

L23 Decomposition of SSM

1. Model $y \sim N(X\beta, \sigma^2 I_n)$, $X \in R^{n \times p}$, $\text{rank}(X) = p$ and $1_n \notin \mathcal{R}(X)$.

(1) ANOVA table for testing on $H_0 : \beta = 0$.

Source	SS	DF	MS	F	$P_r > F$
Model	$\text{SSM} = y'XX^+y$	p	MSM	MSM/MSE	$P(F(p, n-p) > F_{ob})$
Error	$\text{SSE} = y'(I - XX^+)y$	$n-p$	MSE		
U.Total	$\text{U.SSTO} = y'I_n y$	n			

(2) ANOVA table for testing on $H_0 : H\beta = 0$, $H \in R^{q \times p}$, $\text{rank}(H) = q$.

Denote previous SSE = $\text{SSE}_r - \text{SSE}$ as SSH associated with Hypothesis.

$\text{SSH} = y'\{XX^+ - [X(I - H^+H)][X(I - H^+H)]^+\}y$ with DF $p - (p - q) = q$. Then

Source	SS	DF	MS	F	$P_r > F$
Hypothesis	SSH	q	MSH	MSH/MSE	$P(F(q, n-p) > F_{ob})$
Error	SSE	$n-p$	MSE		

(3) SSH is part of SSM

$\{XX^+ - [X(I - H^+H)][X(I - H^+H)]^+\} = XX^+ \{XX^+ - [X(I - H^+H)][X(I - H^+H)]^+\}$

implies that SSH is part of SSM. Thus with $\text{SSH}^\perp = y'[X(I - H^+H)][X(I - H^+H)]^+y$,

$\text{SSM} = \text{SSH} + \text{SSH}^\perp$. We therefore have combined ANOVA table

Source	SS	DF	MS	F	$P_r > F$
Model	SSM	p	MSM	MSM/MSE	$P(F(p, n-p) > F_{ob})$
H	SSH	q	MSH	MSH/MSE	$P(F(q, n-p) > F_{ob})$
H^\perp	SSH^\perp	$p - q$	MSH^\perp		
Error	SSE	$n-p$	MSE		
U.Total	U.SSTO	n			

Ex1: $\text{SSH} = \|\{XX^+ - [X(I - H^+H)][X(I - H^+H)]^+\}y\|^2$,

$\text{SSH}^\perp = \|[X(I - H^+H)][X(I - H^+H)]^+y\|^2$ and

$\{XX^+ - [X(I - H^+H)][X(I - H^+H)]^+\}y \perp [X(I - H^+H)][X(I - H^+H)]^+y$.

Ex2: Decomposition of $\text{SSA} = y'AA^+y$ where $\text{rank}(A) = r$.

For given $r_1 + \dots + r_k = r$, in the compact form of EVD $AA^+ = PP'$ where

$P \in R^{p \times r}$ and $P'P = I_r$, break P as $P = (P_1, \dots, P_r)$ where $P_i \in R^{p \times r_i}$. Then

$AA^+ = PP' = \sum_{i=1}^k P_i P_i'$. Let $A_i = P_i P_i' = A_i A_i^+$ and $\text{SSA}_i = y'A_i A_i^+ y$. Then

$\text{SSA} = \sum_{i=1}^k \text{SSA}_i$ where SSA_i , $i = 1, \dots, k$, are SSs.

From $PP' = P_1 P_1' + \dots + P_k P_k'$, $PP' P_i P_i' = P_i P_i'$. So $A_i = AA^+ A_i$. Hence SSA_i is part of SSA.

2. Model $y \sim N(X\beta, \sigma^2 I_n)$, $X \in R^{n \times p}$, $\text{rank}(X) = p$ and $1_n \in \mathcal{R}(X)$.

(1) ANOVA table for global F-test.

Source	SS	DF	MS	F	$P_r > F$
Model	$\text{SSM} = y'(XX^+ - 11^+)y$	$p - 1$	MSM	MSM/MSE	$P(F(p-1, n-p) > F_{ob})$
Error	$\text{SSE} = y'(I - XX^+)y$	$n - p$	MSE		
C.Total	$\text{C.SSTO} = y'(I_n - 11^+)y$	$n - 1$			

(2) ANOVA table for testing on $H_0 : H\beta = 0$, $H \in R^{q \times p}$, $\text{rank}(H) = q$.

