

STATS 206
Applied Multivariate Analysis
Lecture 3: Inferences About a Mean Vector

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Agenda

- Hotelling's T^2 test
- Likelihood ratio test and Hotelling's T^2
- Confidence regions
- Large sample inferences
- Dealing with missing values
- Effect of correlation among observations

Plausibility (Hypothesis Test) of a Mean Vector Problem Formulation

$\mathbf{X}_1, \dots, \mathbf{X}_n$: random sample from a normal population $\sim N_p(\boldsymbol{\mu}, \boldsymbol{\Sigma})$

- Our focus: the population mean $\boldsymbol{\mu}$
 - Is $\boldsymbol{\mu}_0$ (a known vector) plausible for $\boldsymbol{\mu}$?
- Formulation as a test of the two competing hypotheses:

$$H_0 : \boldsymbol{\mu} = \boldsymbol{\mu}_0 \quad \text{and} \quad H_1 : \boldsymbol{\mu} \neq \boldsymbol{\mu}_0$$

H_0 : the null hypothesis; H_1 : the alternative hypothesis

- How to proceed? Start with the univariate case first (next page)

Plausibility (Hypothesis Test) of a Mean The Univariate Case ($p = 1$)

X_1, \dots, X_n : normal sample with mean μ

- Test of the two hypotheses: $H_0 : \mu = \mu_0$ and $H_1 : \mu \neq \mu_0$
- Let $\bar{X} = \frac{1}{n} \sum_{j=1}^n X_j$, $s^2 = \frac{1}{n-1} \sum_{j=1}^n (X_j - \bar{X})^2$

Test statistic : $t = \frac{\bar{X} - \mu_0}{s/\sqrt{n}} \sim \text{Student's } t \text{ with } (n-1) \text{ deg. of freedom}$

Squared distance : $t^2 = n(\bar{X} - \mu_0)(s^2)^{-1}(\bar{X} - \mu_0)$

- **Reject H_0** at significance level α if and only if the observed

$$n(\bar{x} - \mu_0)(s^2)^{-1}(\bar{x} - \mu_0) > t_{n-1}^2(\alpha/2)$$

$t_{n-1}(\alpha/2)$: the upper 100($\alpha/2$)th percentile of the t dist. (above)

Plausibility (Hypothesis Test) of a Mean Vector The multivariate Case ($p \geq 2$) (i)

$\mathbf{X}_1, \dots, \mathbf{X}_n$: normal sample $\sim N_p(\boldsymbol{\mu}, \boldsymbol{\Sigma})$

- Testing $H_0 : \boldsymbol{\mu} = \boldsymbol{\mu}_0$ against $H_1 : \boldsymbol{\mu} \neq \boldsymbol{\mu}_0$
- Generalization

$$p = 1 : t^2 = n(\bar{X} - \mu_0)(s^2)^{-1}(\bar{X} - \mu_0)$$

$$p \geq 2 : \text{Test statistic : Hotelling's } T^2$$

$$T^2 = n(\bar{\mathbf{X}} - \boldsymbol{\mu}_0)' \mathbf{S}^{-1} (\bar{\mathbf{X}} - \boldsymbol{\mu}_0) \sim \frac{(n-1)p}{(n-p)} F_{p, n-p}$$

- $\bar{\mathbf{X}}_{p \times 1} = \frac{1}{n} \sum_{j=1}^n \mathbf{X}_j$, $\mathbf{S}_{p \times p} = \frac{1}{n-1} \sum_{j=1}^n (\mathbf{X}_j - \bar{\mathbf{X}})(\mathbf{X}_j - \bar{\mathbf{X}})'$
- $\boldsymbol{\mu}_0 = [\mu_{10}, \dots, \mu_{p0}]'$
- F_{c_1, c_2} : F -dist. with c_1 and c_2 deg. of freedom

Plausibility (Hypothesis Test) of a Mean Vector

The multivariate Case ($p \geq 2$) (ii)

$\mathbf{X}_1, \dots, \mathbf{X}_n$: normal sample $\sim N_p(\boldsymbol{\mu}, \boldsymbol{\Sigma})$

- $F_{c_1, c_2}(\alpha)$: the upper (100α) th percentile of F_{c_1, c_2}

For all values of $\boldsymbol{\mu}, \boldsymbol{\Sigma}$

$$T^2 = n(\bar{\mathbf{X}} - \boldsymbol{\mu})' \mathbf{S}^{-1} (\bar{\mathbf{X}} - \boldsymbol{\mu}) \sim \frac{(n-1)p}{(n-p)} F_{p, n-p}$$

$$\Rightarrow P \left[T^2 > \frac{(n-1)p}{(n-p)} F_{p, n-p}(\alpha) \right]$$

$$= P \left[n(\bar{\mathbf{X}} - \boldsymbol{\mu})' \mathbf{S}^{-1} (\bar{\mathbf{X}} - \boldsymbol{\mu}) > \frac{(n-1)p}{(n-p)} F_{p, n-p}(\alpha) \right] = \alpha$$

$$\bar{\mathbf{X}} = \frac{1}{n} \sum_{j=1}^n \mathbf{X}_j \quad \mathbf{S} = \frac{1}{n-1} \sum_{j=1}^n (\mathbf{X}_j - \bar{\mathbf{X}})(\mathbf{X}_j - \bar{\mathbf{X}})'$$

Plausibility (Hypothesis Test) of a Mean Vector

The multivariate Case ($p \geq 2$) (iii)

$\mathbf{X}_1, \dots, \mathbf{X}_n$: normal sample $\sim N_p(\boldsymbol{\mu}, \boldsymbol{\Sigma})$

$H_0 : \boldsymbol{\mu} = \boldsymbol{\mu}_0$ and $H_1 : \boldsymbol{\mu} \neq \boldsymbol{\mu}_0$

- $F_{c_1, c_2}(\alpha)$: the upper (100α) th percentile of F_{c_1, c_2}

Reject H_0 at significance level α if and only if the observed

$$n(\bar{\mathbf{x}} - \boldsymbol{\mu}_0)' \mathbf{S}^{-1} (\bar{\mathbf{x}} - \boldsymbol{\mu}_0) > \frac{(n-1)p}{(n-p)} F_{p, n-p}(\alpha)$$

