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

Orthogonal Linear Combinations

Under the model

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

two estimable linear combinations $c_1'\beta$ and $c_2'\beta$ are *orthogonal* if and only if their best linear unbiased estimators $c_1'\hat{\beta}$ and $c_2'\hat{\beta}$ are uncorrelated.

Orthogonal Linear Combinations

Recall $c'_k\beta$ is estimable iff there exists a_k such that $c'_k=a'_kX$.

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

Thus, estimable linear combinations $c_1'\beta$ and $c_2'\beta$ are orthogonal if and only if $c_1'(X'X)^-c_2=0$.

Orthogonal Contrasts

A linear combinations $c'\beta$ is a *contrast* if and only if c'1 = 0.

Two estimable contrasts $c_1'\beta$ and $c_2'\beta$ that are orthogonal are called *orthogonal contrasts*.

Suppose $c'_1\beta, \ldots, c'_q\beta$ are pairwise orthogonal linear combinations.

Let $C' = [c_1, \ldots, c_q]$. Then

$$C(X'X)^{-}C' = \begin{bmatrix} c'_{1}(X'X)^{-}c_{1} & c'_{1}(X'X)^{-}c_{2} & \cdots & c'_{1}(X'X)^{-}c_{q} \\ c'_{2}(X'X)^{-}c_{1} & c'_{2}(X'X)^{-}c_{2} & \cdots & c'_{2}(X'X)^{-}c_{q} \\ \vdots & \vdots & \ddots & \vdots \\ c'_{q}(X'X)^{-}c_{1} & c'_{q}(X'X)^{-}c_{2} & \cdots & c'_{q}(X'X)^{-}c_{q} \end{bmatrix}$$

$$= \begin{bmatrix} c'_{1}(X'X)^{-}c_{1} & 0 & \cdots & 0 \\ 0 & c'_{2}(X'X)^{-}c_{2} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & c'_{q}(X'X)^{-}c_{q} \end{bmatrix}.$$

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

$$\hat{oldsymbol{eta}}' oldsymbol{C}' [oldsymbol{C}(X'X)^{-}oldsymbol{C}']^{-1} oldsymbol{C}\hat{oldsymbol{eta}} \ = \sum_{k=1}^{q} \hat{oldsymbol{eta}}' oldsymbol{c}_{k} [oldsymbol{c}_{k}'(X'X)^{-}oldsymbol{c}_{k}]^{-1} oldsymbol{c}_{k}' \hat{oldsymbol{eta}} \ = \sum_{k=1}^{q} (oldsymbol{c}_{k}'\hat{oldsymbol{eta}})^{2} / oldsymbol{c}_{k}'(X'X)^{-}oldsymbol{c}_{k}.$$

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

Example: Balanced Two-Factor Diet-Drug Experiment

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

Example: Balanced Two-Factor Diet-Drug Experiment

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

Thus, in this case,

$$c_1'(X'X)^-c_2 = c_1'c_2/2$$

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

Example: Balanced Two-Factor Diet-Drug Experiment It follows that

$$c'_1\beta = [1, 1, 1, -1, -1, -1]\beta$$
 $c'_2\beta = [1, -1, 0, 1, -1, 0]\beta$
 $c'_3\beta = [1, 1, -2, 1, 1, -2]\beta$
 $c'_4\beta = [1, -1, 0, -1, 1, 0]\beta$
 $c'_5\beta = [1, 1, -2, -1, -1, 2]\beta$

comprise a set of pairwise orthogonal contrasts.

Connection to the ANOVA Table

Source	Sum of Squares	DF
Diets	$y'(P_2-P_1)y$	2 - 1 = 1
Drugs	$\mathbf{y}'(\mathbf{P}_3 - \mathbf{P}_2)\mathbf{y}$	4 - 2 = 2
$Diets \times Drugs$	$y'(P_4-P_3)y$	6 - 4 = 2
Error	$oldsymbol{y}'(oldsymbol{I}-oldsymbol{P}_4)oldsymbol{y}$	12 - 6 = 6
C. Total	$y'(I - P_1)y$	12 - 1 = 11

Connection to the ANOVA Table

SS		DF
$y'(P_2-P_1)y =$	$(c_1'\hat{m{eta}})^2/c_1'(X'X)^-c_1$	1
$y'(P_3 - P_2)y =$	$({m c}_2'\hat{m eta})^2/{m c}_2'(X'X)^-{m c}_2 + ({m c}_3'\hat{m eta})^2/{m c}_3'(X'X)^-{m c}_3$	2
$y'(P_4 - P_3)y =$	$(c_4'\hat{oldsymbol{eta}})^2/c_4'(X'X)^-c_4+(c_5'\hat{oldsymbol{eta}})^2/c_5'(X'X)^-c_5$	2
$y'(I-P_4)y$		6
$y'(I - P_1)y$		11

