

Maximum Likelihood Theory

Max Turgeon

STAT 4690—Applied Multivariate Analysis

Sufficient Statistics i

- We saw in the previous lecture that the multivariate normal distribution is completely determined by its mean vector $\mu \in \mathbb{R}^p$ and its covariance matrix Σ .
- Therefore, given a sample $\mathbf{Y}_1, \dots, \mathbf{Y}_n \sim N_p(\mu, \Sigma)$ ($n > p$), we only need to estimate (μ, Σ) .
 - Obvious candidates: sample mean $\bar{\mathbf{Y}}$ and sample covariance S_n .

Sufficient Statistics ii

- Write down the *likelihood*:

$$\begin{aligned} L &= \prod_{i=1}^n \left(\frac{1}{\sqrt{(2\pi)^p |\Sigma|}} \exp \left(-\frac{1}{2} (\mathbf{y}_i - \mu)^T \Sigma^{-1} (\mathbf{y}_i - \mu) \right) \right) \\ &= \frac{1}{(2\pi)^{np/2} |\Sigma|^{n/2}} \exp \left(-\frac{1}{2} \sum_{i=1}^n (\mathbf{y}_i - \mu)^T \Sigma^{-1} (\mathbf{y}_i - \mu) \right) \end{aligned}$$

- If we take the (natural) logarithm of L and drop any term that does not depend on (μ, Σ) , we get

$$\ell = -\frac{n}{2} \log |\Sigma| - \frac{1}{2} \sum_{i=1}^n (\mathbf{y}_i - \mu)^T \Sigma^{-1} (\mathbf{y}_i - \mu).$$

- If we can re-express the second summand in terms of \bar{Y} and S_n , by the Fisher-Neyman factorization theorem, we will then know that (\bar{Y}, S_n) is jointly **sufficient** for (μ, Σ) .
- First, we have

$$\begin{aligned}\sum_{i=1}^n (\mathbf{y}_i - \mu)(\mathbf{y}_i - \mu)^T &= \sum_{i=1}^n (\mathbf{y}_i - \bar{\mathbf{y}} + \bar{\mathbf{y}} - \mu)(\mathbf{y}_i - \bar{\mathbf{y}} + \bar{\mathbf{y}} - \mu)^T \\ &= \sum_{i=1}^n \left((\mathbf{y}_i - \bar{\mathbf{y}})(\mathbf{y}_i - \bar{\mathbf{y}})^T + (\mathbf{y}_i - \bar{\mathbf{y}})(\bar{\mathbf{y}} - \mu)^T \right. \\ &\quad \left. + (\bar{\mathbf{y}} - \mu)(\mathbf{y}_i - \bar{\mathbf{y}})^T + (\bar{\mathbf{y}} - \mu)(\bar{\mathbf{y}} - \mu)^T \right) \\ &= \sum_{i=1}^n (\mathbf{y}_i - \bar{\mathbf{y}})(\mathbf{y}_i - \bar{\mathbf{y}})^T + n(\bar{\mathbf{y}} - \mu)(\bar{\mathbf{y}} - \mu)^T \\ &= (n-1)S_n + n(\bar{\mathbf{y}} - \mu)(\bar{\mathbf{y}} - \mu)^T.\end{aligned}$$

- Next, using the fact that $\text{tr}(ABC) = \text{tr}(BCA)$, we have

$$\begin{aligned}\sum_{i=1}^n (\mathbf{y}_i - \boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1} (\mathbf{y}_i - \boldsymbol{\mu}) &= \text{tr} \left(\sum_{i=1}^n (\mathbf{y}_i - \boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1} (\mathbf{y}_i - \boldsymbol{\mu}) \right) \\ &= \text{tr} \left(\sum_{i=1}^n \boldsymbol{\Sigma}^{-1} (\mathbf{y}_i - \boldsymbol{\mu}) (\mathbf{y}_i - \boldsymbol{\mu})^T \right) \\ &= \text{tr} \left(\boldsymbol{\Sigma}^{-1} \sum_{i=1}^n (\mathbf{y}_i - \boldsymbol{\mu}) (\mathbf{y}_i - \boldsymbol{\mu})^T \right) \\ &= (n - 1) \text{tr} \left(\boldsymbol{\Sigma}^{-1} S_n \right) \\ &\quad + n \text{tr} \left(\boldsymbol{\Sigma}^{-1} (\bar{\mathbf{y}} - \boldsymbol{\mu}) (\bar{\mathbf{y}} - \boldsymbol{\mu})^T \right) \\ &= (n - 1) \text{tr} \left(\boldsymbol{\Sigma}^{-1} S_n \right) \\ &\quad + n (\bar{\mathbf{y}} - \boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1} (\bar{\mathbf{y}} - \boldsymbol{\mu}).\end{aligned}$$