Plausibility (Hypothesis Test) of a Mean Vector

The multivariate Case ($p \geq 2$) (iv)

Remark: recall $(n - 1)\mathbf{S} = \sum_{j=1}^n (\mathbf{X}_j - \bar{\mathbf{X}})(\mathbf{X}_j - \bar{\mathbf{X}})' \sim \mathbf{W}_{p,n-1}(\Sigma)$

$$\begin{aligned}
 p = 1 : t^2 &= \underbrace{\sqrt{n}(\bar{X} - \mu_0)}_{\text{univariate normal}} \left(\underbrace{s^2}_{\substack{\text{scaled } \chi^2 \text{ random variable} \\ \text{divided by deg. of freedom}}} \right)^{-1} \underbrace{\sqrt{n}(\bar{X} - \mu_0)}_{\text{univariate normal}} \\
 p \geq 2 : T^2 &= \left[\underbrace{\sqrt{n}(\bar{\mathbf{X}} - \boldsymbol{\mu}_0)}_{N_p(\mathbf{0}, \Sigma)} \right]' \left(\underbrace{\mathbf{S}}_{\substack{\text{Wishart random matrix} \\ (\mathbf{W}_{p,n-1}(\Sigma)) \text{ divided by} \\ \text{deg. of freedom}}} \right)^{-1} \left[\underbrace{\sqrt{n}(\bar{\mathbf{X}} - \boldsymbol{\mu}_0)}_{N_p(\mathbf{0}, \Sigma)} \right]
 \end{aligned}$$

Example 1: Testing a Multivariate Mean Vector

Sweat Data

X_1 : Sweat rate; X_2 : Sodium; X_3 : Potassium (from $n = 20$ individuals)							
No	X_1	X_2	X_3	No	X_1	X_2	X_3
1	3.7	48.5	9.3	11	3.9	36.9	12.7
2	5.7	65.1	8	12	4.5	58.8	12.3
3	3.8	47.2	10.9	13	3.5	27.8	9.8
4	3.2	53.2	12	14	4.5	40.2	8.4
5	3.1	55.5	9.7	15	1.5	13.5	10.1
6	4.6	36.1	7.9	16	8.5	56.4	7.1
7	2.4	24.8	14	17	4.5	71.6	8.2
8	7.2	33.1	7.6	18	6.5	52.8	10.9
9	6.7	47.4	8.5	19	4.1	44.1	11.2
10	5.4	54.1	11.3	20	5.5	40.9	9.4

Table 5.1 in the textbook

Example 1: Testing a Multivariate Mean Vector

Calculating T^2 of the Sweat Data

- Assuming the data are multivariate normal (need to be checked first!)
- $\mu_0 = [4, 50, 10]'$
- Test hypothesis $H_0 : \mu = \mu_0$ against $H_1 : \mu \neq \mu_0$
- $\alpha = 0.10$
- It can be shown that $(n = 20, p = 3)$

$$T^2 = 9.7388 > \underbrace{\frac{(n-1)p}{(n-p)} F_{p, n-p}(\alpha)}_{\text{critical value here}} \bigg|_{\substack{\alpha=0.1 \\ n=20 \\ p=3}} = 8.1726$$

\implies Reject H_0 at $\alpha = 0.1$ (level of significance)

Example 1: Testing a Multivariate Mean Vector

Calculating T^2 of the Sweat Data (MATLAB)

```
%%%%%%%%% Calculating Hotelling's  $T^2$  (T2)%%%%%%%%%  
load T5_1.dat  
mu_0 = [4; 50; 10];  
X = T5_1;  
[n, p] = size(X);  
X_Mean = (1/n) * X' * ones(n,1);  
S = (1/(n-1)) * X' * (eye(n) - (1/n) * ones(n,1) * ones(1,n)) * X;  
T2 = n * (X_Mean - mu_0)' * inv(S) * (X_Mean - mu_0);  
  
%%%%%%%%% Evaluating the critical value (CV)%%%%%%%%%  
alpha = 0.10;  
CV = (n-1) * p * finv(1-alpha, p, n-p)/(n-p);
```

Invariance Property of Hotelling's T^2

Transformation: $\mathbf{Y}_{p \times 1} = \mathbf{C}_{p \times p} \mathbf{X}_{p \times 1} + \mathbf{d}_{p \times 1}$ (\mathbf{C} : non-singular)

- Previous techniques

$$\bar{\mathbf{y}} = \mathbf{C}\bar{\mathbf{x}} + \mathbf{d}, \quad \boldsymbol{\mu}_{\mathbf{Y}} = \mathbf{C}\boldsymbol{\mu} + \mathbf{d}$$

$$\mathbf{S}_{\mathbf{y}} = \frac{1}{n-1} \sum_{j=1}^n (\mathbf{y}_j - \bar{\mathbf{y}})(\mathbf{y}_j - \bar{\mathbf{y}})' = \mathbf{CSC}'$$

- Let $\boldsymbol{\mu}_{\mathbf{Y},0} = \mathbf{C}\boldsymbol{\mu}_0 + \mathbf{d}$

$$T^2 = n(\bar{\mathbf{y}} - \boldsymbol{\mu}_{\mathbf{y},0})' \mathbf{S}_{\mathbf{y}}^{-1} (\bar{\mathbf{y}} - \boldsymbol{\mu}_{\mathbf{y},0}) \quad (\text{for } \mathbf{y}_1, \dots, \mathbf{y}_n)$$

$$= n[\mathbf{C}(\bar{\mathbf{x}} - \boldsymbol{\mu}_0)]' (\mathbf{CSC}')^{-1} [\mathbf{C}(\bar{\mathbf{x}} - \boldsymbol{\mu}_0)]$$

$$= n(\bar{\mathbf{x}} - \boldsymbol{\mu}_0)' \mathbf{C}' (\mathbf{C}')^{-1} \mathbf{S}^{-1} \mathbf{C}^{-1} \mathbf{C} (\bar{\mathbf{x}} - \boldsymbol{\mu}_0)$$

$$= n(\bar{\mathbf{x}} - \boldsymbol{\mu}_0)' \mathbf{S}^{-1} (\bar{\mathbf{x}} - \boldsymbol{\mu}_0) \quad (\text{for } \mathbf{x}_1, \dots, \mathbf{x}_n)$$

