

# Bayesian Inference

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# Outline of the course

This course provides theory and practice of the **Bayesian** approach to statistical inference. Applications are performed with the statistical package **R**.

Topics:

- ▶ Bayesian Updating through Bayes' Theorem
- ▶ Prior Distributions
- ▶ Multi-parameter Problems
- ▶ Summarizing Posterior Information
- ▶ **The Multivariate Normal Model**
- ▶ Prediction
- ▶ Asymptotics
- ▶ Markov chain Monte Carlo Methods

# The Multivariate Normal Distribution

## Definition

Let  $X$  be a  $p \times 1$  real random vector.  $X$  follows the multivariate normal distribution with mean vector  $\mu$  and covariance matrix  $\Sigma$ , i.e.  $X \sim N_p(\mu, \Sigma)$ , if and only if its pdf is

$$f(x \mid \mu, \Sigma) = (2\pi)^{-p/2} |\Sigma|^{-1/2} \exp \left\{ -\frac{1}{2} (x - \mu)' \Sigma^{-1} (x - \mu) \right\},$$

where  $\mu$  is a  $p \times 1$  real vector and  $\Sigma$  is a  $p \times p$  symmetric and positive definite matrix.

## Random Sample from the Multivariate Normal Distribution

Let  $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n$  be an i.i.d sample from a random variable  $\mathbf{X} \sim N_p(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ .

The pdf of the  $i$ th observation,  $\mathbf{x}_i$ , is

$$f(\mathbf{x}_i | \boldsymbol{\mu}, \boldsymbol{\Sigma}) = (2\pi)^{-p/2} |\det(\boldsymbol{\Sigma})|^{-1/2} \exp \left[ -\frac{1}{2}(\mathbf{x}_i - \boldsymbol{\mu})' \boldsymbol{\Sigma}^{-1}(\mathbf{x}_i - \boldsymbol{\mu}) \right],$$

where  $\boldsymbol{\mu}$  is the  $p \times 1$  mean vector and  $\boldsymbol{\Sigma}$  is the  $p \times p$  symmetric and positive definite covariance matrix.

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$$f(\mathbf{x}_i | \mu, \Sigma) = (2\pi)^{-p/2} |\det(\Sigma)|^{-1/2} \exp \left[ -\frac{1}{2}(\mathbf{x}_i - \mu)' \Sigma^{-1}(\mathbf{x}_i - \mu) \right],$$

where  $\mu$  is the  $p \times 1$  mean vector and  $\Sigma$  is the  $p \times p$  symmetric and positive definite covariance matrix.

We will use the multivariate random sample to estimate the unknown parameters,  $\mu, \Sigma$ , of the multivariate normal model.

# The Likelihood Function

The likelihood function of the observed data is

$$\begin{aligned}L(\mu, \Sigma) &= \prod_{i=1}^n f(\mathbf{x}_i | \mu, \Sigma) \\&= \prod_{i=1}^n (2\pi)^{-p/2} |\det(\Sigma)|^{-1/2} \exp \left[ -\frac{1}{2} (\mathbf{x}_i - \mu)' \Sigma^{-1} (\mathbf{x}_i - \mu) \right] \\&= (2\pi)^{-np/2} |\det(\Sigma)|^{-n/2} \\&\quad \times \exp \left[ -\frac{1}{2} \sum_{i=1}^n (\mathbf{x}_i - \mu)' \Sigma^{-1} (\mathbf{x}_i - \mu) \right]\end{aligned}$$

Note that the likelihood function is well-defined only if  $\det(\Sigma)$  is strictly positive. This reflects the assumption made above that  $\Sigma$  is positive definite, which implies that the search of a maximum likelihood estimator of  $\Sigma$  is restricted to the space of positive definite matrices.

