

Minimization by use of differentiation

Show that  $T^2 = \min_{\underline{\beta}} n (\underline{\bar{x}} - K\underline{\beta})^T S^{-1} (\underline{\bar{x}} - K\underline{\beta})$

$$\begin{aligned} R &= (\underline{\bar{x}} - K\underline{\beta})^T S^{-1} (\underline{\bar{x}} - K\underline{\beta}) \\ &= \underline{\bar{x}}^T S^{-1} \underline{\bar{x}} - \underline{\bar{x}}^T S^{-1} K\underline{\beta} - \underline{\beta}^T K^T S^{-1} \underline{\bar{x}} + \underline{\beta}^T K^T S^{-1} K\underline{\beta} \\ &= \underline{\bar{x}}^T S^{-1} \underline{\bar{x}} - 2\underline{\beta}^T K^T S^{-1} \underline{\bar{x}} + \underline{\beta}^T K^T S^{-1} K\underline{\beta} \end{aligned}$$

Differentiation wrt  $\underline{\beta}$  leads to

$$\begin{aligned} \frac{dR}{d\underline{\beta}} &= \underline{0} - 2K^T S^{-1} \underline{\bar{x}} + K^T S^{-1} K\underline{\beta} + (\underline{\beta}^T K^T S^{-1} K)^T \\ &= -2K^T S^{-1} \underline{\bar{x}} + 2K^T S^{-1} K\underline{\beta} = \underline{0} \quad \text{for} \end{aligned}$$

$$\underline{\beta} = \underline{\beta}^* = (K^T S^{-1} K)^{-1} K^T S^{-1} \underline{\bar{x}}$$

$$\begin{aligned} T^2 &= n R_{\min} = n (\underline{\bar{x}}^T S^{-1} \underline{\bar{x}} - 2\underline{\bar{x}}^T S^{-1} K (K^T S^{-1} K)^{-1} K^T S^{-1} \underline{\bar{x}} \\ &\quad + \underline{\bar{x}}^T S^{-1} K (K^T S^{-1} K)^{-1} K^T S^{-1} K (K^T S^{-1} K)^{-1} K^T S^{-1} \underline{\bar{x}}) \\ &= n (\underline{\bar{x}}^T S^{-1} \underline{\bar{x}} - \underline{\bar{x}}^T S^{-1} K (K^T S^{-1} K)^{-1} K^T S^{-1} \underline{\bar{x}}) \\ &= n (\underline{\bar{x}}^T S^{-1} \underline{\bar{x}} - \underline{\bar{x}}^T S^{-1} K \underline{\beta}^*) \end{aligned}$$

$$T^2 \sim T^2(d-k, n-1) = \frac{(n-1)(d-k)}{n-d+k} F(d-k, n-d+k),$$

where  $k = \text{rank } K$

Ex .

**EXAMPLE 2.4** The height, in millimeters, of the ramus bone in the jaws of 20 boys was measured at ages 8,  $8\frac{1}{2}$ , 9, and  $9\frac{1}{2}$ , and the results from Elston and Grizzle [1962] are given in Table 3.4. A main objective of the study was to establish a standard growth curve for the use of orthodontists, and it is clear from the sample means that a straight line should provide a satisfactory fit for the age range considered. Following Grizzle and Allen [1969], we can use orthogonal polynomials and consider the model

$$\mu_j = \beta_0 + 2\beta_1(t_j - \bar{t}) \quad (j = 1, 2, 3, 4),$$

where age 8 is chosen as the time origin so that  $t_j = j - 1$ . Then  $\mu = K\beta$ , where

$$K\beta = \begin{pmatrix} 1 & -3 \\ 1 & -1 \\ 1 & 1 \\ 1 & 3 \end{pmatrix} \begin{pmatrix} \beta_0 \\ \beta_1 \end{pmatrix},$$