ANOVA Table with Additional Partitioning

Source	SS	DF
Diet	$(c_1'\hat{\beta})^2/c_1'(X'X)^-c_1$	1
Drug 1 − Drug 2	$(c_2'\hat{\beta})^2/c_2'(X'X)^-c_2$	1
$(Drug\ 1 + Drug\ 2)/2 - Drug\ 3$	$(c_3'\hat{\beta})^2/c_3'(X'X)^-c_3$	1
$Diet \times (Drug \ 1 - Drug \ 2)$	$(c_4'\hat{m{eta}})^2/c_4'(X'X)^-c_4$	1
$Diet \times [(Drug 1 + Drug 2)/2 - Drug 3]$	$(c_5'\hat{\beta})^2/c_5'(X'X)^-c_5$	1
Error	$y'(I-P_4)y$	6
C.Total	$\mathbf{y}'(\mathbf{I} - \mathbf{P}_1)\mathbf{y}$	11

Additional Partitioning of ANOVA Sums of Squares

The previous example shows how the Drug and Diet \times Drug sums of squares can each be partitioned into two single-degree of freedom sums of squares corresponding to estimable orthogonal contrasts.

More generally, any ANOVA sum of squares with q degrees of freedom can be partitioned into q single-degree-of-freedom sums of squares corresponding to q estimable orthogonal linear combinations $c'_1\beta, \ldots, c'_a\beta$.

Proof of ANOVA Partitioning

To see that such a partitioning is always possible, first recall from the last set of slides that an ANOVA sum of squares

$$\mathbf{y}'(\mathbf{P}_{j+1}-\mathbf{P}_j)\mathbf{y}=\hat{\boldsymbol{\beta}}'\mathbf{C}'[\mathbf{C}(\mathbf{X}'\mathbf{X})^{-}\mathbf{C}']^{-1}\mathbf{C}\hat{\boldsymbol{\beta}},$$

where C is any matrix $q \times p$ matrix of rank $q = r_{j+1} - r_j$ whose row space is the same as the row space of $(P_{j+1} - P_j)X$.

Proof of ANOVA Partitioning (continued)

Now let a_1, \ldots, a_q be an orthogonal basis for $C(P_{j+1} - P_j)$.

Then, $\forall k = 1, \ldots, q$,

$$\boldsymbol{a}_k \in \mathcal{C}(\boldsymbol{P}_{j+1} - \boldsymbol{P}_j) \implies \exists \boldsymbol{v}_k \ni \boldsymbol{a}_k = (\boldsymbol{P}_{j+1} - \boldsymbol{P}_j)\boldsymbol{v}_k.$$

 $\forall k = 1, ..., q$, let $c'_k = a'_k X$. Then $c'_k \beta$ is estimable.

Also, $\forall k \neq \ell$,

$$c'_{k}(X'X)^{-}c_{\ell} = a'_{k}X(X'X)^{-}X'a_{\ell}$$

$$= a'_{k}P_{X}a_{\ell} = a'_{k}P_{X}(P_{j+1} - P_{j})v_{\ell}$$

$$= a'_{k}(P_{j+1} - P_{j})v_{\ell} = a'_{k}a_{\ell} = 0$$

so that $c'_1\beta,\ldots,c'_q\beta$ are orthogonal linear combinations.

Proof of ANOVA Partitioning (continued)

Let
$$extbf{\emph{C}}' = [extbf{\emph{c}}_1, \dots, extbf{\emph{c}}_q] = [extbf{\emph{X}}' extbf{\emph{a}}_1, \dots, extbf{\emph{X}}' extbf{\emph{a}}_q] = extbf{\emph{X}}'[extbf{\emph{a}}_1, \dots, extbf{\emph{a}}_q]$$

Is the row space of C the same as the row space of $(P_{j+1}-P_j)X$? Equivalently, is $\mathcal{C}(C')=\mathcal{C}(X'(P_{j+1}-P_j))$?

$$C' = X'[a_1, \ldots, a_q] = X'[(P_{j+1} - P_j)v_1, \ldots, (P_{j+1} - P_j)v_q]$$

= $X'(P_{j+1} - P_j)[v_1, \ldots, v_q] \implies C(C') \subseteq C(X'(P_{j+1} - P_j)).$

Also, $X'(P_{j+1}-P_j)=X'[a_1,\ldots,a_q]M=C'M$, for some $q\times n$ matrix M because a_1,\ldots,a_q comprises a basis for $\mathcal{C}(P_{j+1}-P_j)$. Thus, $\mathcal{C}(X'(P_{j+1}-P_j))\subseteq\mathcal{C}(C')$.

Proof of ANOVA Partitioning (continued)

Thus, we have $C(X'(P_{j+1} - P_j)) = C(C')$.

It follows that

$$\mathbf{y}'(\mathbf{P}_{j+1} - \mathbf{P}_j)\mathbf{y} = \hat{\boldsymbol{\beta}}' \mathbf{C}' [\mathbf{C}(\mathbf{X}'\mathbf{X})^{-} \mathbf{C}']^{-1} \mathbf{C} \hat{\boldsymbol{\beta}}$$

$$= \sum_{k=1}^{q} \hat{\boldsymbol{\beta}}' \mathbf{c}_{k} [\mathbf{c}'_{k}(\mathbf{X}'\mathbf{X})^{-} \mathbf{c}_{k}]^{-1} \mathbf{c}'_{k} \hat{\boldsymbol{\beta}}$$

$$= \sum_{k=1}^{q} (\mathbf{c}'_{k} \hat{\boldsymbol{\beta}})^{2} / \mathbf{c}'_{k} (\mathbf{X}'\mathbf{X})^{-} \mathbf{c}_{k}.$$

ANOVA Partitioning is Not Always Necessary

Just because we can partition ANOVA sums of squares does not mean we need to partition ANOVA sums of squares.