# The Log-likelihood Function

The log-likelihood function is

$$l(\mu, \Sigma) = -\frac{np}{2} \ln(2\pi) - \frac{n}{2} \ln(\det(\Sigma)) - \frac{1}{2} \sum_{i=1}^n (\mathbf{x}_i - \mu)' \Sigma^{-1} (\mathbf{x}_i - \mu)$$

For convenience, the log-likelihood function can be also parameterised in terms of the precision matrix,  $\Sigma^{-1}$ , i.e.

$$l(\mu, \Sigma^{-1}) = -\frac{np}{2} \ln(2\pi) + \frac{n}{2} \ln(\det(\Sigma^{-1})) - \frac{1}{2} \sum_{i=1}^n (\mathbf{x}_i - \mu)' \Sigma^{-1} (\mathbf{x}_i - \mu)$$

## Preliminaries: Linear Algebra

- ▶ If  $c$  is a scalar, then the trace of  $c$  equals  $c$ :  $tr(c) = c$ .
- ▶ If two matrices  $A$  and  $B$  are such that the products  $AB$  and  $BA$  are both well defined, then  $tr(AB) = tr(BA)$ .
- ▶ The trace is a linear operator: if  $A$  and  $B$  are two matrices and  $a$  and  $b$  are two scalars, then  $tr(aA + bB) = atr(A) + btr(B)$ .
- ▶ The gradient of the trace of the product of two matrices  $A$  and  $B$  with respect to  $A$  is  $\frac{\partial}{\partial A} tr(BA) = B'$ .
- ▶ The gradient of the natural logarithm of the determinant of  $A$  is  $\frac{\partial}{\partial A} \ln(\det(A)) = (A^{-1})'$ .
- ▶ If  $\mathbf{x}$  is a  $p \times 1$  vector and  $A$  is a  $p \times p$  symmetric matrix, then  $\frac{\partial}{\partial \mathbf{x}} \mathbf{x}' A \mathbf{x} = 2A\mathbf{x}$ .



## The Log-likelihood Function Revisited

$$l(\mu, \Sigma^{-1}) = -\frac{np}{2} \ln(2\pi) + \frac{n}{2} \ln(\det(\Sigma^{-1})) - \frac{1}{2} \sum_{i=1}^n (\mathbf{x}_i - \mu)' \Sigma^{-1} (\mathbf{x}_i - \mu)$$

## The Log-likelihood Function Revisited

$$\begin{aligned}l(\mu, \Sigma^{-1}) &= -\frac{np}{2} \ln(2\pi) + \frac{n}{2} \ln(\det(\Sigma^{-1})) - \frac{1}{2} \sum_{i=1}^n (\mathbf{x}_i - \mu)' \Sigma^{-1} (\mathbf{x}_i - \mu) \\ &= \frac{np}{2} \ln(2\pi) + \frac{n}{2} \ln(\det(\Sigma^{-1})) - \frac{1}{2} \text{tr} \left[ \sum_{i=1}^n (\mathbf{x}_i - \mu)' \Sigma^{-1} (\mathbf{x}_i - \mu) \right]\end{aligned}$$

## The Log-likelihood Function Revisited

$$\begin{aligned}l(\mu, \Sigma^{-1}) &= -\frac{np}{2} \ln(2\pi) + \frac{n}{2} \ln(\det(\Sigma^{-1})) - \frac{1}{2} \sum_{i=1}^n (\mathbf{x}_i - \mu)' \Sigma^{-1} (\mathbf{x}_i - \mu) \\&= \frac{np}{2} \ln(2\pi) + \frac{n}{2} \ln(\det(\Sigma^{-1})) - \frac{1}{2} \text{tr} \left[ \sum_{i=1}^n (\mathbf{x}_i - \mu)' \Sigma^{-1} (\mathbf{x}_i - \mu) \right] \\&= \frac{np}{2} \ln(2\pi) + \frac{n}{2} \ln(\det(\Sigma^{-1})) - \frac{1}{2} \text{tr} \left[ \sum_{i=1}^n (\mathbf{x}_i - \mu)(\mathbf{x}_i - \mu)' \Sigma^{-1} \right]\end{aligned}$$