TABLE 3.4 Ramus Height of 20 Boys<sup>a</sup>

Individual	Age in Years			
	8	8½	9	9½
1	47.8	48.8	49.0	49.7
2	46.4	47.3	47.7	48.4
3	46.3	46.8	47.8	48.5
4	45.1	45.3	46.1	47.2
5	47.6	48.5	48.9	49.3
6	52.5	53.2	53.3	53.7
7	51.2	53.0	54.3	54.5
8	49.8	50.0	50.3	52.7
9	48.1	50.8	52.3	54.4
10	45.0	47.0	47.3	48.3
11	51.2	51.4	51.6	51.9
12	48.5	49.2	53.0	55.5
13	52.1	52.8	53.7	55.0
14	48.2	48.9	49.3	49.8
15	49.6	50.4	51.2	51.8
16	50.7	51.7	52.7	53.3
17	47.2	47.7	48.4	49.5
18	53.3	54.6	55.1	55.3
19	46.2	47.5	48.1	48.4
20	46.3	47.6	51.3	51.8
Mean	48.655	49.625	50.570	51.450
s. d.	2.52	2.54	2.63	2.73

<sup>a</sup>Reproduced from R. C. Elston and J. E. Grizzle [1962]. "Estimation of time-response curves and their confidence bands." *Biometrics*, **18**, 148-159, Table 2. With permission from The Biometric Society.

and  $\mathbf{K}$  has orthogonal columns. Now

$$\bar{x}' = (48.655, 49.625, 50.570, 51.450),$$

$$\mathbf{S} = \begin{pmatrix} 6.330 & 6.189 & 5.777 & 5.548 \\ - & 6.449 & 6.153 & 5.923 \\ - & - & 6.918 & 6.946 \\ - & - & - & 7.465 \end{pmatrix},$$

and

$$\begin{aligned} \beta^* &= (\mathbf{K}'\mathbf{S}^{-1}\mathbf{K})^{-1}\mathbf{K}'\mathbf{S}^{-1}\bar{x} \\ &= \begin{pmatrix} 50.050 \\ 0.465 \end{pmatrix}. \end{aligned}$$

Hence

$$\begin{aligned} T_0^2 &= n(\bar{x} - \mathbf{K}\beta^*)'\mathbf{S}^{-1}(\bar{x} - \mathbf{K}\beta^*) \\ &= n(\bar{x}'\mathbf{S}^{-1}\bar{x} - \bar{x}'\mathbf{S}^{-1}\mathbf{K}\beta^*) \\ &= 0.20113, \end{aligned}$$

and we compare

$$F_0 = T_0^2 \frac{20 - 4 + 2}{19(4 - 2)} = 0.095$$

with  $F_{2,18}^\alpha$ . Since  $F_0$  is so low, we do not reject the straight line model.

## Confidence intervals

$\underline{x}_i \sim N_d(\underline{\mu}, \Sigma)$ ,  $i=1, \dots, n$  independent

$$\underline{a}^T \bar{\underline{x}} \sim N\left(\underline{a}^T \underline{\mu}, \frac{\underline{a}^T \Sigma \underline{a}}{n}\right)$$

Confidence intervals for pre specified linear combinations of  $\mu_1, \dots, \mu_d$ ,  $\underline{a}^T \underline{\mu}$ , with confidence level  $1 - \alpha$ :

$$\underline{a}^T \underline{\mu} = \underline{a}^T \bar{\underline{x}} \pm t_{1-\frac{\alpha}{2}}(n-1) \sqrt{\frac{\underline{a}^T S \underline{a}}{n}}$$

Confidence intervals for  $r$  pre specified linear combinations  $\underline{a}_i^T \underline{\mu}$ ,  $i=1, \dots, r$ , each with confidence level  $1 - \frac{\alpha}{r}$ :

$$\underline{a}_i^T \underline{\mu} = \underline{a}_i^T \bar{\underline{x}} \pm t_{1-\frac{\alpha}{2r}}(n-1) \sqrt{\frac{\underline{a}_i^T S \underline{a}_i}{n}}, \quad i=1, \dots, r$$

(Bonferroni intervals)

Combined confidence level for the  $r$  intervals:

$$\begin{aligned} 1 - \alpha_0 &= P\left(\bigcap_i (|t_i(n-1)| < t_{1-\frac{\alpha}{2r}}(n-1))\right) \\ &= 1 - P\left(\bigcup_i (|t_i(n-1)| > t_{1-\frac{\alpha}{2r}}(n-1))\right) \\ &\geq 1 - \sum_i P(|t_i(n-1)| > t_{1-\frac{\alpha}{2r}}(n-1)) \\ &= 1 - r \frac{\alpha}{r} = 1 - \alpha, \end{aligned}$$

thus  $1 - \alpha_0 \geq 1 - \alpha$

Assume that  $\underline{a}_1, \dots, \underline{a}_r$  are ordered, so  $\underline{a}_1, \dots, \underline{a}_q$  are linear independent and that  $\underline{a}_{q+1}, \dots, \underline{a}_r$  are all linear dependent of  $\underline{a}_1, \dots, \underline{a}_q$

