9. Orthogonal Linear Combinations, Contrasts, and Additional Partitioning of ANOVA Sums of Squares

Introduction

Orthogonal contrasts are

- designed to be independent of one another (within the same model)
- useful because they allow testing of multiple hypotheses simultaneously without inflating the probability of a Type I error.
- constructed such that they do not overlap in terms of the information they provide about the data.

Orthogonal Linear Combinations

GMMNE

Under the model

$$\boldsymbol{y} = \boldsymbol{X}\boldsymbol{\beta} + \boldsymbol{\epsilon},\ \boldsymbol{\epsilon} \sim \mathcal{N}(\boldsymbol{0}, \sigma^2 \boldsymbol{I}),$$

two estimable linear combinations $\boldsymbol{c}_1^\top \boldsymbol{\beta}$ and $\boldsymbol{c}_2^\top \boldsymbol{\beta}$ are *orthogonal* if and only if their $\underbrace{\text{best linear unbiased estimators}}_{\text{Blues}}$ $\boldsymbol{c}_1^\top \widehat{\boldsymbol{\beta}}$ and $\boldsymbol{c}_2^\top \widehat{\boldsymbol{\beta}}$ are uncorrelated.

Orthogonal Linear Combinations

Recall $\boldsymbol{c}_k^\top \boldsymbol{\beta}$ is estimable if and only if there exists $\boldsymbol{a}_k$ such that $\boldsymbol{c}_k^\top = \boldsymbol{a}_k^\top \boldsymbol{X}$.

$X\hat{\beta} = P_X y$

$$
\begin{aligned}
\text{Cov}(\boldsymbol{c}_1^\top \widehat{\boldsymbol{\beta}}, \boldsymbol{c}_2^\top \widehat{\boldsymbol{\beta}}) &= \\
&= \text{Cov}(\boldsymbol{a}_1^\top \boldsymbol{X}\widehat{\boldsymbol{\beta}}, \boldsymbol{a}_2^\top \boldsymbol{X}\widehat{\boldsymbol{\beta}}) = \text{Cov}(\boldsymbol{a}_1^\top \boldsymbol{P}_{\boldsymbol{X}}\boldsymbol{y}, \boldsymbol{a}_2^\top \boldsymbol{P}_{\boldsymbol{X}}\boldsymbol{y}) \\
&= \boldsymbol{a}_1^\top \boldsymbol{P}_{\boldsymbol{X}} \text{Cov}(\boldsymbol{y}, \boldsymbol{y}) \boldsymbol{P}_{\boldsymbol{X}}^\top \boldsymbol{a}_2 = \boldsymbol{a}_1^\top \boldsymbol{P}_{\boldsymbol{X}} \text{Var}(\boldsymbol{y}) \boldsymbol{P}_{\boldsymbol{X}}^\top \boldsymbol{a}_2 \\
&= \boldsymbol{a}_1^\top \boldsymbol{P}_{\boldsymbol{X}} (\sigma^2 \boldsymbol{I}) \boldsymbol{P}_{\boldsymbol{X}}^\top \boldsymbol{a}_2 = \sigma^2 \boldsymbol{a}_1^\top \boldsymbol{P}_{\boldsymbol{X}} \boldsymbol{P}_{\boldsymbol{X}} \boldsymbol{a}_2 \\
&= \sigma^2 \boldsymbol{a}_1^\top \boldsymbol{P}_{\boldsymbol{X}} \boldsymbol{a}_2 = \sigma^2 \boldsymbol{a}_1^\top \boldsymbol{X}(\boldsymbol{X}^\top \boldsymbol{X})^- \boldsymbol{X}^\top \boldsymbol{a}_2 = \sigma^2 \boldsymbol{c}_1^\top (\boldsymbol{X}^\top \boldsymbol{X})^- \boldsymbol{c}_2.
\end{aligned}
$$

Thus, estimable linear combinations $\boldsymbol{c}_1^\top \boldsymbol{\beta}$ and $\boldsymbol{c}_2^\top \boldsymbol{\beta}$ are orthogonal if and only if $\boldsymbol{c}_1^\top (\boldsymbol{X}^\top \boldsymbol{X})^- \boldsymbol{c}_2 = 0$.

