Theorem 3.7.

Consider model

\[ X = Z\beta + \varepsilon \]

(1)

with assumption A1 (\( \varepsilon \) is distributed as \( N_n(0, \sigma^2 I_n) \) with an unknown \( \sigma^2 > 0 \)).

(i) The LSE \( \hat{l}^\tau \hat{\beta} \) is the UMVUE of \( l^\tau \beta \) for any estimable \( l^\tau \beta \).

(ii) The UMVUE of \( \sigma^2 \) is \( \hat{\sigma}^2 = (n - r)^{-1} \| X - Z\hat{\beta} \|^2 \), where \( r \) is the rank of \( Z \).

Proof of (i)

Let \( \hat{\beta} \) be an LSE of \( \beta \). By \( Z^\tau Zb = Z^\tau X \),

\[ (X - Z\hat{\beta})^\tau Z(\hat{\beta} - \beta) = (X^\tau Z - X^\tau Z)(\hat{\beta} - \beta) = 0 \]

and, hence,
Theorem 3.7.
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\[ X = Z\beta + \varepsilon \]  

with assumption A1 (\(\varepsilon\) is distributed as \(N_n(0, \sigma^2 I_n)\) with an unknown \(\sigma^2 > 0\)).

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Proof of (i) continue ......

\[ \| X - Z\beta \|^2 = \| X - Z\hat{\beta} + Z\hat{\beta} - Z\beta \|^2 \]
\[ = \| X - Z\hat{\beta} \|^2 + \| Z\hat{\beta} - Z\beta \|^2 \]
\[ = \| X - Z\hat{\beta} \|^2 - 2\beta^\tau Z^\tau X + \| Z\beta \|^2 + \| Z\hat{\beta} \|^2. \]

Using this result and assumption A1, we obtain the following joint Lebesgue p.d.f. of \( X \):

\[ (2\pi\sigma^2)^{-n/2} \exp \left\{ \frac{\beta^\tau Z^\tau X}{\sigma^2} - \frac{\| X - Z\hat{\beta} \|^2 + \| Z\hat{\beta} \|^2}{2\sigma^2} - \frac{\| Z\beta \|^2}{2\sigma^2} \right\}. \]

By Proposition 2.1 and the fact that \( Z\hat{\beta} = Z(Z^\tau Z)^{-1}Z^\tau X \) is a function of \( Z^\tau X \), the statistic \( (Z^\tau X, \| X - Z\hat{\beta} \|^2) \) is complete and sufficient for \( \theta = (\beta, \sigma^2) \).

Note that \( \hat{\beta} \) is a function of \( Z^\tau X \) and, hence, a function of the complete sufficient statistic. If \( l^\tau \beta \) is estimable, then \( l^\tau \hat{\beta} \) is unbiased for \( l^\tau \beta \) (Theorem 3.6) and, hence, \( l^\tau \hat{\beta} \) is the UMVUE of \( l^\tau \beta \).
Proof of (ii)

From $\|X - Z\beta\|^2 = \|X - \hat{Z}\beta\|^2 + \|\hat{Z}\beta - Z\beta\|^2$ and $E(\hat{Z}\beta) = Z\beta$ (Theorem 3.6),

$$E\|X - \hat{Z}\beta\|^2 = E(X - Z\beta)^\tau(X - Z\beta) - E(\beta - \hat{\beta})^\tau Z^\tau Z(\beta - \hat{\beta})$$

$$= \text{tr} \left( \text{Var}(X) - \text{Var}(\hat{Z}\beta) \right)$$

$$= \sigma^2[n - \text{tr} \left( Z(Z^\tau Z)^{-1} Z^\tau Z(Z^\tau Z)^{-1} Z^\tau \right)]$$

$$= \sigma^2[n - \text{tr} \left( (Z^\tau Z)^{-1} Z^\tau \right)].$$

Since each row of $Z \in \mathcal{R}(Z)$, $\hat{Z}\beta$ does not depend on the choice of $(Z^\tau Z)^{-1}$ in $\hat{\beta} = (Z^\tau Z)^{-1} Z^\tau X$ (Theorem 3.6).

- Hence, we can evaluate $\text{tr}((Z^\tau Z)^{-1} Z^\tau Z)$ using a particular $(Z^\tau Z)^{-1}$.

From the theory of linear algebra, there exists a $p \times p$ matrix $C$ such that $CC^\tau = I_p$ and

$$C^\tau(Z^\tau Z)C = \begin{pmatrix} \Lambda & 0 \\ 0 & 0 \end{pmatrix},$$
Proof of (ii)

From $\|X - Z\beta\|^2 = \|X - Z\hat{\beta}\|^2 + \|Z\hat{\beta} - Z\beta\|^2$ and $E(Z\hat{\beta}) = Z\beta$ (Theorem 3.6),

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$$= \text{tr} \left( \text{Var}(X) - \text{Var}(Z\hat{\beta}) \right)$$

$$= \sigma^2 [n - \text{tr} \left( Z(Z^\tau Z)^{-1} Z^\tau Z(Z^\tau Z)^{-1} Z^\tau \right)]$$

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Since each row of $Z \in \mathcal{R}(Z)$, $Z\hat{\beta}$ does not depend on the choice of $(Z^\tau Z)^{-1}$ in $\hat{\beta} = (Z^\tau Z)^{-1} Z^\tau X$ (Theorem 3.6).