Let  $A = [a_1 \dots a_q]^T$ ,  $A$   $q \times d$ ,  $\text{rank } A = q$  ( $\leq d$ ),  
and  $\underline{q} = A\underline{\mu}$

$$n(A\bar{\underline{x}} - A\underline{\mu})^T (ASA^T)^{-1} (A\bar{\underline{x}} - A\underline{\mu}) \sim T^2(q, n-1)$$

$$\Leftrightarrow n(\hat{\underline{q}} - \underline{q})^T (ASA^T)^{-1} (\hat{\underline{q}} - \underline{q}) \sim T^2(q, n-1)$$

$$1 - \alpha = P\left( (\hat{\underline{q}} - \underline{q})^T (ASA^T)^{-1} (\hat{\underline{q}} - \underline{q}) < T_{1-\alpha}^2(q, n-1) \frac{1}{n} \right)$$

$$= P\left( \sup_{\underline{h} \neq \underline{0}} \frac{(\underline{h}^T (\hat{\underline{q}} - \underline{q}))^2}{\underline{h}^T ASA^T \underline{h}} < T_{1-\alpha}^2(q, n-1) \frac{1}{n} \right) \text{ cf. A7.6}$$

$$= P\left( \forall \underline{h} \neq \underline{0} : (\underline{h}^T (\hat{\underline{q}} - \underline{q}))^2 < T_{1-\alpha}^2(q, n-1) \frac{\underline{h}^T ASA^T \underline{h}}{n} \right)$$

$$= P\left( \forall \underline{h} \neq \underline{0} : |\underline{h}^T \hat{\underline{q}} - \underline{h}^T \underline{q}| < \sqrt{T_{1-\alpha}^2(q, n-1) \frac{\underline{h}^T ASA^T \underline{h}}{n}} \right)$$

Hence confidence intervals with confidence level  $1 - \alpha$   
for any  $\underline{h}^T \underline{q}$ :

$$\underline{h}^T \underline{q} = \underline{h}^T \hat{\underline{q}} \pm \sqrt{T_{1-\alpha}^2(q, n-1) \frac{\underline{h}^T ASA^T \underline{h}}{n}} \quad (\text{Scheffé intervals})$$

or - with  $\underline{h}^T \underline{q} = \underline{h}^T A \underline{\mu}$  -

$$\underline{h}^T A \underline{\mu} = \underline{h}^T A \bar{\underline{x}} \pm \sqrt{T_{1-\alpha}^2(q, n-1) \frac{\underline{h}^T ASA^T \underline{h}}{n}}$$

Any of the linear combinations  $\underline{a}_i^T \underline{\mu}$ ,  $i = 1, \dots, r$   
arise from a suitable choice of  $\underline{h}$ , as

$$\underline{h}^T \underline{q} = (\underline{h}_1 \underline{a}_1^T + \dots + \underline{h}_q \underline{a}_q^T) \underline{\mu}$$

For the combined confidence level  $1 - \alpha_0$  of the intervals

$$\underline{a}_i^T \underline{\mu} = \underline{a}_i^T \bar{\underline{x}} \pm \sqrt{T_{1-\alpha}^2(q, n-1) \frac{\underline{a}_i^T S \underline{a}_i}{n}}, \quad i = 1, \dots, r$$

we have  $1 - \alpha_0 \geq 1 - \alpha$ , as the  $r$  intervals constitute  
a subset of all the covered intervals

Bonferroni intervals are in general shorter than Scheffé intervals as

$$\begin{aligned} \left( t_{1-\frac{\alpha}{2q}}(n-1) \right)^2 &= F_{1-\frac{\alpha}{q}}(1, n-1) < q F_{1-\alpha}(q, n-1) \quad (\text{empirical}) \\ &\leq \frac{(n-1)q}{n-q} F_{1-\alpha}(q, n-1) = T_{1-\alpha}^2(q, n-1) \end{aligned}$$