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# Maximum Likelihood Estimation

To obtain the maximum likelihood estimators of  $\mu, \Sigma$  we need to solve the system

$$\frac{\partial l(\mu, \Sigma^{-1})}{\partial \mu} \Big|_{\hat{\mu}, \hat{\Sigma}^{-1}} = \mathbf{0} \quad (1)$$

$$\frac{\partial l(\mu, \Sigma^{-1})}{\partial \Sigma^{-1}} \Big|_{\hat{\mu}, \hat{\Sigma}^{-1}} = \mathbf{0} \quad (2)$$

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$$(1) \Rightarrow -\hat{\Sigma}^{-1} \sum_{i=1}^n (\mathbf{x}_i - \hat{\mu}) = \mathbf{0} \Rightarrow \hat{\mu} = \frac{1}{n} \sum_{i=1}^n \mathbf{x}_i = \bar{\mathbf{x}}$$

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$$(2) \Rightarrow \frac{n}{2} \hat{\Sigma} - \frac{1}{2} \sum_{i=1}^n (\mathbf{x}_i - \hat{\mu})(\mathbf{x}_i - \hat{\mu})' \Rightarrow \hat{\Sigma} = \frac{1}{n} \sum_{i=1}^n (\mathbf{x}_i - \bar{\mathbf{x}})(\mathbf{x}_i - \bar{\mathbf{x}})'$$

# Conjugate Analysis for the Multivariate Normal Model

## The Inverse Wishart Distribution

Let  $\Sigma$  be a  $p \times p$  symmetric and positive definite matrix.  $\Sigma$  follows the inverse Wishart distribution, i.e.  $\Sigma \sim IW(A, d)$ , if and only if its pdf is

$$f(\Sigma) = k^{-1} |A|^{d/2} |\Sigma|^{-(d+p+1)/2} \exp \left\{ -\frac{1}{2} \text{tr} \Sigma^{-1} A \right\},$$

where  $k = 2^{dp/2} \pi^{p(p-1)/4} \prod_{i=1}^p \Gamma((d+1-i)/2)$ ,  $A$  is a  $p \times p$  symmetric and positive definite matrix and  $d$  is a positive scalar.



# Conjugate Analysis for the Multivariate Normal Model

## The Normal - Inverse Wishart Distribution

$(\mu, \Sigma) \sim NIW(A, d, a, c)$ , where  $A$  is a  $p \times p$  symmetric and positive definite matrix,  $a$  is a  $p \times 1$  real vector and  $d, c$  are positive scalars.

Joint distribution for  $(\mu, \Sigma)$  of the form

$$f(\mu, \Sigma) = f(\mu | \Sigma)f(\Sigma)$$

where  $f(\Sigma) \equiv IW(A, d)$  and  $f(\mu | \Sigma) \equiv N_p(a, c^{-1}\Sigma)$ .

## Conjugate Analysis for the Multivariate Normal Model

Let  $X_1, X_2, \dots, X_n$  be a random sample from the multivariate normal distribution  $N_p(\mu, \Sigma)$ .

Likelihood of  $x = (x_1, x_2, \dots, x_n)$ :

$$\begin{aligned} f(x \mid \mu, \Sigma) &\propto \prod_{i=1}^n |\Sigma|^{-1/2} \exp \left\{ -\frac{1}{2} (x_i - \mu)' \Sigma^{-1} (x_i - \mu) \right\} \\ &= |\Sigma|^{-n/2} \exp \left\{ -\frac{1}{2} \sum_{i=1}^n (x_i - \mu)' \Sigma^{-1} (x_i - \mu) \right\} \end{aligned}$$

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where  $\bar{x} = \frac{1}{n} \sum_{i=1}^n x_i$ ,  $S = \frac{1}{n} \sum_{i=1}^n (x_i - \bar{x})(x_i - \bar{x})'$ .