- Hence, we can evaluate $\text{tr}((Z^\tau Z)^{-1} Z^\tau Z)$ using a particular $(Z^\tau Z)^{-1}$. From the theory of linear algebra, there exists a $p \times p$ matrix $C$ such that $CC^\tau = I_p$ and

$$C^\tau (Z^\tau Z) C = \begin{pmatrix} \Lambda & 0 \\ 0 & 0 \end{pmatrix},$$
Proof of (ii) continue ......

Then, a particular choice of \((Z^\tau Z)^{-}\) is

\[
(Z^\tau Z)^{-} = C \begin{pmatrix} \Lambda^{-1} & 0 \\ 0 & 0 \end{pmatrix} C^\tau
\]

(2)

and

\[
(Z^\tau Z)^{-} Z^\tau Z = C \begin{pmatrix} I_r & 0 \\ 0 & 0 \end{pmatrix} C^\tau
\]

whose trace is \(r\).

Hence \(\hat{\sigma}^2\) is the UMVUE of \(\sigma^2\), since it is a function of the complete sufficient statistic and

\[
E\hat{\sigma}^2 = (n - r)^{-1} E\|X - Z\hat{\beta}\|^2 = \sigma^2.
\]

Residual vector

The vector \(X - Z\hat{\beta}\) is called the residual vector and \(\|X - Z\hat{\beta}\|^2\) is called the sum of squared residuals and is denoted by \(SSR\).

The estimator \(\hat{\sigma}^2\) is then equal to \(SSR/(n - r)\).
Proof of (ii) continue ......

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Residual vector

- The vector \(X - Z\hat{\beta}\) is called the residual vector and \(\|X - Z\hat{\beta}\|^2\) is called the sum of squared residuals and is denoted by SSR.
- The estimator \(\hat{\sigma}^2\) is then equal to \(SSR/(n - r)\).
More properties

In general,

\[ \text{Var}(l^\tau \hat{\beta}) = l^\tau (Z^\tau Z)^{-1} Z^\tau \text{Var}(\varepsilon) Z(Z^\tau Z)^{-1} l. \] (3)

If \( l \in \mathcal{R}(Z) \) and \( \text{Var}(\varepsilon) = \sigma^2 I_n \) (assumption A2), then the use of the generalized inverse matrix in (2) leads to \( \text{Var}(l^\tau \hat{\beta}) = \sigma^2 l^\tau (Z^\tau Z)^{-1} l \), which attains the Cramér-Rao lower bound under assumption A1 (Proposition 3.2).

Since \( X - Z\hat{\beta} = [I_n - Z(Z^\tau Z)^{-1} Z^\tau]X \) and \( l^\tau \hat{\beta} = l^\tau (Z^\tau Z)^{-1} Z^\tau X \) are linear in \( X \), they are normally distributed under assumption A1.

Also, using the generalized inverse matrix in (2), we obtain that

\[ [I_n - Z(Z^\tau Z)^{-1} Z^\tau]Z(Z^\tau Z)^{-1} = Z(Z^\tau Z)^{-1} - Z(Z^\tau Z)^{-1} Z^\tau Z(Z^\tau Z)^{-1} = 0, \]

which implies that \( \hat{\sigma}^2 \) and \( l^\tau \hat{\beta} \) are independent (Exercise 58 in §1.6) for any estimable \( l^\tau \beta \).
Furthermore,

\[ [Z(Z^\tau Z)^{-}Z^\tau]^2 = Z(Z^\tau Z)^{-}Z^\tau \]

(i.e., \( Z(Z^\tau Z)^{-}Z^\tau \) is a projection matrix) and

\[ SSR = X^\tau [I_n - Z(Z^\tau Z)^{-}Z^\tau]X. \]

The rank of \( Z(Z^\tau Z)^{-}Z^\tau \) is \( \text{tr}(Z(Z^\tau Z)^{-}Z^\tau) = r. \)

Similarly, the rank of the projection matrix \( I_n - Z(Z^\tau Z)^{-}Z^\tau \) is \( n - r. \)

From

\[ X^\tau X = X^\tau [Z(Z^\tau Z)^{-}Z^\tau]X + X^\tau [I_n - Z(Z^\tau Z)^{-}Z^\tau]X \]

and Theorem 1.5 (Cochran’s theorem), \( SSR/\sigma^2 \) has the chi-square distribution \( \chi^2_{n-r}(\delta) \) with

\[ \delta = \sigma^{-2} \beta^\tau Z^\tau [I_n - Z(Z^\tau Z)^{-}Z^\tau]Z\beta = 0. \]
Thus, we have proved the following result.