Confidence interval for any not pre specified  $\mu_{\sim}^T$  can be achieved by choosing  $A = I_d$ , hence  $q = d$  and  $g = \mu_{\sim}^T$ :

$$\mu_{\sim}^T = \mu_{\sim}^T \bar{x}_{\sim} \pm \sqrt{T_{1-\alpha}^2(d, n-1) \frac{\mu_{\sim}^T S \mu_{\sim}}{n}}, \quad \text{confidence level } 1-\alpha$$

Confidence intervals for contrasts can be achieved by choosing  $A = FC_2$ , where  $C_2$  originates from section 3.4.2 and  $F$  is  $(d-1) \times (d-1)$  non-singular.

Confidence interval for any contrast  $c^T \mu_{\sim}$ ,  $c^T = \mu_{\sim}^T A = \mu_{\sim}^T FC_2$ , with confidence level  $1-\alpha$ :

$$c^T \mu_{\sim} = c^T \bar{x}_{\sim} \pm \sqrt{T_{1-\alpha}^2(d-1, n-1) \frac{c^T S c}{n}}, \quad c^T \mathbf{1}_d = 0$$

Bonferroni interval for one among  $r$  specified contrasts:

$$c^T \mu_{\sim} = c^T \bar{x}_{\sim} \pm t_{1-\frac{\alpha}{2r}}(n-1) \sqrt{\frac{c^T S c}{n}}, \quad c^T \mathbf{1}_d = 0, \quad \text{confidence level } 1-\frac{\alpha}{r}$$

EXAMPLE 3.5 Consider Example 3.2 (Section 3.4.2) and the cork data of Table 3.3. If we are interested in a confidence interval for each  $\mu_j$ , then we can use (3.29) with  $\mathbf{a}'_1 = (1, 0, \dots, 0)$ , and so on, namely,

$$\bar{x}_j \pm k_\alpha \left( \frac{s_{jj}}{n} \right)^{1/2} \quad (j = 1, 2, 3, 4).$$

With  $n = 28$ ,  $r = q = d = 4$ , and  $\alpha = 0.05$ , the two methods give the following values of  $k_\alpha$ : From Appendix D1,  $t_{27}^{0.05/8} = 2.676$  [see (3.28)] for the Bonferroni method and  $(T_{4,27,0.05}^2)^{1/2} = \{[4(27)/24]F_{4,24}^{0.05}\}^{1/2} = 3.537$  [see (3.33) and (3.30)] for the Scheffé method. We require the elements of  $\bar{\mathbf{x}}$  and the diagonal elements  $s_{jj}$  of  $\mathbf{S}$ , where

$$\bar{\mathbf{x}} = \begin{pmatrix} 50.536 \\ 46.179 \\ 49.679 \\ 45.179 \end{pmatrix} \begin{matrix} \text{N} \\ \text{E} \\ \text{S} \\ \text{W} \end{matrix} \quad \text{and} \quad \mathbf{S} = \begin{pmatrix} 290.406 & 223.753 & 288.438 & 226.271 \\ - & 219.930 & 229.060 & 171.374 \\ - & - & 350.004 & 259.541 \\ - & - & - & 226.004 \end{pmatrix}.$$

Using the Bonferroni intervals, we obtain the following:

$$\mu_1: 50.54 \pm 8.62,$$

$$\mu_2: 46.18 \pm 7.50,$$

$$\mu_3: 49.68 \pm 9.46,$$

$$\mu_4: 45.18 \pm 7.60.$$

Since the test for  $H_0: \mu_1 = \mu_2 = \mu_3 = \mu_4$  was significant at the 1% level, we can see which contrasts  $\mathbf{c}'\bar{\mathbf{x}}$  are responsible for the rejection of  $H_0$ . In Example 3.3 (Section 3.4.2) the contrast  $\mu_1 - \mu_2 + \mu_3 - \mu_4$  ( $= \text{N} + \text{S} - \text{E} - \text{W}$ ) with  $\mathbf{c}' = (1, -1, 1, -1)$  was regarded as a likely candidate. Using (3.35), a 99% confidence interval for this contrast is

$$8.86 \pm \left\{ \frac{3(27)}{25} F_{3,25}^{0.01} \right\}^{1/2} \{128.718/28\}^{1/2},$$