## Conjugate Analysis for the Multivariate Normal Model

Let  $\sum_{i=1}^n (x_i - \mu)' \Sigma^{-1} (x_i - \mu) = C$ . Then

$$C = n\mu' \Sigma^{-1} \mu - n\bar{x}' \Sigma^{-1} \mu - n\mu' \Sigma^{-1} \bar{x} + \sum_{i=1}^n x_i' \Sigma^{-1} x_i$$

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$$\begin{aligned}
 C &= n\mu' \Sigma^{-1} \mu - n\bar{x}' \Sigma^{-1} \mu - n\mu' \Sigma^{-1} \bar{x} + \sum_{i=1}^n x_i' \Sigma^{-1} x_i \\
 &= n(\mu - \bar{x})' \Sigma^{-1} (\mu - \bar{x}) - n\bar{x}' \Sigma^{-1} \bar{x} + \sum_{i=1}^n x_i' \Sigma^{-1} x_i \\
 &= n(\mu - \bar{x})' \Sigma^{-1} (\mu - \bar{x}) + \sum_{i=1}^n (x_i - \bar{x})' \Sigma^{-1} (x_i - \bar{x}) \\
 &= n(\mu - \bar{x})' \Sigma^{-1} (\mu - \bar{x}) + \sum_{i=1}^n \text{tr} \Sigma^{-1} (x_i - \bar{x})(x_i - \bar{x})' \\
 &= n(\mu - \bar{x})' \Sigma^{-1} (\mu - \bar{x}) + n \text{tr} \Sigma^{-1} S
 \end{aligned}$$

where  $\bar{x} = \frac{1}{n} \sum_{i=1}^n x_i$ ,  $S = \frac{1}{n} \sum_{i=1}^n (x_i - \bar{x})(x_i - \bar{x})'$ .



## Conjugate Analysis for the Multivariate Normal Model

Likelihood of  $x$ :

$$f(x | \mu, \Sigma) \propto |\Sigma|^{-n/2} \exp \left\{ -\frac{n}{2} (\mu - \bar{x})' \Sigma^{-1} (\mu - \bar{x}) - \frac{n}{2} \text{tr} \Sigma^{-1} S \right\}$$

Conjugate prior for  $(\mu, \Sigma)$ : Normal-Inverse Wishart

$$\begin{aligned} f(\mu, \Sigma) &\propto |\Sigma|^{-(d+p+2)/2} \exp \left\{ -\frac{c}{2} (\mu - a)' \Sigma^{-1} (\mu - a) - \frac{1}{2} \text{tr} \Sigma^{-1} A \right\} \\ &\equiv NIW(A, d, a, c), \end{aligned}$$

where  $A$  is a  $p \times p$  symmetric and positive definite matrix,  $a$  is a  $p \times 1$  real vector and  $d, c$  are positive scalars.

# The Joint Posterior

$$f(\mu, \Sigma | x) \propto f(x | \mu, \Sigma)f(\mu, \Sigma) \propto |\Sigma|^{-(d+p+2+n)/2} \exp\{-Q/2\},$$

$$Q = \text{tr}\Sigma^{-1}(S + A) + c(\mu - a)'\Sigma^{-1}(\mu - a) + n(\mu - \bar{x})'\Sigma^{-1}(\mu - \bar{x})$$

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$$\begin{aligned} Q &= \text{tr}\Sigma^{-1}(S + A) + c(\mu - a)' \Sigma^{-1}(\mu - a) + n(\mu - \bar{x})' \Sigma^{-1}(\mu - \bar{x}) \\ &= \text{tr}\Sigma^{-1}(S + A) + c\mu' \Sigma^{-1}\mu + ca' \Sigma^{-1}a - c\mu' \Sigma^{-1}a - ca' \Sigma^{-1}\mu \\ &\quad + n\mu' \Sigma^{-1}\mu + n\bar{x}' \Sigma^{-1}\bar{x} - n\mu' \Sigma^{-1}\bar{x} - n\bar{x}' \Sigma^{-1}\mu \end{aligned}$$

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where  $c^* = c + n$ ,  $a^* = (c + n)^{-1}(ca + n\bar{x})$  and  $A^* = A + S + nc(c + n)^{-1}(a - \bar{x})(a - \bar{x})'$ .