Denote previous SSE = $\text{SSE}_r - \text{SSE}$ as SSH associated with Hypothesis.

$\text{SSH} = y'\{XX^+ - [X(I - H^+H)][X(I - H^+H)]^+\}y$ with DF $p - (p - q) = q$. Then

Source	SS	DF	MS	F	$Pr > F$
Hypothesis	SSH	q	MSH	MSH/MSE	$P(F(q, n - p) > F_{ob})$
Error	SSE	$n - p$	MSE		

(3) SSH may or may not be part of SSM

$$\begin{aligned} \text{Recall: } SSB = y'BB^+y \text{ is part of } SSA = y'AA^+y &\iff B = AT \text{ for some } T \\ &\iff BB^+ = AA^+BB^+ \end{aligned}$$

Thus

$$\begin{aligned} SSH \text{ is part of } SSM \\ \iff XX^+ - [X(I - H^+H)][X(I - H^+H)]^+ \\ \quad = (XX^+ - 11^+)\{XX^+ - [X(I - H^+H)][X(I - H^+H)]^+\} \\ \iff 0 = -11^+ + 11^+[X(I - H^+H)][X(I - H^+H)]^+ \\ \iff 11^+ = 11^+[X(I - H^+H)][X(I - H^+H)]^+ \\ \iff 1_n \in \mathcal{R}[X(I - H^+H)]. \end{aligned}$$

3. Contrast tests

(1) Test on q contrasts

In ANOVA of p treatments with response means $\mu_i, i = 1, \dots, p$.

Test on $H_0 : H\mu = 0$ where $H \in R^{q \times p}$, $\text{rank}(H) = q$ and $H1_p = 0$ is a test on q contrasts.

(2) Testing on a hypothesized equivalent groups in treatments is a testing on a group contrasts.

For example when $p = 4$, the hypothesis on groups (μ_1, μ_3) and (μ_2, μ_4) is $H_0 : H\mu = 0$ where $H = \begin{pmatrix} 1 & 0 & -1 & 0 \\ 0 & 1 & 0 & -1 \end{pmatrix}$. Clearly $H1_4 = 0$.

(3) Implementation via SAS

Suppose response y and treatment id with values A, B, C and D are stored in file ex.dat.

```
data a;
  infile "D:\ex.dat";
  input y id $ @@;
proc glm;
  class id;
  model y=id/nouni;
  contrast "group" id 1 0 -1 0, id 0 1 0 -1;
run;
```

The output displays

	MS	DF	F	$Pr > F_{ob}$
Contrast	MSH	2	MSH/MSE	$P(F(2, n - 4) > F_{ob})$

L24: Analysis of Covariance model

1. Analysis of covariance model (ANCOVA)

(1) ANOVA model

For observed $y \in R^n$, $y = X\beta + \epsilon$, $E(\epsilon) = 0 \in R^n$, is a linear model since $E(y) = X\beta$ is a linear function of β and hence $E(y)$ is in a linear space $S = \mathcal{R}(X)$.

For ANOVA $y = \mu_i + \epsilon$ with $E(\epsilon) = 0 \in R$, $i = 1, 2, 3$, suppose y_1 and y_2 are from $y = \mu_1 + \epsilon$; y_3 is from $y = \mu_2 + \epsilon$ and y_4 is from $y = \mu_3 + \epsilon$.

Then $y = \begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \mu_1 \\ \mu_2 \\ \mu_3 \end{pmatrix} + \epsilon$, $E(\epsilon) = 0 \in R^4$. Rewrite $y = \mu + \alpha_i + \epsilon$ with

$E(\epsilon) = 0 \in R$ and $\alpha_1 + \alpha_2 + \alpha_3 = 0$. Then $y = \begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{pmatrix} = \begin{pmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ 1 & 0 & 1 \\ 1 & -1 & -1 \end{pmatrix} \begin{pmatrix} \mu \\ \alpha_1 \\ \alpha_2 \end{pmatrix} + \epsilon$,

$E(\epsilon) = 0 \in R^4$. So one-way ANOVA is a linear model.