that is,  $8.86 \pm 8.35$  or  $[0.51, 17.21]$ , which does not contain zero. Corresponding intervals for pairwise contrasts are

$$\mu_1 - \mu_2: 4.36 \pm 5.83,$$

$$\mu_1 - \mu_3: 0.86 \pm 5.86,$$

$$\mu_1 - \mu_4: 5.36 \pm 5.88,$$

$$\mu_3 - \mu_2: 3.50 \pm 7.78,$$

$$\mu_2 - \mu_4: 1.00 \pm 7.47,$$

$$\mu_3 - \mu_4: 4.50 \pm 5.55,$$

and all of these contain zero. Since  $H_0$  is rejected if and only if at least one interval for a contrast does not contain zero, we see that the contrast  $(\text{N} + \text{S} - \text{E} - \text{W})$  is responsible for the rejection of  $H_0$ .

Test for blockwise independence / two blocks

$$\underline{x}_i \sim N_d(\underline{\mu}, \Sigma), \quad i=1, \dots, n, \text{ independent, } n-1 \geq d$$

$$\text{Partition: } \underline{x}_i = \begin{bmatrix} y_i \\ z_i \end{bmatrix} \quad \underline{\mu} = \begin{bmatrix} \underline{\mu}_1 \\ \underline{\mu}_2 \end{bmatrix} \quad \Sigma = \begin{bmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{bmatrix}$$

$$y_i \text{ } d_1\text{-dim.}, \quad z_i \text{ } d_2\text{-dim.}, \quad d_1 + d_2 = d, \text{ assume } d_1 \geq d_2$$

$$H_0: y_i \text{ and } z_i \text{ independent} \Leftrightarrow \Sigma_{12} = 0 \text{ cf. th. 2.1 (iv)}$$

The likelihood ratio:

$$l = \frac{\sup_{\underline{\mu}_1, \underline{\mu}_2, \Sigma_{11}, \Sigma_{22}} L_1(\underline{\mu}_1, \Sigma_{11}) L_2(\underline{\mu}_2, \Sigma_{22})}{\sup_{\underline{\mu}, \Sigma} L(\underline{\mu}, \Sigma)}$$

$$= \frac{L_1(\hat{\underline{\mu}}_1, \hat{\Sigma}_{11}) L_2(\hat{\underline{\mu}}_2, \hat{\Sigma}_{22})}{L(\hat{\underline{\mu}}, \hat{\Sigma})}$$

$$= \frac{(2\pi e)^{-\frac{nd_1}{2}} (\det \hat{\Sigma}_{11})^{-\frac{n}{2}} (2\pi e)^{-\frac{nd_2}{2}} (\det \hat{\Sigma}_{22})^{-\frac{n}{2}}}{(2\pi e)^{-\frac{nd}{2}} (\det \hat{\Sigma})^{-\frac{n}{2}}}$$

$$= \left( \frac{\det \hat{\Sigma}_{11} \det \hat{\Sigma}_{22}}{\det \hat{\Sigma}} \right)^{-\frac{n}{2}}$$

$$l^{\frac{2}{n}} = \frac{\det \hat{\Sigma}}{\det \hat{\Sigma}_{11} \det \hat{\Sigma}_{22}} = \frac{n^{d_1} n^{d_2} \det Q}{n^d \det Q_{11} \det Q_{22}} = \frac{\det Q}{\det Q_{11} \det Q_{22}}$$

$$= \frac{\det Q_{11} \det (Q_{22} - Q_{21} Q_{11}^{-1} Q_{12})}{\det Q_{11} \det Q_{22}} = \frac{\det Q_{22 \cdot 1}}{\det Q_{22}}$$

$$= \frac{\det E}{\det (E+H)}, \quad \text{where } H = Q_{21} Q_{11}^{-1} Q_{12} \\ E = Q_{22 \cdot 1} = Q_{22} - H$$

$$\left. \begin{aligned} H &\sim W_{d_2}(d_1, \Sigma_{22}), H_0 \text{ true} \\ E &\sim W_{d_2}(n-d_1-1, \Sigma_{22}), H_0 \text{ true} \end{aligned} \right\} \begin{array}{l} \text{indep. of corollary} \\ \text{to lemma 2.10} \end{array}$$

$$l^{\frac{2}{n}} = \Lambda = \frac{\det E}{\det(E+H)} \sim U(d_2, d_1, n-d_1-1), H_0 \text{ true,}$$

cf. def. of U distribution, p.40

$U(d_2, d_1, n-d_1-1) = U(d_1, d_2, n-d_2-1)$ , thus  
interchange of  $y_i$  and  $z_i$  leads to the same test statistic

