + \mathbf{A}_1) \boldsymbol{\theta} \right\} \quad (28)$$

Full conditional

From the previous slide, recall that

$$p(\boldsymbol{\theta} \mid \mathbf{y}, \Sigma) \propto \exp\{\boldsymbol{\theta}^T(b_o + b_1) - \frac{1}{2}\boldsymbol{\theta}^T(A_o + A_1)\boldsymbol{\theta}\}$$

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

$$b_n = b_o + b_1 = \Omega^{-1}\mu + \Sigma^{-1}n\bar{y}$$

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

Interpretations

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

$$\mu_n = A_n^{-1}b_n = [\Omega^{-1} + n\Sigma^{-1}]^{-1}(b_o + b_1) \quad (29)$$

$$= [\Omega^{-1} + n\Sigma^{-1}]^{-1}(\Omega^{-1}\mu + \Sigma^{-1}n\bar{y}) \quad (30)$$

$$\Sigma_n = A_n^{-1} = [\Omega^{-1} + n\Sigma^{-1}]^{-1} \quad (31)$$

inverse Wishart distribution

Let us now consider a prior distribution on $\Sigma_{p \times p}$, which must be a positive definite matrix, meaning that $\mathbf{x}^T \Sigma \mathbf{x} > 0$ for all \mathbf{x} .

Suppose $\Sigma_{p \times p} \sim \text{inverseWishart}(\nu_o, S_o^{-1})$ where ν_o is a scalar and S_o^{-1} is a matrix, where $\nu_o > p - 1$ and S_o must be positive definite.

It can be shown that

$$E[\Sigma] = \frac{1}{\nu_o - p - 1} S_o.$$

(See Hoff, p. 110.)

Then

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

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

$$\mathbf{y} \mid \boldsymbol{\theta}, \Sigma \sim \text{MVN}(\boldsymbol{\theta}, \Sigma).$$

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

$$\Sigma \sim \text{inverseWishart}(\nu_o, S_o^{-1}).$$

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

$$\mathbf{y} \mid \boldsymbol{\theta}, \Sigma \sim \text{MVN}(\boldsymbol{\theta}, \Sigma).$$

$$\Sigma \sim \text{inverseWishart}(\nu_o, S_o^{-1}).$$

Continued

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

$$p(\mathbf{y} \mid \boldsymbol{\theta}, \Sigma) \quad (32)$$

$$\propto \det(\Sigma)^{-n/2} \exp\left\{-\sum_i (\mathbf{y}_i - \boldsymbol{\theta})^T \Sigma^{-1} (\mathbf{y}_i - \boldsymbol{\theta})/2\right\} \quad (33)$$

$$\propto \det(\Sigma)^{-n/2} \exp\left\{-\text{tr}\left(\sum_i (\mathbf{y}_i - \boldsymbol{\theta})(\mathbf{y}_i - \boldsymbol{\theta})^T \Sigma^{-1}/2\right)\right\} \quad (34)$$

$$\propto \det(\Sigma)^{-n/2} \exp\left\{-\text{tr}(S_{\boldsymbol{\theta}} \Sigma^{-1}/2)\right\} \quad (35)$$

where $S_{\boldsymbol{\theta}} = \sum_i (\mathbf{y}_i - \boldsymbol{\theta})(\mathbf{y}_i - \boldsymbol{\theta})^T$.

Note that

$$\sum_k b_k^T A b_k = \text{tr}(B B^T A),$$

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

Continued

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

$$p(\Sigma \mid \mathbf{y}, \boldsymbol{\theta}) \tag{36}$$

$$= p(\Sigma) \times p(\mathbf{y} \mid \boldsymbol{\theta}, \Sigma) \tag{37}$$

$$\propto \det(\Sigma)^{-(\nu_o + p + 1)/2} \times \exp\{-\text{tr}(S_o \Sigma^{-1})/2\} \tag{38}$$

$$\times \det(\Sigma)^{-n/2} \exp\{-\text{tr}(S_\theta \Sigma^{-1})/2\} \tag{39}$$

$$\propto \det(\Sigma)^{-(\nu_o + n + p + 1)/2} \exp\{-\text{tr}((S_o + S_\theta) \Sigma^{-1})/2\} \tag{40}$$

This implies that

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

Continued

Suppose that we wish now to take

$$\boldsymbol{\theta} \mid \mathbf{y}, \Sigma \sim MVN(\mu_n, \Sigma_n)$$

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

$$\Sigma \mid \mathbf{y}, \boldsymbol{\theta} \sim \text{inverseWishart}(\nu_n, S_n^{-1})$$

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 \mathbf{y} 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 \mathbf{y} 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)
```

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,] 0.3142638 -1.853812
```

Evaluation

Evaluate the multivariate normal density at a single value using the `dmvnorm` 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,]  0.7245722 -0.7351094
## [2,] -1.0091095 -0.2835473
## [3,]  1.2940061  1.5560460
```

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]
```

```
##           [,1]      [,2]  
## [1,]  0.07578133 -0.2834182  
## [2,] -0.28341824  1.0790756
```

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, where $i = 1, \dots, n$.