Maximum Likelihood Estimators

- Going back to the log-likelihood, we get:

$$\ell = -\frac{n}{2} \log|\Sigma| - \frac{(n-1)}{2} \text{tr}(\Sigma^{-1}S_n) - \frac{n}{2}(\bar{\mathbf{y}} - \mu)^T \Sigma^{-1}(\bar{\mathbf{y}} - \mu).$$

- Since Σ^{-1} is positive definite, for Σ fixed, the log-likelihood is maximised at

$$\hat{\mu} = \bar{\mathbf{y}}.$$

- With extra effort, it can be shown that $-\log|\Sigma| - \frac{(n-1)}{n} \text{tr}(\Sigma^{-1}S_n)$ is maximised at

$$\hat{\Sigma} = \frac{(n-1)}{n} S_n = \frac{1}{n} \sum_{i=1}^n (\mathbf{y}_i - \bar{\mathbf{y}})(\mathbf{y}_i - \bar{\mathbf{y}})^T.$$

- In other words:* $(\bar{\mathbf{Y}}, \hat{\Sigma})$ are the **maximum likelihood estimators** for (μ, Σ) .

Maximum Likelihood Estimators

- Since the multivariate normal density is “well-behaved”, we can deduce the usual properties:
 - **Consistency:** $(\bar{\mathbf{Y}}, \hat{\Sigma})$ converges in probability to (μ, Σ) .
 - **Efficiency:** Asymptotically, the covariance of $(\bar{\mathbf{Y}}, \hat{\Sigma})$ achieves the Cramér-Rao lower bound.
 - **Invariance:** For any transformation $(g(\mu), G(\Sigma))$ of (μ, Σ) , its MLE is $(g(\bar{\mathbf{Y}}), G(\hat{\Sigma}))$.

Visualizing the likelihood

```
library(mvtnorm)
set.seed(123)

n <- 50; p <- 2

mu <- c(1, 2)
Sigma <- matrix(c(1, 0.5, 0.5, 1), ncol = p)

Y <- rmvnorm(n, mean = mu, sigma = Sigma)
```

Visualizing the likelihood

```
loglik <- function(mu, sigma, data = Y) {  
  # Compute quantities  
  y_bar <- colMeans(Y)  
  Sn <- cov(Y)  
  Sigma_inv <- solve(sigma)  
  
  # Compute quadratic form  
  quad_form <- drop(t(y_bar - mu) %*% Sigma_inv %*%  
                    (y_bar - mu))  
  
  -0.5*n*log(det(sigma)) -  
    0.5*(n - 1)*sum(diag(Sigma_inv %*% Sn)) -  
    0.5*n*quad_form  
}
```

```

grid_xy <- expand.grid(seq(0.5, 1.5,
                          length.out = 32),
                      seq(1, 3,
                          length.out = 32))

contours <- purrr::map_df(seq_len(nrow(grid_xy)),
                          function(i) {
# Where we will evaluate loglik
mu_obs <- as.numeric(grid_xy[i,])
# Evaluate at the pop covariance
z <- loglik(mu_obs, sigma = Sigma)
# Output data.frame
data.frame(x = mu_obs[1],
           y = mu_obs[2],
           z = z)
})

```

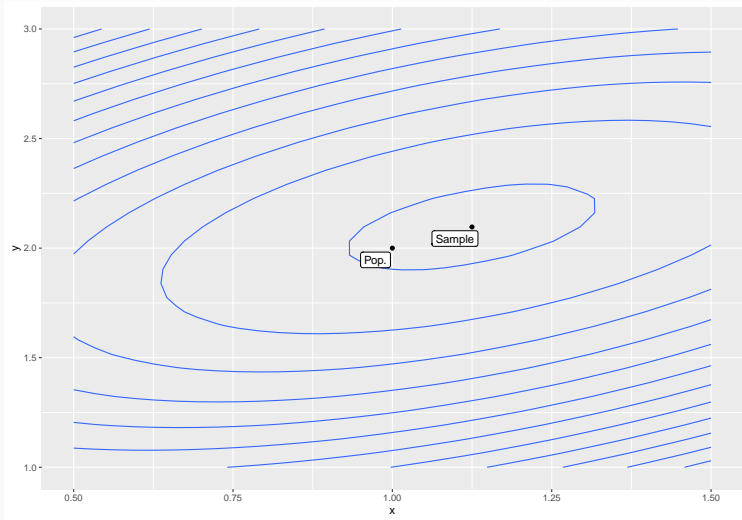
Visualizing the likelihood i

```
library(tidyverse)
library(ggplot2)
# Create df with pop and sample means
data_means <- data.frame(x = c(mu[1], mean(Y[,1])),
                          y = c(mu[2], mean(Y[,2])),
                          label = c("Pop.", "Sample"))
```