- Testing $H_0 : \boldsymbol{\mu} = \boldsymbol{\mu}_0$ of $\mathbf{x} \iff$ testing $H_0 : \boldsymbol{\mu}_{\mathbf{Y}} = \boldsymbol{\mu}_{\mathbf{Y},0}$ of \mathbf{y}

Likelihood Ratio Tests of $H_0 : \mu = \mu_0$ (i)

- Likelihood ratio test of $H_0 : \mu = \mu_0$ against $H_1 : \mu \neq \mu_0$
- Recall: Maximum of the multivariate normal likelihood [unknown (μ, Σ)]

$$\max_{\mu, \Sigma} L(\mu, \Sigma) = \frac{1}{(2\pi)^{np/2} |\hat{\Sigma}|^{n/2}} e^{-np/2}$$

where the maximum is achieved using the following estimates

$$\hat{\Sigma} = \frac{1}{n} \sum_{j=1}^n (\mathbf{x}_j - \bar{\mathbf{x}})(\mathbf{x}_j - \bar{\mathbf{x}})'$$

$$\hat{\mu} = \bar{\mathbf{x}} = \frac{1}{n} \sum_{j=1}^n \mathbf{x}_j$$

Likelihood Ratio Tests of $H_0 : \mu = \mu_0$ (ii)

- Under the hypothesis $H_0 : \mu = \mu_0$ (unknown Σ only)
(multivariate normal distribution)

$$L(\mu_0, \Sigma) = \frac{1}{(2\pi)^{np/2} |\Sigma|^{n/2}} \exp \left(-\frac{1}{2} \sum_{j=1}^n (\mathbf{x}_j - \mu_0)' \Sigma^{-1} (\mathbf{x}_j - \mu_0) \right)$$
$$\max_{\Sigma} L(\mu_0, \Sigma) = \frac{1}{(2\pi)^{np/2} |\hat{\Sigma}_0|^{n/2}} e^{-np/2}$$

where the maximum here is achieved using the following estimate

$$\hat{\Sigma}_0 = \frac{1}{n} \sum_{j=1}^n (\mathbf{x}_j - \mu_0)(\mathbf{x}_j - \mu_0)'$$

Likelihood Ratio Tests of $H_0 : \mu = \mu_0$ (iii)

- (Normal population) Is μ_0 plausible for μ ? Check

$$\text{Likelihood Ratio} = \Lambda = \underbrace{\frac{\max_{\Sigma} L(\mu_0, \Sigma)}{\max_{\mu, \Sigma} L(\mu, \Sigma)}}_{\text{Likelihood ratio statistic}} = \left(\frac{|\hat{\Sigma}|}{|\hat{\Sigma}_0|} \right)^{n/2}$$

- Equivalently, check Wilks' lambda $= \Lambda^{2/n} = |\hat{\Sigma}|/|\hat{\Sigma}_0|$
- c_α : the lower (100α) th percentile of the dist. of Λ

Likelihood ratio test **rejects** H_0 if

$$\Lambda = \left(\frac{|\hat{\Sigma}|}{|\hat{\Sigma}_0|} \right)^{n/2} = \left(\frac{\sum_{j=1}^n (\mathbf{x}_j - \bar{\mathbf{x}})(\mathbf{x}_j - \bar{\mathbf{x}})'}{\sum_{j=1}^n (\mathbf{x}_j - \mu_0)(\mathbf{x}_j - \mu_0)'} \right)^{n/2} < c_\alpha$$

Likelihood Ratio Tests of $H_0 : \mu = \mu_0$ (iv)

Hotelling's T^2 and Wilks' lambda $\Lambda^{2/n}$

$$\Lambda^{2/n} = |\hat{\Sigma}|/|\hat{\Sigma}_0| = \left(1 + \frac{T^2}{n-1}\right)^{-1}$$

- Proof:

$$\hat{\Sigma}_0 = \hat{\Sigma} + (\bar{\mathbf{x}} - \mu_0)(\bar{\mathbf{x}} - \mu_0)' \quad (\text{Need some algebra here!})$$

$$\begin{aligned} |\hat{\Sigma}_0| &= |\hat{\Sigma} + (\bar{\mathbf{x}} - \mu_0)(\bar{\mathbf{x}} - \mu_0)'| \stackrel{(*)}{=} |\hat{\Sigma}| |1 + (\bar{\mathbf{x}} - \mu_0)' \hat{\Sigma}^{-1} (\bar{\mathbf{x}} - \mu_0)| \\ &= |\hat{\Sigma}| \left| 1 + \frac{n}{n-1} (\bar{\mathbf{x}} - \mu_0)' \mathbf{S}^{-1} (\bar{\mathbf{x}} - \mu_0) \right| = |\hat{\Sigma}| \left(1 + \frac{T^2}{n-1} \right) \end{aligned}$$

$$(*) : |\mathbf{A}_{m \times m} + \mathbf{a}_{m \times 1}(\mathbf{b}_{m \times 1})'| = |\mathbf{A}|(1 + \mathbf{b}'\mathbf{A}^{-1}\mathbf{a}) \quad (\mathbf{A} \text{ non-singular})$$

- For normal samples, test based on $T^2 \iff$ test based on Λ ($\Lambda^{2/n}$)
- $T^2 = (n-1)(|\hat{\Sigma}_0|/|\hat{\Sigma}| - 1)$: no need to calculate \mathbf{S}^{-1}