(2) Regression model

Regression $y = \beta_1 x_1 + \beta_2 x_2 + \epsilon$, $E(\epsilon) = 0 \in R$, with data can be expressed as $y = X\beta + \epsilon$ where $E(\epsilon) = 0 \in R^n$, $\beta = \begin{pmatrix} \beta_1 \\ \beta_2 \end{pmatrix}$ and the two columns of X are observed x_1 and x_2 .

(3) ANCOVA model

Suppose one initially has ANOVA model $y = X\delta + \epsilon$ and later adds regression part $Z\gamma$ into the model to have $y = X\delta + Z\gamma + \epsilon$. This model is called ANCOVA model since the later added regressors are called covariates.

Comment: Write ANCOVA $y = X\delta + Z\gamma + \epsilon$ as $y = (X, Z)\beta + \epsilon$ where $\beta = \begin{pmatrix} \delta \\ \gamma \end{pmatrix}$.

Clearly this a linear model.

2. Estimable parameters and BLUE

(1) Recall: LSE and estimable parameters

For linear model $y = X\beta + \epsilon$, $E(\epsilon) = 0$

$$\begin{aligned} \hat{\beta} \text{ is LSE for } \beta &\stackrel{\text{def}}{\iff} \|y - X\beta\|^2 \geq \|y - X\hat{\beta}\|^2 \text{ for all } \beta \iff X\hat{\beta} = \pi(y|\mathcal{R}(X)) \\ &\iff X\hat{\beta} = XX^+y \iff \hat{\beta} \in X^+y + \mathcal{N}(X) \end{aligned}$$

So $\text{LSE}(\beta) = X^+y + \mathcal{N}(X)$.

$$\begin{aligned} H\beta \text{ is estimable} &\stackrel{\text{def}}{\iff} \exists L \text{ such that } E(Ly) = H\beta \iff \exists L \text{ such that } LX\beta = H\beta \\ &\iff LX = H \iff \exists L \text{ such that } H\beta = L(X\beta). \end{aligned}$$

So $E(y) = X\beta$ is estimable since $X = IX$.

Comment: $H\beta$ is estimable $\iff H\hat{\beta}$ is unique. Clearly the unique value is HX^+y .

(2) Estimator for σ^2 and BLUE

Suppose $Y = X\beta + \epsilon$, $\epsilon \sim N(0, \sigma^2 I_n)$. Then $\text{SSE} = \|y - X\hat{\beta}\|^2 = y'(I - XX^+)y$. $\frac{\text{SSE}}{n - \text{rank}(X)}$ is UE for σ^2 , $\frac{\text{SSE}}{n}$ is MLE for σ^2 . For estimable $H\beta$, the unique $H\hat{\beta}$ is a BLUE.

(3) ANCOVA model

For $y = (X, Z)\beta + \epsilon$ where $\beta = \begin{pmatrix} \delta \\ \gamma \end{pmatrix}$ and $\epsilon \sim N(0, \sigma^2 I_n)$, $E(y) \in S = \mathcal{R}[(X, Z)]$.

$\hat{\beta}$ is a LSE for $\beta \iff (X, Z)\hat{\beta} = (X, Z)(X, Z)^+y$.

SSE = $y'[I - (X, Z)(X, Z)^+]y$.

Comment: Fit the linear model framework, X is replaced by (X, Z) . Thus we need to explore more on $\mathcal{R}[(X, Z)]$ and $(X, Z)(X, Z)^+$.

3. Some specifics for ANCOVA

(1) For $y = (X, Z)\beta + \epsilon$

- (i) $E(y) \in \mathcal{R}[(X, Z)] = \mathcal{R}(X) + \mathcal{R}(Z)$
- (ii) $\mathcal{R}[(X, Z)] = \mathcal{R}(X) \dot{+} \mathcal{R}[(X, (I - XX^+)Z)]$
- (iii) $\mathcal{R}[(X, Z)] = \mathcal{R}[(I - ZZ^+)X] \dot{+} \mathcal{R}(Z)$.