Visualizing the likelihood ii

```
contours %>%  
  ggplot(aes(x, y)) +  
  geom_contour(aes(z = z)) +  
  geom_point(data = data_means) +  
  geom_label_repel(data = data_means,  
                  aes(label = label))
```

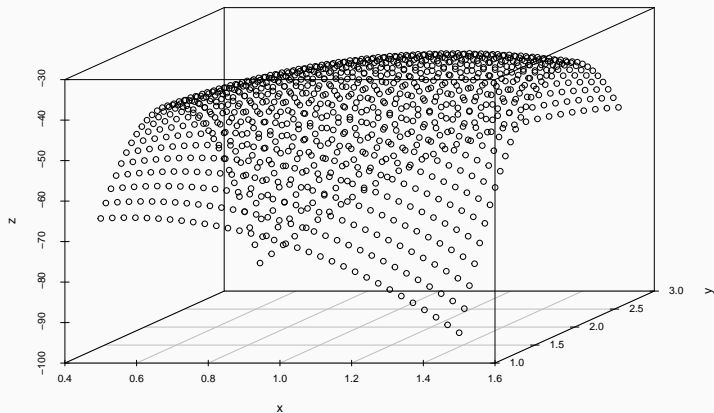
Visualizing the likelihood iii



Visualizing the likelihood iv

```
library(scatterplot3d)  
with(contours, scatterplot3d(x, y, z))
```


Visualizing the likelihood v



Sampling Distributions

- Recall the univariate case:
 - $\bar{X} \sim N(\mu, \sigma^2/n)$;
 - $\frac{(n-1)s^2}{\sigma^2} \sim \chi^2(n-1)$;
 - \bar{X} and s^2 are independent.
- In the multivariate case, we have similar results:
 - $\bar{\mathbf{Y}} \sim N_p\left(\mu, \frac{1}{n}\Sigma\right)$;
 - $(n-1)S_n = n\hat{\Sigma}$ follows a *Wishart* distribution with $n-1$ degrees of freedom;
 - $\bar{\mathbf{Y}}$ and S_n are independent.

Wishart Distribution

- Suppose $\mathbf{Z}_1, \dots, \mathbf{Z}_n \sim N_p(0, \Sigma)$ are independently distributed. Then we say that

$$W = \sum_{i=1}^n \mathbf{Z}_i \mathbf{Z}_i^T$$

follows a *Wishart distribution* $W_n(\Sigma)$ with n degrees of freedom.

- Note that since $E(\mathbf{Z}_i \mathbf{Z}_i^T) = \Sigma$, we have $E(W) = n\Sigma$.
- From the previous slide: $\sum_{i=1}^n (\mathbf{Y}_i - \bar{\mathbf{Y}})(\mathbf{Y}_i - \bar{\mathbf{Y}})^T$ has the same distribution as $\sum_{i=1}^{n-1} \mathbf{Z}_i \mathbf{Z}_i^T$ for some choice of $\mathbf{Z}_1, \dots, \mathbf{Z}_{n-1} \sim N_p(0, \Sigma)$.

Useful Properties

- If $W_1 \sim W_{n_1}(\Sigma)$ and $W_2 \sim W_{n_2}(\Sigma)$ are independent, then

$$W_1 + W_2 \sim W_{n_1+n_2}(\Sigma).$$

- If $W \sim W_n(\Sigma)$ and C is $q \times p$, then

$$CWC^T \sim W_n(C\Sigma C^T).$$

Density function

- Let Σ be a fixed $p \times p$ positive definite matrix. The density of the Wishart distribution with n degrees of freedom, with $n \geq p$, is given by

$$w_n(A; \Sigma) = \frac{|A|^{(n-p-1)/2} \exp\left(-\frac{1}{2}\text{tr}(\Sigma^{-1}A)\right)}{2^{np/2} \pi^{p(p-1)/4} |\Sigma|^{n/2} \prod_{i=1}^p \left(\frac{1}{2}(n-i+1)\right)},$$

where A is ranging over all $p \times p$ positive definite matrices.

Eigenvalue density function

- For a random matrix $A \sim W_n(I_p)$ with $n \geq p$, the joint distribution of its eigenvalues $\lambda_1 \geq \dots \geq \lambda_p$ has density

$$C_{n,p} \exp\left(-\frac{1}{2} \sum_{i=1}^p \lambda_i\right) \prod_{i=1}^p \lambda_i^{(n-p-1)/2} \prod_{i < j} |\lambda_i - \lambda_j|,$$

for some constant $C_{n,p}$.

- We will study this distribution in STAT 7200–Multivariate Analysis I