$H_0$  is rejected for small values of  $l$ , equivalent  
are small values of  $\Lambda$

$$\Lambda = \prod_{j=1}^{d_2} (1 - \theta_j) \text{ cf for instance formula (2.48)}$$

The  $\theta_j$ 's are the ordered eigenvalues of

$$H(E+H)^{-1} = Q_{21} Q_{11}^{-1} Q_{12} Q_{22}^{-1} = S_{21} S_{11}^{-1} S_{12} S_{22}^{-1}$$

Use of the U-R-principle:

$$H_{0ab} = \underline{a}^T \Sigma_{12} \underline{b} = 0 \text{ equiv. with } \frac{\underline{a}^T \Sigma_{12} \underline{b}}{\sqrt{\underline{a}^T \Sigma_{11} \underline{a}} \sqrt{\underline{b}^T \Sigma_{22} \underline{b}}} = 0$$

$$H_{0ab} : \sigma_{ab} = 0 \text{ equivalent to } \rho_{ab} = 0$$

$\rho_{ab}$  is the correlation coefficient between  $\underline{a}^T \underline{y}$  and  $\underline{b}^T \underline{z}$

The empirical correlation coefficient  $r_{ab}$ :

$$r_{ab} = \frac{s_{ab}}{s_a s_b} = \frac{\underline{a}^T S_{12} \underline{b}}{\sqrt{\underline{a}^T S_{11} \underline{a}} \sqrt{\underline{b}^T S_{22} \underline{b}}}, \text{ as}$$



$$\begin{aligned}
 s_a^2 &= \frac{1}{n-1} \sum_i (\underline{a}^T y_i - \underline{a}^T \bar{y})^2 \\
 &= \frac{1}{n-1} \sum_i (\underline{a}^T y_i - \underline{a}^T \bar{y}) (\underline{a}^T y_i - \underline{a}^T \bar{y})^T \\
 &= \frac{1}{n-1} \underline{a}^T \left( \sum_i (y_i - \bar{y})(y_i - \bar{y})^T \right) \underline{a} \\
 &= \frac{1}{n-1} \underline{a}^T Q_{11} \underline{a} = \underline{a}^T S_{11} \underline{a}
 \end{aligned}$$

analogous  $s_b^2$  and  $S_{ab}$

Acceptance area for  $H_{0ab}$ :  $r_{ab}^2 \leq k \Leftrightarrow \frac{(\underline{a}^T S_{12} \underline{b})^2}{\underline{a}^T S_{11} \underline{a} \underline{b}^T S_{22} \underline{b}} \leq k$

$$\begin{aligned}
 \bigcap_{a, b} \{(Y, Z) : r_{ab}^2 \leq k\} &= \{(Y, Z) : \sup_{a, b} r_{ab}^2 \leq k\} \\
 &= \{(Y, Z) : \Theta_{\max} \leq k\},
 \end{aligned}$$

where  $\Theta_{\max}$  is the largest eigenvalue of  $S_{11}^{-1} S_{12} S_{22}^{-1} S_{21}$  or of  $S_{22}^{-1} S_{21} S_{11}^{-1} S_{12}$ , cf. A 7.7 (and A 1.4), or of  $S_{21} S_{11}^{-1} S_{12} S_{22}^{-1}$  cf. A 1.4  $\Leftrightarrow \Theta_{\max}$  is the largest root in  $\det(S_{21} S_{11}^{-1} S_{12} S_{22}^{-1} - \theta I_{d_2}) = 0$  1)

The test is called Roy's maximum root test

Pillai's test variable:

$$V^{(s)} = \sum_j \theta_j = \text{tr}(H(E+H)^{-1}) = \text{tr}(S_{21} S_{11}^{-1} S_{12} S_{22}^{-1}) \quad 2)$$

1) percentiles for  $\Theta_{\max}$  in table D 14

2) - -  $V^{(s)}$  - - D 16