Denote each student's pair of scores \mathbf{Y}_i

$$\mathbf{Y}_i = \begin{pmatrix} Y_{i,1} \\ Y_{i,2} \end{pmatrix} = \begin{pmatrix} \text{score on first test} \\ \text{score on second test} \end{pmatrix}$$

Model set up

$$\mathbf{Y}_i \mid \boldsymbol{\theta}, \Sigma \sim \text{MVN}(\boldsymbol{\theta}, \Sigma).$$

$$\boldsymbol{\theta} \sim \text{MVN}(\boldsymbol{\mu}_0, \Lambda_0)$$

$$\Sigma \sim \text{inverseWishart}(\nu_o, S_o^{-1}).$$

Let $\boldsymbol{\theta} = (\theta_1, \theta_2)$.

$i = 1, \dots, n$.

Prior settings

$$\mathbf{Y}_i \mid \boldsymbol{\theta}, \Sigma \sim \text{MVN}(\boldsymbol{\theta}, \Sigma).$$

$$\boldsymbol{\theta} \sim \text{MVN}(\boldsymbol{\mu}_0, \Lambda_0)$$

$$\Sigma \sim \text{inverseWishart}(\nu_o, S_o^{-1}).$$

The exam was designed to give average scores of around 50 out of 100, so $\boldsymbol{\mu}_0 = (50, 50)^T$ would be a good choice for our prior mean.

Prior settings

$$\mathbf{Y}_i \mid \boldsymbol{\theta}, \Sigma \sim \text{MVN}(\boldsymbol{\theta}, \Sigma).$$

$$\boldsymbol{\theta} \sim \text{MVN}(\boldsymbol{\mu}_0, \Lambda_0)$$

$$\Sigma \sim \text{inverseWishart}(\nu_o, S_o^{-1}).$$

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 $P(\theta_j \notin [0, 100]) = 0.05$.

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)

$$\mathbf{Y}_i \mid \boldsymbol{\theta}, \Sigma \sim \text{MVN}(\boldsymbol{\theta}_j, \Sigma).$$

$$\boldsymbol{\theta} \sim \text{MVN}(\boldsymbol{\mu}_0, \Lambda_0)$$

$$\Sigma \sim \text{inverseWishart}(\nu_o, S_o^{-1}).$$

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 $\nu_o = p + 2 = 4$, which is the mean of the inverse Wishart distribution (Hoff, p. 100).

Load in data

```
# read in data
Y <- structure(c(59, 43, 34, 32, 42, 38, 55, 67, 64,
                 45, 49, 72, 34, 70, 34, 50, 41, 52,
                 60, 34, 28, 35, 77, 39, 46, 26, 38,
                 43, 68, 86, 77, 60, 50, 59, 38, 48,
                 55, 58, 54, 60, 75, 47, 48, 33),
               .Dim = c(22L, 2L), .Dimnames = list(NULL,
               c("pretest", "posttest")))
# number of observations
```

Quick calculations

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

```
## [1] 22
```

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

```
## pretest posttest
```

```
## 47.18182 53.86364
```

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
```

Gibbs sampler

```
## Loading required package: coda
## Loading required package: MASS
## ##
## ## Markov Chain Monte Carlo Package (MCMCpack)
## ## Copyright (C) 2003-2022 Andrew D. Martin, Kevin M. Quinn
## ##
## ## Support provided by the U.S. National Science Foundation
## ## (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 \mathbf{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 \mathbf{X} and $\theta^{(s+1)}$
 - b) Sample $\Sigma^{(s+1)} \sim \text{inverseWishart}(\nu_n, S_n^{-1})$

Gibbs sampler

```
THETA <- SIGMA <- NULL
set.seed(1)
for (s in 1:5000) {
  ## update theta
  Ln <- solve(solve(L0) + n*solve(Sigma))
  mun <- Ln %*% (solve(L0) %*% mu0 +
                n*solve(Sigma) %*% ybar)
  theta <- rmvnorm(1, mun, Ln)

  ## update Sigma
  Sn <- S0 + (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))
}
```


Posterior inference

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

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

that approximates $p(\boldsymbol{\theta}, \boldsymbol{\Sigma} \mid y_1, \dots, y_n)$.