Proof. (i) $\mathcal{R}[(X, Z)] = \left\{ (X, Z) \begin{pmatrix} r_1 \\ r_2 \end{pmatrix} : \begin{pmatrix} r_1 \\ r_2 \end{pmatrix} \right\} = \{Xr_1 + Zr_2 : r_1, r_2\}$
 $= \{Xr_1 : r_1\} + \{Zr_2 : r_2\} = \mathcal{R}(X) + \mathcal{R}(Z)$.

For (ii) note that $(X, Z) = [X, (I - XX^+)Z] \begin{pmatrix} I & X^+Z \\ 0 & I \end{pmatrix}$

and $[X, (I - XX^+)Z] = (X, Z) \begin{pmatrix} I & -X^+Z \\ 0 & I \end{pmatrix}$. So

$\mathcal{R}[(X, Z)] = \mathcal{R}[(X, (I - XX^+)Z)] = \mathcal{R}(X) + \mathcal{R}[(I - XX^+)Z] = \mathcal{R}(X) \dot{+} \mathcal{R}[(I - XX^+)Z]$.

The last equal sign holds since $X'(I - XX^+)Z = 0$. The proof of (iii) is skipped.

(2) $(X, Z)(X, Z)^+ = XX^+ + [(I - XX^+)Z][(I - XX^+)Z]^+$ and
 $(X, Z)(X, Z)^+ = [(I - ZZ^+)Z][(I - ZZ^+)Z]^+ + ZZ^+$.

Proof. First $(X, Z)(X, Z)^+ = [X, (I - XX^+)Z][X, (I - XX^+)Z]^+$ since they are the projection matrices onto the same space $\mathcal{R}[(X, Z)] = \mathcal{R}[(X, (I - XX^+)Z)]$.

Secondly $[X, (I - XX^+)Z]^+ = \begin{pmatrix} X^+ \\ [(I - XX^+)Z]^+ \end{pmatrix}$ since $X'(I - XX^+)Z = 0$.

Consequently $(X, Z)(X, Z)^+ = XX^+ + [(I - XX^+)Z][(I - XX^+)Z]^+$. The second equation can be proved similarly.

(3) If $\mathcal{R}(X) \cap \mathcal{R}(Z) = \{0\}$, then

- (i) $\text{rank}(X) = \text{rank}[(I - ZZ^+)X]$ and $\text{rank}(Z) = \text{rank}[(I - XX^+)Z]$
- (ii) $\mathcal{R}(X') = \mathcal{R}[X'(I - ZZ^+)]$ and $\mathcal{R}(Z') = \mathcal{R}[Z'(I - XX^+)]$

Proof. We first show the second equation in (i). Under $\mathcal{R}(X) \cap \mathcal{R}(Z) = \{0\}$,

$$\begin{aligned} \text{rank}[(X, Z)] &= \dim[\mathcal{R}[(X, Z)]] = \dim[\mathcal{R}(X) + \mathcal{R}(Z)] \\ &= \dim[\mathcal{R}(X)] + \dim[\mathcal{R}(Z)] - \dim[\mathcal{R}(X) \cap \mathcal{R}(Z)] \\ &= \text{rank}(X) + \text{rank}(Z). \end{aligned}$$

$$\begin{aligned} \text{But } \text{rank}[(X, Z)] &= \dim[\mathcal{R}[(X, (I - XX^+)Z)]] = \dim[\mathcal{R}(X) \dot{+} \mathcal{R}[(I - XX^+)Z]] \\ &= \dim[\mathcal{R}(X)] + \dim[\mathcal{R}[(I - XX^+)Z]] \\ &= \text{rank}(X) + \text{rank}[(I - XX^+)Z]. \end{aligned}$$

Thus $\text{rank}(Z) = \text{rank}[(I - XX^+)Z]$.

For the first equation in (ii) note that $\mathcal{R}[X'(I - ZZ^+)] \subset \mathcal{R}(X')$. But by (i) the two spaces share the same dimension. Thus $\mathcal{R}(X') = \mathcal{R}[X'(I - ZZ^+)]$.