Orthogonal Contrasts

A linear combination $\boldsymbol{c}^\top \boldsymbol{\beta}$ is a *contrast* if and only if $\boldsymbol{c}^\top \mathbf{1} = 0$.

Two estimable contrasts $\boldsymbol{c}_1^\top \boldsymbol{\beta}$ and $\boldsymbol{c}_2^\top \boldsymbol{\beta}$ that are orthogonal are called *orthogonal contrasts*.

That is,

1. $\boldsymbol{c}_1^\top \boldsymbol{\beta}$ and $\boldsymbol{c}_2^\top \boldsymbol{\beta}$ are orthogonal: $\boxed{\boldsymbol{c}_1^\top (\boldsymbol{X}^\top \boldsymbol{X})^- \boldsymbol{c}_2} = 0$
2. $\mathrm{Cov}(\boxed{\boldsymbol{c}_1^\top \widehat{\boldsymbol{\beta}}}, \boxed{\boldsymbol{c}_2^\top \widehat{\boldsymbol{\beta}}}) = 0$
3. contrast coefficients add to zero $\boldsymbol{c}_1^\top \mathbf{1} = \boldsymbol{c}_2^\top \mathbf{1} = 0$

Suppose $c_1^\top \beta, \ldots, c_q^\top \beta$ are pairwise orthogonal linear combinations.

Let $C^\top = [c_1, \ldots, c_q]$. Then, $C(X^\top X)^- C^\top =$

these are all $= 0$

$$= \begin{bmatrix} c_1^\top (X^\top X)^- c_1 & c_1^\top (X^\top X)^- c_2 & \cdots & c_1^\top (X^\top X)^- c_q \\ c_2^\top (X^\top X)^- c_1 & c_2^\top (X^\top X)^- c_2 & \cdots & c_2^\top (X^\top X)^- c_q \\ \vdots & \vdots & \ddots & \vdots \\ c_q^\top (X^\top X)^- c_1 & c_q^\top (X^\top X)^- c_2 & \cdots & c_q^\top (X^\top X)^- c_q \end{bmatrix}$$

$$= \begin{bmatrix} c_1^\top (X^\top X)^- c_1 & 0 & \cdots & 0 \\ 0 & c_2^\top (X^\top X)^- c_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & c_q^\top (X^\top X)^- c_q \end{bmatrix}.$$

When C has rank q, it follows that the sum of squares

$$\widehat{\boldsymbol{\beta}}^\top \boldsymbol{C}^\top[\boldsymbol{C}(\boldsymbol{X}^\top\boldsymbol{X})^-\boldsymbol{C}^\top]^{-1}\boldsymbol{C}\widehat{\boldsymbol{\beta}} = \sum_{k=1}^{q} \underbrace{\widehat{\boldsymbol{\beta}}^\top \boldsymbol{c}_k[\boldsymbol{c}_k^\top(\boldsymbol{X}^\top\boldsymbol{X})^-\boldsymbol{c}_k]^{-1}\boldsymbol{c}_k^\top\widehat{\boldsymbol{\beta}}}_{q \text{ 1-df sums of squares}}$$

$$\boxed{(C\widehat{\beta})^\top\{C(X^\top X)^- C^\top\}^{-1}C\widehat{\beta}} = \sum_{k=1}^{q}(\boldsymbol{c}_k^\top\widehat{\boldsymbol{\beta}})^2/\boldsymbol{c}_k^\top(\boldsymbol{X}^\top\boldsymbol{X})^-\boldsymbol{c}_k.$$