Glance at Gibbs sampler

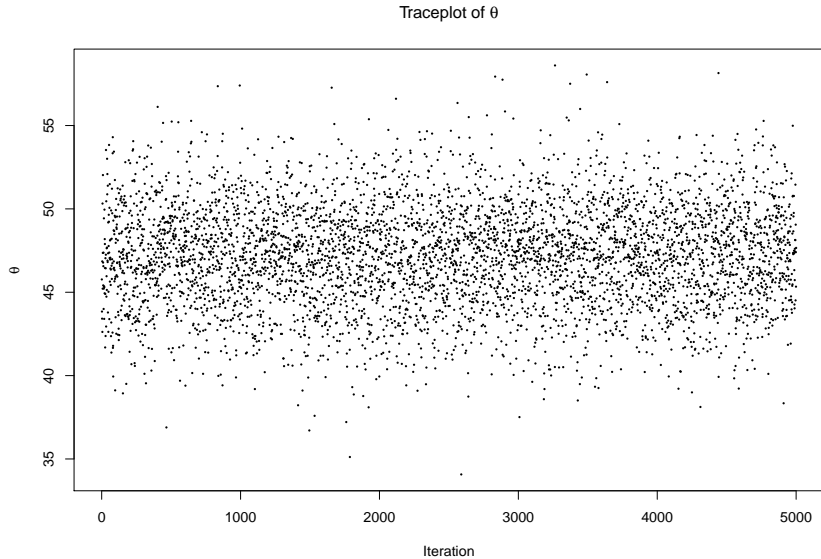
```
head(THETA)
```

```
##           [,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
```

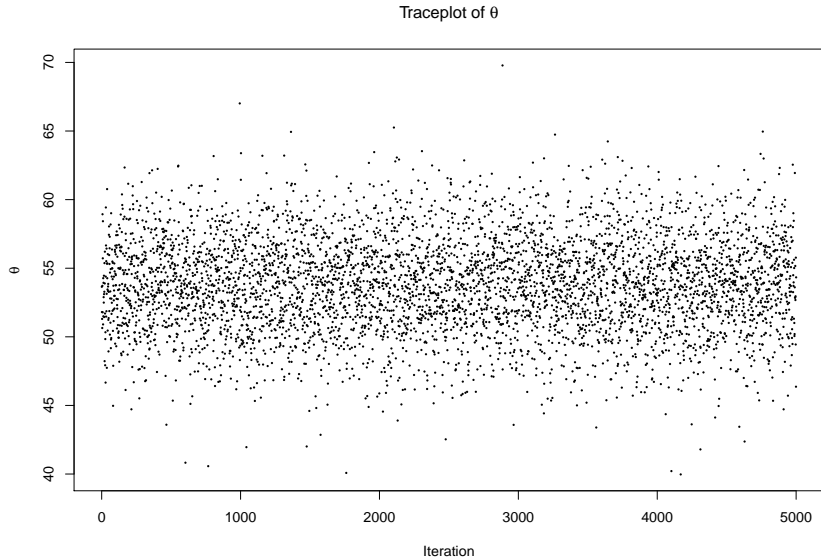
```
head(SIGMA)
```

```
##           [,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
## [6,] 289.4997 246.9184 246.9184 319.9786
```