General Likelihood Ratio Method

- General observations: $\mathbf{X}_1 = \mathbf{x}_1, \dots, \mathbf{X}_n = \mathbf{x}_n$
- θ : vector of unknown population parameters ($\theta \in \Theta$)
- $H_0 : \theta \in \Theta_0$ vs. $H_1 : \theta \notin \Theta_0$ ($\Theta_0 \subset \Theta$; Θ : whole parameter space)
- General likelihood ratio test statistic: Λ

Reject H_0 if

$$\Lambda = \frac{\max_{\theta \in \Theta_0} L(\theta)}{\max_{\theta \in \Theta} L(\theta)} < c \text{ (a suitably chosen constant)}$$

- Remark:

$$-2 \ln \Lambda \xrightarrow{\text{approximately}} \chi^2_{\nu - \nu_0} \quad (n \rightarrow \infty)$$

ν : dimension of Θ ; ν_0 : dimension of Θ_0

Confidence Regions (i)

- For a general random sample $\mathbf{X} = [\mathbf{X}_1, \dots, \mathbf{X}_n]'$
Unknown parameter vector $\boldsymbol{\theta} \in \Theta$ (parameter space)

$$R(\mathbf{X}) : 100(1 - \alpha)\% \text{ confidence region} \iff \underbrace{P[\boldsymbol{\theta} \in R(\mathbf{X})]}_{\text{calculated under the true but unknown } \boldsymbol{\theta}} = 1 - \alpha$$

- Recall: for a p -dimensional normal population, $\forall \boldsymbol{\mu}, \boldsymbol{\Sigma}$

$$P \left[T^2 = n(\bar{\mathbf{X}} - \boldsymbol{\mu})' \mathbf{S}^{-1} (\bar{\mathbf{X}} - \boldsymbol{\mu}) \leq \frac{(n-1)p}{(n-p)} F_{p, n-p}(\alpha) \right] = 1 - \alpha$$

$$\mathbf{S} = \frac{1}{n-1} \sum_{j=1}^n (\mathbf{X}_j - \bar{\mathbf{X}})(\mathbf{X}_j - \bar{\mathbf{X}})'$$

$$F_{c_1, c_2}(\alpha) : \text{the upper } (100\alpha)\text{th percentile of } F_{c_1, c_2}$$

Confidence Regions (ii)

- Given $\mathbf{x}_1, \dots, \mathbf{x}_n$: observations from a p -dim normal population
 $100(1 - \alpha)\%$ confidence region for the mean $\boldsymbol{\mu}$ of a p -dim. normal dist.

$$\left\{ \boldsymbol{\mu} : n(\bar{\mathbf{x}} - \boldsymbol{\mu})' \mathbf{S}^{-1} (\bar{\mathbf{x}} - \boldsymbol{\mu}) \leq \frac{(n-1)p}{(n-p)} F_{p, n-p}(\alpha) \right\}$$
$$\left[\bar{\mathbf{x}} = \frac{1}{n} \sum_{j=1}^n \mathbf{x}_j, \quad \mathbf{S} = \frac{1}{n-1} \sum_{j=1}^n (\mathbf{x}_j - \bar{\mathbf{x}})(\mathbf{x}_j - \bar{\mathbf{x}})' \right]$$

- Relation to testing $H_0 : \boldsymbol{\mu} = \boldsymbol{\mu}_0$ vs. $H_1 : \boldsymbol{\mu} \neq \boldsymbol{\mu}_0$

The above confidence region consists of all $\boldsymbol{\mu}_0$ with which H_0 would not be rejected by the T^2 test at significance level α .

Confidence Regions (iii)

- $100(1 - \alpha)\%$ confidence region for the mean $\boldsymbol{\mu}$ of a p -dim. normal dist.

$$\underbrace{\left\{ \boldsymbol{\mu} : n(\bar{\mathbf{x}} - \boldsymbol{\mu})' \mathbf{S}^{-1} (\bar{\mathbf{x}} - \boldsymbol{\mu}) \leq \frac{(n-1)p}{(n-p)} F_{p, n-p}(\alpha) = c^2 \right\}}_{100(1-\alpha)\% \text{ confidence ellipsoid}}$$

- Given that: $\mathbf{S} \mathbf{e}_i = \lambda_i \mathbf{e}_i, i = 1, \dots, p$

Center of the confidence ellipsoid = $\bar{\mathbf{x}}$

Axes of the confidence ellipsoid = $\pm c \sqrt{\lambda_i} \mathbf{e}_i$

$$= \pm \sqrt{\lambda_i} \sqrt{\frac{(n-1)p}{n(n-p)} F_{p, n-p}(\alpha)} \mathbf{e}_i$$

(similar to constant prob. density contour analysis of $N_p(\boldsymbol{\mu}, \boldsymbol{\Sigma})$)

Simultaneous Confidence Intervals (i)

$$\mathbf{X} \sim N_p(\boldsymbol{\mu}, \boldsymbol{\Sigma}) \implies Z = \mathbf{a}'\mathbf{X} \sim N(\mathbf{a}'\boldsymbol{\mu}, \mathbf{a}'\boldsymbol{\Sigma}\mathbf{a}); \quad \mathbf{a} \neq \mathbf{0}$$

$$\mathbf{X}_1, \dots, \mathbf{X}_n: \text{ random sample } \sim N_p(\boldsymbol{\mu}, \boldsymbol{\Sigma}); \quad Z_j = \mathbf{a}'\mathbf{X}_j, \forall j$$

$$\bar{\mathbf{x}} (\mathbf{S}): \text{ sample mean (cov. matrix) from } \mathbf{x}_1, \dots, \mathbf{x}_n$$