Thus, the sum of squares $\widehat{\boldsymbol{\beta}}^\top \boldsymbol{C}^\top[\boldsymbol{C}(\boldsymbol{X}^\top\boldsymbol{X})^-\boldsymbol{C}^\top]^{-1}\boldsymbol{C}\widehat{\boldsymbol{\beta}}$ with q degrees of freedom can be partitioned into q single-degree-of-freedom sums of squares $(\boldsymbol{c}_1^\top\widehat{\boldsymbol{\beta}})^2/\boldsymbol{c}_1^\top(\boldsymbol{X}^\top\boldsymbol{X})^-\boldsymbol{c}_1, \ldots, (\boldsymbol{c}_q^\top\widehat{\boldsymbol{\beta}})^2/\boldsymbol{c}_q^\top(\boldsymbol{X}^\top\boldsymbol{X})^-\boldsymbol{c}_q$, corresponding to orthogonal linear combinations.

Example: Balanced Two-Factor Diet-Drug Experiment

$$\begin{bmatrix} y_{111} \\ y_{112} \\ y_{121} \\ y_{122} \\ y_{131} \\ y_{132} \\ y_{211} \\ y_{212} \\ y_{221} \\ y_{222} \\ y_{231} \\ y_{232} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} \mu_{11} \\ \mu_{12} \\ \mu_{13} \\ \mu_{21} \\ \mu_{22} \\ \mu_{23} \end{bmatrix} + \begin{bmatrix} \epsilon_{111} \\ \epsilon_{112} \\ \epsilon_{121} \\ \epsilon_{122} \\ \epsilon_{131} \\ \epsilon_{132} \\ \epsilon_{211} \\ \epsilon_{212} \\ \epsilon_{221} \\ \epsilon_{222} \\ \epsilon_{231} \\ \epsilon_{232} \end{bmatrix}$$

$$\boldsymbol{y} = \boldsymbol{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}, \quad \boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \sigma^2 \boldsymbol{I})$$

Example: Balanced Two-Factor Diet-Drug Experiment

$$X^\top X = \begin{bmatrix} 2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2 \end{bmatrix} \quad (X^\top X)^{-1} = \begin{bmatrix} \frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2} \end{bmatrix}$$

Thus, in this case,

$$c_1^\top (X^\top X)^- c_2 = \boxed{c_1^\top c_2 / 2}$$

so that linear combinations $c_1^\top \beta$ and $c_2^\top \beta$ are orthogonal if and only if $c_1^\top c_2 = 0$.

Example: Balanced Two-Factor Diet-Drug Experiment

It follows that

main diet effect

$$\mathbf{c}_1^\top \boldsymbol{\beta} = [\overbrace{1, \; 1, \; 1}^{\text{diet 1}}, \overbrace{-1, -1, -1}^{\text{diet 2}}]\boldsymbol{\beta}$$

$\frac{1}{3} \quad \frac{1}{3} \quad \frac{1}{3} \quad -\frac{1}{3} \quad -\frac{1}{3} \quad -\frac{1}{3}$

diet 1 $\bar{\mu}_{1.}$ vs. $\bar{\mu}_{2.}$

test for drug main effect

$$\mathbf{c}_2^\top \boldsymbol{\beta} = [1, -1, \; 0, \; 1, -1, \; 0]\boldsymbol{\beta}$$

drug 1 vs. drug 2 within each diet

$$\mathbf{c}_3^\top \boldsymbol{\beta} = [1, \; 1, -2, \; 1, \; 1, -2]\boldsymbol{\beta}$$

$\mu_{11} + \mu_{12} - 2\mu_{13} = 0$

$\frac{\mu_{11} + \mu_{12}}{2} = \mu_{13}$

test for the interaction term

$$\mathbf{c}_4^\top \boldsymbol{\beta} = [1, -1, \; 0, -1, \; 1, \; 0]\boldsymbol{\beta}$$

$$\mathbf{c}_5^\top \boldsymbol{\beta} = [1, \; 1, -2, -1, -1, \; 2]\boldsymbol{\beta}$$

end lecture 18

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comprise a set of pairwise orthogonal contrasts.