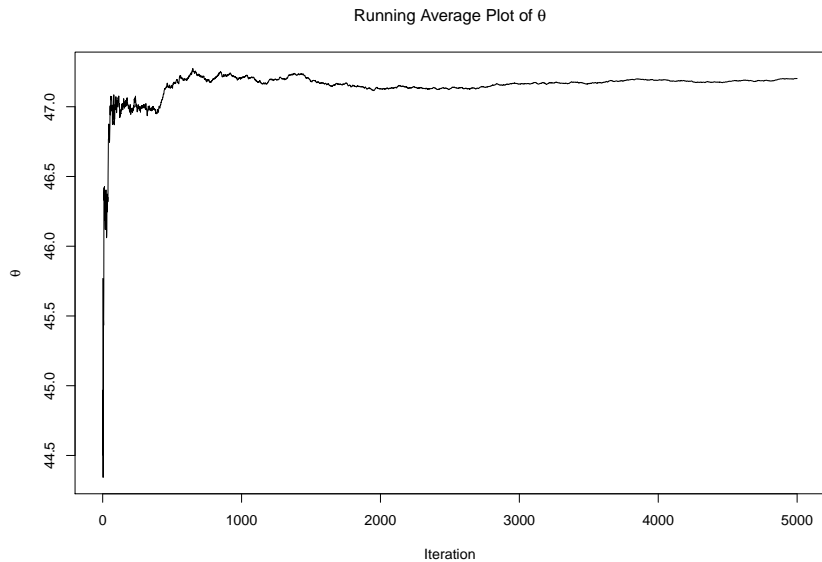
Traceplot of θ_1



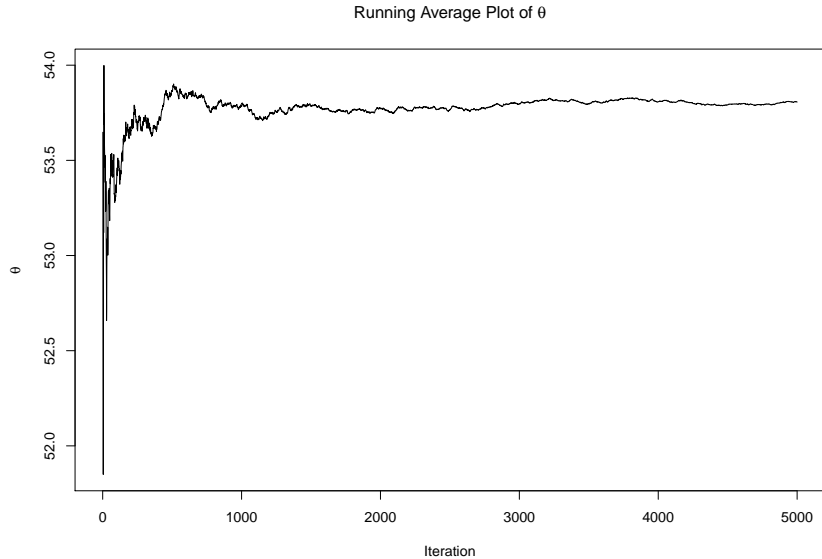
Traceplot of θ_2



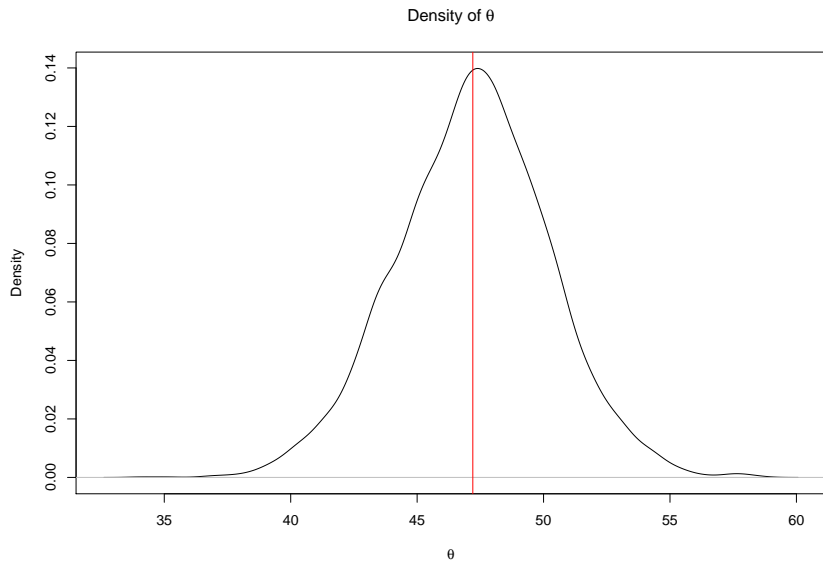
Running average plot of θ_1



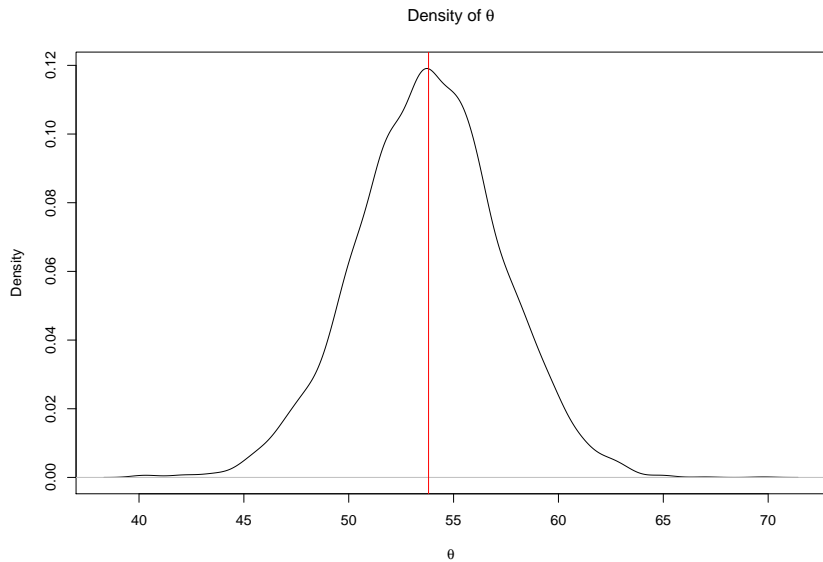
Running average plot of θ_2



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 quantify this by calculating

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

```
mean(THETA[,2] > THETA[,1])
```

```
## [1] 0.9926
```

Detailed Takeaways on Background

- ▶ Understanding vectors, matrices and notation
- ▶ Understanding how to write multivariate notation for a conceptual problem
- ▶ Understanding how to write general multivariate notation
- ▶ Background on linear algebra
- ▶ Determinants, traces, quadratic forms
- ▶ Knowing how to do simple proofs such as the exercises from class

Detailed Takeaways on Multivariate Normal Models

- ▶ The multivariate normal distribution (MVN)
- ▶ Exercise with the MVN
- ▶ MVN-MVN semi-conjugacy
- ▶ The inverse wishart distribution
- ▶ MVN-inverse wishart semi-conjugacy
- ▶ The MVN-MVN-inverse wishart model
- ▶ Applying a Gibbs sampler
- ▶ How to draw samples from the MVN and inverse wishart distributions
- ▶ Case study on reading comprehension

Proof of Lemma 1

$$\text{tr}(AB) = \text{tr}(BA)$$

Proof: Suppose that $A_{n \times n}$ and $B_{n \times n}$.

Recall that by definition $\text{tr}(A) = \sum_{i=1}^n a_{ii}$. By definition

$$\text{tr}(AB) = \sum_{i=1}^n (AB)_{ii} \tag{41}$$

$$\sum_{i=1}^n \sum_{j=1}^n a_{ij} b_{ji} \tag{42}$$

$$\sum_{i=1}^n \sum_{j=1}^n b_{ji} a_{ij} \tag{43}$$

$$= \sum_{i=1}^n (BA)_{ii} = \text{tr}(BA) \tag{44}$$

Exam II Preparation