- Sample mean and var. of z_1, \dots, z_n : $\bar{z} = \mathbf{a}'\bar{\mathbf{x}}, s_z^2 = \mathbf{a}'\mathbf{S}\mathbf{a}$
- $100(1 - \alpha)\%$ confidence interval for $\mu_Z = \mathbf{a}'\boldsymbol{\mu}$ (given \mathbf{a} , unknown σ_Z^2)

$$\mathbf{a}'\bar{\mathbf{x}} - t_{n-1}(\alpha/2) \frac{\sqrt{\mathbf{a}'\mathbf{S}\mathbf{a}}}{\sqrt{n}} \leq \mathbf{a}'\boldsymbol{\mu} \leq \mathbf{a}'\bar{\mathbf{x}} + t_{n-1}(\alpha/2) \frac{\sqrt{\mathbf{a}'\mathbf{S}\mathbf{a}}}{\sqrt{n}}$$

$$\text{using Student's } t : |t| = \left| \frac{\bar{z} - \mu_Z}{s_z/\sqrt{n}} \right| = \left| \frac{\sqrt{n}(\mathbf{a}'\bar{\mathbf{x}} - \mathbf{a}'\boldsymbol{\mu})}{\sqrt{\mathbf{a}'\mathbf{S}\mathbf{a}}} \right| \leq t_{n-1}(\alpha/2)$$

Simultaneous Confidence Intervals (ii)

- A simultaneous region satisfies: $\forall \mathbf{a} : t^2 = \left(\frac{\sqrt{n}(\mathbf{a}'\bar{\mathbf{x}} - \mathbf{a}'\boldsymbol{\mu})}{\sqrt{\mathbf{a}'\mathbf{S}\mathbf{a}}} \right)^2 \leq c^2$
- If $\max_{\mathbf{a}} t^2 \leq c^2$, then the above holds.

$$\begin{aligned} \max_{\mathbf{a}} t^2 &= \max_{\mathbf{a}} \frac{n(\mathbf{a}'(\bar{\mathbf{x}} - \boldsymbol{\mu}))^2}{\mathbf{a}'\mathbf{S}\mathbf{a}} = n \left[\max_{\mathbf{a}} \frac{(\mathbf{a}'(\bar{\mathbf{x}} - \boldsymbol{\mu}))^2}{\mathbf{a}'\mathbf{S}\mathbf{a}} \right] \\ &= n(\bar{\mathbf{x}} - \boldsymbol{\mu})'\mathbf{S}^{-1}(\bar{\mathbf{x}} - \boldsymbol{\mu}) \\ &= T^2 \end{aligned}$$

Maximum achieved with $\mathbf{a} = b \cdot \mathbf{S}^{-1}(\bar{\mathbf{x}} - \boldsymbol{\mu})$ ($b \neq 0$: constant)

- Recall: $T^2 \sim \frac{(n-1)p}{n-p} F_{p, n-p}$

Simultaneous Confidence Intervals (iii)

If: $\mathbf{X}_1, \dots, \mathbf{X}_n$: random sample $\sim N_p(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ ($\boldsymbol{\Sigma}$ positive definite)

Then: simultaneously for all \mathbf{a} ,

$$\left(\mathbf{a}'\bar{\mathbf{X}} - \sqrt{\frac{p(n-1)}{n(n-p)} F_{p,n-p}(\alpha) \mathbf{a}'\mathbf{S}\mathbf{a}}, \quad \mathbf{a}'\bar{\mathbf{X}} + \sqrt{\frac{p(n-1)}{n(n-p)} F_{p,n-p}(\alpha) \mathbf{a}'\mathbf{S}\mathbf{a}} \right)$$

will contain $\mathbf{a}'\boldsymbol{\mu}$ with prob. $(1 - \alpha)$.

- The simultaneous intervals are referred to as T^2 -intervals.

Simultaneous Confidence Intervals (iv)

- Choices of $\mathbf{a} = [1, 0, \dots, 0]', [0, 1, \dots, 0]', \dots, [0, \dots, 0, 1]'$

$$\Rightarrow \bar{x}_j - \sqrt{\frac{p(n-1)}{(n-p)} F_{p,n-p}(\alpha)} \sqrt{\frac{s_{jj}}{n}} \leq \mu_j \leq \bar{x}_j + \sqrt{\frac{p(n-1)}{(n-p)} F_{p,n-p}(\alpha)} \sqrt{\frac{s_{jj}}{n}}, \quad j = 1, \dots, p$$

all hold simultaneously with confidence coefficient $1 - \alpha$

Simultaneous Confidence Intervals (v)

- Let $\mathbf{a} = [0, \dots, 0, a_i, 0, \dots, 0, a_k, 0, \dots, 0]'$, $a_i = 1, a_k = -1$

$$\begin{aligned} \Rightarrow \bar{x}_i - \bar{x}_k - \sqrt{\frac{p(n-1)}{(n-p)} F_{p, n-p}(\alpha)} \sqrt{\frac{s_{ii} - 2s_{ik} + s_{kk}}{n}} \\ \leq \mu_i - \mu_k \\ \leq \bar{x}_i - \bar{x}_k + \sqrt{\frac{p(n-1)}{(n-p)} F_{p, n-p}(\alpha)} \sqrt{\frac{s_{ii} - 2s_{ik} + s_{kk}}{n}} \end{aligned}$$

One-at-a-Time Intervals

- Consider each component μ_j one at a time, for $j = 1, \dots, p$:

$$\bar{x}_j - t_{n-1}(\alpha/2) \sqrt{\frac{s_{jj}}{n}} \leq \mu_j \leq \bar{x}_j + t_{n-1}(\alpha/2) \sqrt{\frac{s_{jj}}{n}}$$

- No clue of $P[\text{all } t\text{-intervals above contain the } \mu_j\text{'s}]$ in general
- When X_i 's are independent

$$P[\text{all } t\text{-intervals above contain the } \mu_j\text{'s}] = (1 - \alpha)^p$$

- The T^2 -interval is wider than the individual interval for each μ_j .
(Comparison next page)

Comparison of T^2 and One-at-a-Time Intervals

Critical distance multipliers for both intervals ($1 - \alpha = 0.95$)

sample size n	$t_{n-1}(0.025)$	$\sqrt{\frac{p(n-1)}{(n-p)}} F_{p,n-p}(0.05)$	
		$p = 4$	$p = 10$
15	2.1448	4.1338	11.5144
25	2.0639	3.6032	6.3796
50	2.0096	3.3117	5.0444
100	1.9842	3.1897	4.6166
∞	1.9600	3.0750	4.2769