## Joint and Conditional Posteriors

$$\begin{aligned} f(\mu, \Sigma | x) &\propto |\Sigma|^{-\frac{d^*+p+2}{2}} \exp\left\{-\frac{c^*}{2}(\mu - a^*)'\Sigma^{-1}(\mu - a^*) - \frac{1}{2}\text{tr}\Sigma^{-1}A^*\right\} \\ &\equiv NIW(A^*, d^*, a^*, c^*), \end{aligned}$$

where  $d^* = d + n$ ,  $c^* = c + n$ ,  $a^* = (c + n)^{-1}(ca + n\bar{x})$  and  $A^* = A + S + nc(c + n)^{-1}(a - \bar{x})(a - \bar{x})'$ .

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$$f(\mu | \Sigma, x) \propto \exp\left\{-\frac{c^*}{2}(\mu - a^*)'\Sigma^{-1}(\mu - a^*)\right\} \equiv N_p(a^*, c\Sigma^{-1})$$

## Joint and Conditional Posteriors

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$$\equiv NIW(A^*, d^*, a^*, c^*),$$

where  $d^* = d + n$ ,  $c^* = c + n$ ,  $a^* = (c + n)^{-1}(ca + n\bar{x})$  and  $A^* = A + S + nc(c + n)^{-1}(a - \bar{x})(a - \bar{x})'$ .

$$f(\mu | \Sigma, x) \propto \exp\left\{-\frac{c^*}{2}(\mu - a^*)'\Sigma^{-1}(\mu - a^*)\right\} \equiv N_p(a^*, c\Sigma^{-1})$$

$$f(\Sigma | \mu, x) \propto |\Sigma|^{-\frac{d^*+p+2}{2}} \exp\left\{-\frac{c^*}{2}(\mu - a^*)'\Sigma^{-1}(\mu - a^*) - \frac{1}{2}\text{tr}\Sigma^{-1}A^*\right\}$$

$$= |\Sigma|^{-\frac{d^*+p+2}{2}} \exp\left\{-\frac{1}{2}\text{tr}\Sigma^{-1}A_\mu^*\right\} \equiv IW(A_\mu^*, d^* + 1),$$

where  $A_\mu^* = A^* + c^*(\mu - a^*)(\mu - a^*)'$ .



Marginal Posterior of  $\Sigma$ 

$$\begin{aligned} f(\Sigma|x) &\propto \int f(\mu, \Sigma | x) d\mu \\ &\propto \int |\Sigma|^{-\frac{d^*+p+2}{2}} \exp\left\{-\frac{c^*}{2}(\mu - a^*)'\Sigma^{-1}(\mu - a^*) - \frac{1}{2}\text{tr}\Sigma^{-1}A^*\right\} d\mu \end{aligned}$$

Marginal Posterior of  $\Sigma$ 

$$\begin{aligned} f(\Sigma|x) &\propto \int f(\mu, \Sigma | x) d\mu \\ &\propto \int |\Sigma|^{-\frac{d^*+p+2}{2}} \exp\left\{-\frac{c^*}{2}(\mu - a^*)'\Sigma^{-1}(\mu - a^*) - \frac{1}{2}\text{tr}\Sigma^{-1}A^*\right\} d\mu \\ &= |\Sigma|^{-\frac{d^*+p+2}{2}} \exp\left\{-\frac{1}{2}\text{tr}\Sigma^{-1}A^*\right\} \\ &\quad \times \int \exp\left\{-\frac{c^*}{2}(\mu - a^*)'\Sigma^{-1}(\mu - a^*)\right\} d\mu \end{aligned}$$