Consider the following Exponential model for an observation x :

$$p(x|a, b) = ab \exp(-abx) \mathbb{1}(x > 0)$$

and suppose the prior is

$$p(a, b) = \exp(-a - b) \mathbb{1}(a, b > 0).$$

Exam II Preparation

1. Write out the $p(a, b \mid x)$. Is is something you know how to sample from? Explain.
2. Derive any conditional distributions needed for a Gibbs sampler.
3. Write pseudo code to illustrate how one would utilize a Gibbs sampler to approximate the posterior distribution.

Solution

1. The posterior distribution can be written as

$$p(a, b \mid x) = ab \exp(-abx) \times \exp(-a - b) \mathbb{1}(a, b, x > 0) \quad (45)$$

This distribution is not something that appears to be a known distribution or looks like it might be something easy to sample from, thus, Gibbs sampling is a natural choice. (Metropolis could be used as well.)

Solution

2. We must derive the full conditionals $a \mid b, x$ and $b \mid a, x$.
Consider

$$p(a \mid b, x) \propto_a p(x, a, b) \quad (46)$$

$$\propto_a a \exp(-abx - a) \mathbb{1}(a > 0) \quad (47)$$

$$= a \exp(-(bx + 1)a) \mathbb{1}(a > 0) \quad (48)$$

$$\propto_a \text{Gamma}(a \mid 2, bx + 1). \quad (49)$$

Solution

It follows that

$$p(b \mid a, x) \propto \text{Gamma}(b \mid 2, ax + 1).$$

Solution

Initialize (a, b) to (a_0, b_0) .

1. For the first iteration of the Gibbs sampler,

Draw a from $a \mid b = b_0, x$

Draw b from $b \mid a = a_1, x$

in order to get (a_1, b_1) .

2. For the second iteration of the Gibbs sampler,

Draw a from $a \mid b = b_1, x$

Draw b from $b \mid a = a_2, x$

in order to get (a_2, b_2) .

M. For the M th iteration of the Gibbs sampler,

Draw a from $a \mid b = b_{M-1}, x$

Draw b from $b \mid a = a_M, x$