Bonferroni Method for Multiple Comparisons (i)

- Motivation: in practice
 - T^2 intervals can be too wide to use
 - Only m (finite) linear combinations needed: $\mathbf{a}_1, \dots, \mathbf{a}_m$
 $\xRightarrow{\text{Bonferroni}}$ Constructing shorter intervals than T^2
- C_i : confidence statement about $\mathbf{a}_i' \boldsymbol{\mu}$, $P(C_i \text{ true}) = 1 - \alpha_i$, $i = 1, \dots, m$

$$P[\text{all } C_i \text{'s true}] = 1 - P[\text{at least one } C_i \text{ false}]$$

$$\begin{aligned} &\stackrel{\text{Bonferroni}}{\geq} 1 - \sum_{i=1}^m P[C_i \text{ false}] = 1 - \sum_{i=1}^m (1 - P[C_i \text{ true}]) \\ &= 1 - (\alpha_1 + \dots + \alpha_m) \end{aligned}$$

control of overall type-I error rate $\sum_i \alpha_i$; flexibility in choosing each α_i

Bonferroni Method for Multiple Comparisons (ii)

- Let $z_i = \mathbf{a}_i' \mathbf{x}_i$; $s_{z,ii} = \mathbf{a}_i' \mathbf{S} \mathbf{a}_i$; without prior info., $\alpha_i = \frac{\alpha}{m}, \forall i$

$$P \left[\bar{z}_i \pm t_{n-1}(\alpha/(2m)) \sqrt{s_{z,ii}/n} \text{ contains } \mathbf{a}_i' \boldsymbol{\mu} \right] = 1 - \alpha/m, \forall i$$

$$P \left[\bar{z}_i \pm t_{n-1}(\alpha/(2m)) \sqrt{\frac{s_{z,ii}}{n}} \text{ contains } \mathbf{a}_i' \boldsymbol{\mu}, \forall i \right] \geq 1 - \sum_{i=1}^m \frac{\alpha}{m} = 1 - \alpha$$

- Set $m = p$, $\mathbf{a}_i = [0, \dots, 0, 1, 0, \dots, 0]'$ (1 at the i -th entry only), $\forall i$:

Then the following intervals (**the Bonferroni intervals**)

$$\bar{x}_i - t_{n-1}(\alpha/(2p)) \sqrt{\frac{s_{ii}}{n}} \leq \mu_i \leq \bar{x}_i + t_{n-1}(\alpha/(2p)) \sqrt{\frac{s_{ii}}{n}}, \quad i = 1, \dots, p$$

hold (simultaneously) with probability $\geq 1 - \alpha$

Comparison of T^2 and Bonferroni Intervals

- Comparing Bonferroni and T^2 intervals (same α_i 's, $\alpha_i = \alpha/p$):

$$t_{n-1}(\alpha/(2p)) \leftarrow \sqrt{\frac{p(n-1)}{n-p}} F_{p,n-p}(\alpha) \text{ (difference in intervals)}$$

$$\frac{\text{Length of Bonferroni interval}}{\text{Length of } T^2 \text{ interval}} = \frac{t_{n-1}(\alpha/(2p))}{\sqrt{\frac{p(n-1)}{n-p}} F_{p,n-p}(\alpha)}$$

- Table of the above ratio ($\alpha_i = \alpha/p, 1 - \alpha = 0.95$)

n	p		
	2	4	10
15	0.8766	0.6928	0.2888
25	0.8947	0.7494	0.4844
50	0.9060	0.7831	0.5828
100	0.9110	0.7976	0.6219
∞	0.9199	0.8122	0.6563

Large Sample Inferences about a Mean Vector (i)

$\mathbf{X}_1, \dots, \mathbf{X}_n$: random sample

(mean: $\boldsymbol{\mu}_{p \times 1}$, finite positive definite covariance matrix: $\boldsymbol{\Sigma}_{p \times p}$)

(no normality assumption!!!)

- Recall: for large $n - p$,

$$n(\bar{\mathbf{X}} - \boldsymbol{\mu})' \mathbf{S}^{-1} (\bar{\mathbf{X}} - \boldsymbol{\mu}) \longrightarrow \chi_p^2 \text{ distributed}$$

$$\implies P[n(\bar{\mathbf{X}} - \boldsymbol{\mu})' \mathbf{S}^{-1} (\bar{\mathbf{X}} - \boldsymbol{\mu}) \leq \chi_p^2(\alpha)] \approx 1 - \alpha$$

$\chi_p^2(\alpha)$: the upper (100α) th percentile of χ_p^2

- Consequences: next page

Large Sample Inferences about a Mean Vector (ii)

$\mathbf{X}_1, \dots, \mathbf{X}_n$: random sample (mean: $\boldsymbol{\mu}$, finite positive def. cov.: $\boldsymbol{\Sigma}$)

(no normality assumption)

- (Asymptotic testing)

For large $n - p$: at significance level approximately α :

reject the hypothesis $H_0 : \boldsymbol{\mu} = \boldsymbol{\mu}_0$ in favor of $H_1 : \boldsymbol{\mu} \neq \boldsymbol{\mu}_0$ if

$$n(\bar{\mathbf{X}} - \boldsymbol{\mu}_0)' \mathbf{S}^{-1} (\bar{\mathbf{X}} - \boldsymbol{\mu}_0) > \chi_p^2(\alpha).$$

- (Asymptotic simultaneous confidence intervals)

For large $n - p$ and for every \mathbf{a}

$$\mathbf{a}' \bar{\mathbf{X}} \pm \sqrt{\chi_p^2(\alpha)} \sqrt{\frac{\mathbf{a}' \mathbf{S} \mathbf{a}}{n}}$$

will contain $\mathbf{a}' \boldsymbol{\mu}$ with probability approximately $1 - \alpha$.