Marginal Posterior of  $\Sigma$ 

$$\begin{aligned} f(\Sigma|x) &\propto \int f(\mu, \Sigma | x) d\mu \\ &\propto \int |\Sigma|^{-\frac{d^*+p+2}{2}} \exp\left\{-\frac{c^*}{2}(\mu - a^*)'\Sigma^{-1}(\mu - a^*) - \frac{1}{2}\text{tr}\Sigma^{-1}A^*\right\} d\mu \\ &= |\Sigma|^{-\frac{d^*+p+2}{2}} \exp\left\{-\frac{1}{2}\text{tr}\Sigma^{-1}A^*\right\} \\ &\quad \times \int \exp\left\{-\frac{c^*}{2}(\mu - a^*)'\Sigma^{-1}(\mu - a^*)\right\} d\mu \\ &\propto |\Sigma|^{-\frac{d^*+p+2}{2}} \exp\left\{-\frac{1}{2}\text{tr}\Sigma^{-1}A^*\right\} \times |\Sigma|^{1/2} \\ &= |\Sigma|^{-\frac{d^*+p+1}{2}} \exp\left\{-\frac{1}{2}\text{tr}\Sigma^{-1}A^*\right\} \equiv IW(A^*, d^*) \end{aligned}$$

Marginal Posterior of  $\mu$ 

$$\begin{aligned} f(\mu|x) &\propto \int f(\mu, \Sigma | x) d\Sigma \\ &\propto \int |\Sigma|^{-\frac{d^*+p+2}{2}} \exp\left\{-\frac{1}{2} \text{tr} \Sigma^{-1} A_{\mu}^*\right\} d\Sigma \end{aligned}$$

Marginal Posterior of  $\mu$ 

$$\begin{aligned}f(\mu|x) &\propto \int f(\mu, \Sigma | x) d\Sigma \\&\propto \int |\Sigma|^{-\frac{d^*+p+2}{2}} \exp\left\{-\frac{1}{2} \text{tr} \Sigma^{-1} A_{\mu}^*\right\} d\Sigma \\&\propto |A_{\mu}^*|^{(d^*+1)/2} \\&= |A^* + c^*(\mu - a^*)(\mu - a^*)'|^{-(d^*+1)/2}\end{aligned}$$

Marginal Posterior of  $\mu$ 

$$\begin{aligned} f(\mu|x) &\propto \int f(\mu, \Sigma | x) d\Sigma \\ &\propto \int |\Sigma|^{-\frac{d^*+p+2}{2}} \exp\left\{-\frac{1}{2} \text{tr} \Sigma^{-1} A_{\mu}^*\right\} d\Sigma \\ &\propto |A_{\mu}^*|^{(d^*+1)/2} \\ &= |A^* + c^*(\mu - a^*)(\mu - a^*)'|^{-(d^*+1)/2} \\ &\equiv t_{d^*+1-p}(a^*, \frac{1}{c^*} A^*) \end{aligned}$$

Marginal Posterior of  $\mu$ 

$$\begin{aligned}
 f(\mu|x) &\propto \int f(\mu, \Sigma | x) d\Sigma \\
 &\propto \int |\Sigma|^{-\frac{d^*+p+2}{2}} \exp\left\{-\frac{1}{2} \text{tr} \Sigma^{-1} A_{\mu}^*\right\} d\Sigma \\
 &\propto |A_{\mu}^*|^{(d^*+1)/2} \\
 &= |A^* + c^*(\mu - a^*)(\mu - a^*)'|^{-(d^*+1)/2} \\
 &\equiv t_{d^*+1-p}(a^*, \frac{1}{c^*} A^*)
 \end{aligned}$$

This is a non-central multivariate Student-t distribution with  $d^* + 1 - p$  degrees of freedom, mean equal to  $a^*$  and covariance matrix equal to  $\frac{1}{(d^*-p-1)c^*} A^*$ .