The goals of an analysis typically involve constructing estimates or conducting tests of scientific interest.

The tests of scientific interest do not necessarily involve orthogonal linear combinations.

For example, suppose the goal of the researchers who conducted the diet-drug study is to determine which of the three drugs is best for enhancing weight gain of pigs on each diet.

SAS Code

```
proc mixed;
  class diet drug;
  model weightgain=diet drug diet*drug;
  lsmeans diet*drug / slice=diet;
  estimate 'drug 1 - drug 2 for diet 1'
           drug 1 -1 0 diet*drug 1 -1 0 0 0 / cl;
  estimate 'drug 1 - drug 3 for diet 1'
         drug 1 0 -1 diet*drug 1 0 -1 0 0 0;
  estimate 'drug 2 - drug 3 for diet 1'
         drug 0 1 -1 diet*drug 0 1 -1 0 0 0;
  estimate 'drug 1 - drug 2 for diet 2'
         drug 1 -1 0 diet*drug 0 0 0 1 -1 0;
  estimate 'drug 1 - drug 3 for diet 2'
         drug 1 0 -1 diet*drug 0 0 0 1 0 -1;
  estimate 'drug 2 - drug 3 for diet 2'
         drug 0 1 -1 diet*drug 0 0 0 1 -1;
run;
```

The Mixed Procedure

Type 3 Tests of Fixed Effects

Effect	Num DF	Den DF	F Value	Pr > F
diet	1	6	61.96	0.0002
drug	2	6	6.04	0.0365
diet*drug	2	6	5.01	0.0526

Tests of Effect Slices

Effect	diet	Num DF	Den DF	F Value	Pr > F
diet*drug	1	2 2	6	9.59	0.0135
diet*drug	2		6	1.46	0.3042

Least Squares Means

Effect	diet	drug	Estimate	Standard Error
diet*drug	1	1	42.5000	0.7832
diet*drug	1	2	40.0500	0.7832
diet*drug	1	3	37.6500	0.7832
diet*drug	2	1	35.7000	0.7832
diet*drug	2	2	33.9500	0.7832
diet*drug	2	3	35.4500	0.7832

Estimates

			Standard	
Label		Estimate	Error DF t	Value Pr > t
drug 1 - drug 2	for diet 1	2.4500	1.1075 6	2.21 0.0689
drug 1 - drug 3	for diet 1	4.8500	1.1075 6	4.38 0.0047
drug 2 - drug 3	for diet 1	2.4000	1.1075 6	2.17 0.0734
drug 1 - drug 2	for diet 2	1.7500	1.1075 6	1.58 0.1652
drug 1 - drug 3	for diet 2	0.2500	1.1075 6	0.23 0.8289
drug 2 - drug 3	for diet 2	-1.5000	1.1075 6	-1.35 0.2244
Label		Lower	Upper	
drug 1 - drug 2	for diet 1	-0.2601	5.1601	
drug 1 - drug 3	for diet 1	2.1399	7.5601	
drug 2 - drug 3	for diet 1	-0.3101	5.1101	
drug 1 - drug 2	for diet 2	-0.9601	4.4601	
drug 1 - drug 3	for diet 2	-2.4601	2.9601	
drug 2 - drug 3	for diet 2	-4.2101	1.2101	

Main Conclusions

For pigs on diet 1, treatment with drug 1 led to significantly greater mean weight gain than treatment with drug 3.

No other differences in mean weight gain between drugs within either diet were statistically significant.

Comments on the Analysis

Note that the main analysis focuses on pairwise comparisons of drugs within each diet.

This involves a set of six contrasts, but the contrasts are not pairwise orthogonal within either diet.

The sums of squares for these contrasts do not add up to any ANOVA sums of squares, but they are the contrasts that best address the researchers' questions.

If we want to control the probability of one or more type I errors, we could use Bonferroni's method. In this case, the adjustment for multiple testing would not change the conclusions.

Comments on the Cell Means vs. Additive Model

We used the cell means model for analysis even though the interactions were not significant at the 0.05 level.

I tend to prefer the cell means model in experiments with a full-factorial treatment design even if interactions are not significant.

The cell means model is less restrictive than an additive model.

The cell means model estimator of error variance σ^2 is not inflated by incorrectly specifying an additive mean structure when the additive mean structure is too restrictive.

Comments on the Cell Means vs. Additive Model

Using the cell means model honors the treatment structure.

Using the cell means model avoids problems with using the data once to select a model and a second time to perform inference.

Some other statisticians may favor a different strategy, especially in experiments with many factors or few degrees of freedom for error.