Note: For large n and large $n - p$, $[p(n - 1)/(n - p)] F_{p, n-p} \approx \chi_p^2(\alpha)$

Dealing with Missing Observations in Normal Samples

- Important assumption: data are **missing at random**!
- One of the methods: **the EM algorithm** (see footnote for a ref.)
- Recall: (multivariate normal distribution)
 1. (**Cond. dist. of a subset**) $\mathbf{Y} = [\mathbf{Y}'_1 \ \mathbf{Y}'_2] \sim N_p(\boldsymbol{\mu}, \boldsymbol{\Sigma})$, $|\boldsymbol{\Sigma}_{22}| > 0$
 $\mathbf{Y}_1 \sim N_q(\boldsymbol{\mu}_1, \boldsymbol{\Sigma}_{11})$, $\mathbf{Y}_2 \sim N_{p-q}(\boldsymbol{\mu}_2, \boldsymbol{\Sigma}_{22})$, $\text{Cov}(\mathbf{Y}_1, \mathbf{Y}_2) = \boldsymbol{\Sigma}_{12}$, $q \leq p$
 $\implies \mathbf{Y}_1 |_{\mathbf{Y}_2=\mathbf{y}_2} \sim N_q(\boldsymbol{\mu}_1 + \boldsymbol{\Sigma}_{12}\boldsymbol{\Sigma}_{22}^{-1}(\mathbf{y}_2 - \boldsymbol{\mu}_2), \boldsymbol{\Sigma}_{11} - \boldsymbol{\Sigma}_{12}\boldsymbol{\Sigma}_{22}^{-1}\boldsymbol{\Sigma}_{21})$
 2. $\mathbf{X}_1, \dots, \mathbf{X}_n$: sample $\sim N_p(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ ($\boldsymbol{\mu}, \boldsymbol{\Sigma}$ unknown, to be estimated)

$$\begin{aligned} & \overline{\mathbf{X}} \text{ and } \mathbf{S}: \text{ sufficient statistics } \implies \text{ so are:} \\ & \mathbf{T}_1 = \sum_j \mathbf{X}_j = n\overline{\mathbf{X}} \quad \text{and} \quad \mathbf{T}_2 = \sum_j \mathbf{X}_j \mathbf{X}'_j = (n-1)\mathbf{S} + n\overline{\mathbf{X}}\overline{\mathbf{X}}' \end{aligned}$$

Dempster, Laird and Rubin, *Maximum Likelihood from Incomplete Data via the EM Algorithm*, Journal of the Royal Statistical Society, Series B (Methodological), Vol. 39, No. 1, (1977), pp. 1-38.

Dealing with Missing Observations in Normal Samples

The EM Algorithm (Assuming Data Missing at Random) (i)

$\mathbf{X}_1, \dots, \mathbf{X}_n$: p -dim. normal sample with unknown $\boldsymbol{\mu}, \boldsymbol{\Sigma}$

- Initializing $\hat{\boldsymbol{\mu}}, \hat{\boldsymbol{\Sigma}}, \hat{\mathbf{T}}_1, \hat{\mathbf{T}}_2$ (for $\mathbf{T}_1, \mathbf{T}_2$, see prev. page)
- E-step: for each vector with missing values: $\mathbf{x}_j = [\mathbf{x}_j^{(1)'}; \mathbf{x}_j^{(2)'}]'$:
($\mathbf{x}_j^{(1)}$: missing, $\mathbf{x}_j^{(2)}$: available)
(\star) $\hat{\mathbf{x}}_j^{(1)} = \mathbb{E}(\mathbf{X}_j^{(1)} | \mathbf{x}_j^{(2)}; \hat{\boldsymbol{\mu}}, \hat{\boldsymbol{\Sigma}}) = \hat{\boldsymbol{\mu}}_1 + \hat{\boldsymbol{\Sigma}}_{12} \hat{\boldsymbol{\Sigma}}_{22}^{-1} (\mathbf{x}_j^{(2)} - \hat{\boldsymbol{\mu}}_2)$
(\diamond) $\widehat{\mathbf{x}_j^{(1)} \mathbf{x}_j^{(1)'}} = \mathbb{E}(\mathbf{X}_j^{(1)} \mathbf{X}_j^{(1)' | \mathbf{x}_j^{(2)}; \hat{\boldsymbol{\mu}}, \hat{\boldsymbol{\Sigma}})$
$$= \hat{\boldsymbol{\Sigma}}_{11} - \hat{\boldsymbol{\Sigma}}_{12} \hat{\boldsymbol{\Sigma}}_{22}^{-1} \hat{\boldsymbol{\Sigma}}_{21} + \hat{\mathbf{x}}_j^{(1)} \hat{\mathbf{x}}_j^{(1)'}$$

(\circ) $\widehat{\mathbf{x}_j^{(1)} \mathbf{x}_j^{(2)'}} = \mathbb{E}(\mathbf{X}_j^{(1)} \mathbf{X}_j^{(2)' | \mathbf{x}_j^{(2)}; \hat{\boldsymbol{\mu}}, \hat{\boldsymbol{\Sigma}}) = \hat{\mathbf{x}}_j^{(1)} \hat{\mathbf{x}}_j^{(2)'}$
(\star): estimate of missing data; use (\star), (\diamond), (\circ) to update $\hat{\mathbf{T}}_1, \hat{\mathbf{T}}_2$

Dealing with Missing Observations in Normal Samples

The EM Algorithm (Assuming Data Missing at Random) (ii)

$\mathbf{X}_1, \dots, \mathbf{X}_n$: p -dim. normal sample with unknown $\boldsymbol{\mu}, \boldsymbol{\Sigma}$

- M-step: compute the updates of ML estimates

$$\hat{\boldsymbol{\mu}} = \frac{\hat{\mathbf{T}}_1}{n}, \quad \hat{\boldsymbol{\Sigma}} = \frac{\hat{\mathbf{T}}_2}{n} - \hat{\boldsymbol{\mu}}\hat{\boldsymbol{\mu}}'$$

- Recursively continue the above E-step and M-step until the difference between updates and previous values are smaller than a given small value.

Effect of Correlation among Observations (i)

- Suppose observations are collected over time
- Time correlation: using the first-order autoregressive (AR (1)) model

$$\mathbf{X}_t - \boldsymbol{\mu} = \boldsymbol{\Phi}(\mathbf{X}_{t-1} - \boldsymbol{\mu}) + \boldsymbol{\varepsilon}_t, \quad \boldsymbol{\varepsilon}_t \sim N_p(\mathbf{0}, \boldsymbol{\Sigma}_{\boldsymbol{\varepsilon}}) (\boldsymbol{\varepsilon}_t : \text{i.i.d. over } t)$$

Also assuming $|\lambda_i(\boldsymbol{\Phi})| < 1, \forall i$

- Clearly,

$$\begin{aligned} \mathbf{X}_t - \boldsymbol{\mu} &= \boldsymbol{\varepsilon}_t + \boldsymbol{\Phi}(\mathbf{X}_{t-1} - \boldsymbol{\mu}) \\ &= \boldsymbol{\varepsilon}_t + \boldsymbol{\Phi}[\boldsymbol{\varepsilon}_{t-1} + \boldsymbol{\Phi}(\mathbf{X}_{t-2} - \boldsymbol{\mu})] \\ &= \boldsymbol{\varepsilon}_t + \boldsymbol{\Phi}\boldsymbol{\varepsilon}_{t-1} + \boldsymbol{\Phi}^2\boldsymbol{\varepsilon}_{t-2} + \dots \end{aligned}$$

$$\boldsymbol{\Sigma}_{\mathbf{X}} = \text{E}(\mathbf{X}_t - \boldsymbol{\mu})(\mathbf{X}_t - \boldsymbol{\mu})' = \sum_{j=0}^{\infty} \boldsymbol{\Phi}^j \boldsymbol{\Sigma}_{\boldsymbol{\varepsilon}} \boldsymbol{\Phi}'^j$$

$$\text{Cov}(\mathbf{X}_t, \mathbf{X}_{t-r}) = \boldsymbol{\Phi}^r \boldsymbol{\Sigma}_{\mathbf{X}}$$

Effect of Correlation among Observations (ii)

- Collect \mathbf{X}_t for n consecutive times to get $\mathbf{X}_1, \dots, \mathbf{X}_n$;

It can be shown that

$$\mathbf{S} = \frac{1}{n-1} \sum_{t=1}^n (\mathbf{X}_t - \bar{\mathbf{X}})(\mathbf{X}_t - \bar{\mathbf{X}})' \rightarrow \Sigma_{\mathbf{x}} \text{ (in prob.) } (n \rightarrow \infty)$$

$$\bar{\mathbf{X}} \rightarrow \boldsymbol{\mu}, \quad \text{Cov} \left(n^{-1/2} \sum_{t=1}^n \mathbf{X}_t \right) \rightarrow \boldsymbol{\Psi} \text{ (in prob.) } (n \rightarrow \infty)$$

$$\text{where } \boldsymbol{\Psi} = (\mathbf{I} - \boldsymbol{\Phi})^{-1} \Sigma_{\mathbf{x}} + \Sigma_{\mathbf{x}} (\mathbf{I} - \boldsymbol{\Phi}')^{-1} - \Sigma_{\mathbf{x}}$$

Furthermore, for large n

$$\begin{aligned} \sqrt{n}(\bar{\mathbf{X}} - \boldsymbol{\mu}) &\approx \text{distributed as } N_p(\mathbf{0}, \boldsymbol{\Psi}) \\ \implies n(\bar{\mathbf{X}} - \boldsymbol{\mu})' \boldsymbol{\Psi}^{-1} (\bar{\mathbf{X}} - \boldsymbol{\mu}) &\approx \text{distributed as } \chi_p^2 \end{aligned}$$

Effect of Correlation among Observations (iii)

- Large n , $\mathbf{X}_1, \dots, \mathbf{X}_n$: i.i.d. ($\mathbf{S} \rightarrow \Sigma_{\mathbf{x}}$ in prob.)

$$\Rightarrow \left\{ \mu : \underbrace{n(\bar{\mathbf{X}} - \mu)' \mathbf{S}^{-1} (\bar{\mathbf{X}} - \mu)}_{\text{asymptotically } n(\bar{\mathbf{X}} - \mu)' \Sigma_{\mathbf{x}}^{-1} (\bar{\mathbf{X}} - \mu) \sim \chi_p^2} \leq \chi_p^2(0.05) \right\}$$

covers μ with prob. 0.95 (asymptotically).

- Large n , $\mathbf{X}_1, \dots, \mathbf{X}_n$: AR(1) [$\Phi = \phi \mathbf{I}$, ($|\phi| < 1$), $\Psi = \frac{1+\phi}{1-\phi} \Sigma_{\mathbf{x}}$],

$$\Rightarrow \left\{ \mu : \underbrace{n(\bar{\mathbf{X}} - \mu)' \mathbf{S}^{-1} (\bar{\mathbf{X}} - \mu)}_{\text{asymptotically } n(\bar{\mathbf{X}} - \mu)' [\frac{1+\phi}{1-\phi} \Psi^{-1}] (\bar{\mathbf{X}} - \mu) \sim \frac{1+\phi}{1-\phi} \chi_p^2} \leq \chi_p^2(0.05) \right\}$$

covers μ with $\underbrace{P[\chi_p^2 \leq (1 - \phi)(1 + \phi)^{-1} \chi_p^2(0.05)]}_{\text{tabulated on next page}}$ (asymptotically).

Effect of Correlation among Observations (iv)

Table:

$P [\chi_p^2 \leq (1 - \phi)(1 + \phi)^{-1} \chi_p^2(0.05)]$				
p	ϕ			
	-0.25	0	0.25	0.5
1	0.9886	0.95	0.8710	0.7422
2	0.9932	0.95	0.8343	0.6316
5	0.9976	0.95	0.7514	0.4052
10	0.9993	0.95	0.6413	0.1934
15	0.9997	0.95	0.5484	0.0902

Conclusion: correlation among observations can cause the coverage prob. to drop significantly (e.g., comparing some of the above with **0.95 in the case with i.i.d. observations**).