**Theorem 3.8.**

Consider model (1) with assumption A1. For any estimable parameter \( l^\tau \beta \), the UMVUE's \( l^\tau \hat{\beta} \) and \( \hat{\sigma}^2 \) are independent; the distribution of \( l^\tau \hat{\beta} \) is \( N(l^\tau \beta, \sigma^2 l^\tau (Z^\tau Z)^{-1}) \); and \( (n-r)\hat{\sigma}^2 / \sigma^2 \) has the chi-square distribution \( \chi^2_{n-r} \).

**Example 3.15.**

In Examples 3.12-3.14, UMVUE's of estimable \( l^\tau \beta \) are the LSE's \( l^\tau \hat{\beta} \), under assumption A1. In Example 3.13,

\[
SSR = \sum_{i=1}^{m} \sum_{j=1}^{n_i} (X_{ij} - \bar{X}_i)^2;
\]

in Example 3.14, if \( c > 1 \),

\[
SSR = \sum_{i=1}^{a} \sum_{j=1}^{b} \sum_{k=1}^{c} (X_{ijk} - \bar{X}_{ij})^2.
\]
Thus, we have proved the following result.

**Theorem 3.8.**
Consider model (1) with assumption A1. For any estimable parameter $l^\tau \beta$, the UMVUE’s $l^\tau \widehat{\beta}$ and $\widehat{\sigma}^2$ are independent; the distribution of $l^\tau \widehat{\beta}$ is $N(l^\tau \beta, \sigma^2 l^\tau (Z^\tau Z)^{-1} l)$; and $(n - r)\widehat{\sigma}^2 / \sigma^2$ has the chi-square distribution $\chi^2_{n-r}$.

**Example 3.15.**
In Examples 3.12-3.14, UMVUE’s of estimable $l^\tau \beta$ are the LSE’s $l^\tau \widehat{\beta}$, under assumption A1. In Example 3.13,

$$SSR = \sum_{i=1}^{m} \sum_{j=1}^{n_i} (X_{ij} - \bar{X}_{i.})^2;$$

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$$SSR = \sum_{i=1}^{a} \sum_{j=1}^{b} \sum_{k=1}^{c} (X_{ijk} - \bar{X}_{ij.})^2.$$
Non normal assumptions

We now study properties of $l^\tau \hat{\beta}$ and $\hat{\sigma}^2$ under assumption A2, i.e., without the normality assumption on $\varepsilon$.

- From Theorem 3.6 and the proof of Theorem 3.7(ii), $l^\tau \hat{\beta}$ (with an $l \in \mathcal{R}(Z)$) and $\hat{\sigma}^2$ are still unbiased without normality.
- In what sense are $l^\tau \hat{\beta}$ and $\hat{\sigma}^2$ optimal beyond being unbiased?
- We have the following result for the LSE $l^\tau \hat{\beta}$.
- Some discussion about $\hat{\sigma}^2$ can be found in Rao (1973, p. 228).

Theorem 3.9

Consider model (1) with assumption A2.

(i) A necessary and sufficient condition for the existence of a linear unbiased estimator of $l^\tau \beta$ (i.e., an unbiased estimator that is linear in $X$) is $l \in \mathcal{R}(Z)$.

(ii) (Gauss-Markov theorem). If $l \in \mathcal{R}(Z)$, then the LSE $l^\tau \hat{\beta}$ is the best linear unbiased estimator (BLUE) of $l^\tau \beta$ in the sense that it has the minimum variance in the class of linear unbiased estimators of $l^\tau \beta$. 
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(i) The sufficiency has been established in Theorem 3.6. Suppose now a linear function of $X$, $c^\tau X$ with $c \in \mathbb{R}^n$, is unbiased for $l^\tau \beta$. Then

$$l^\tau \beta = E(c^\tau X) = c^\tau EX = c^\tau Z\beta.$$  

Since this equality holds for all $\beta$, $l = Z^\tau c$, i.e., $l \in \mathcal{R}(Z)$.

(ii) Let $l \in \mathcal{R}(Z) = \mathcal{R}(Z^\tau Z)$.

- Then $l = (Z^\tau Z)\zeta$ for some $\zeta$ and $l^\tau \hat{\beta} = \zeta^\tau (Z^\tau Z)\hat{\beta} = \zeta^\tau Z^\tau X$ by $Z^\tau Z\hat{\beta} = Z^\tau X$.
- Let $c^\tau X$ be any linear unbiased estimator of $l^\tau \beta$.

From the proof of (i), $Z^\tau c = l$, and

$$\text{Cov}(\zeta^\tau Z^\tau X, c^\tau X - \zeta^\tau Z^\tau X) = E(X^\tau Z\zeta c^\tau X) - E(X^\tau Z\zeta \zeta^\tau Z^\tau X)$$

$$= \sigma^2 \text{tr}(Z\zeta c^\tau) + \beta^\tau Z^\tau Z\zeta c^\tau Z\beta$$

$$- \sigma^2 \text{tr}(Z\zeta \zeta^\tau Z^\tau) - \beta^\tau Z^\tau Z\zeta \zeta^\tau Z^\tau Z\beta$$

$$= \sigma^2 \zeta^\tau l + (l^\tau \beta)^2 - \sigma^2 \zeta^\tau l - (l^\tau \beta)^2$$

$$= 0.$$
Proof of (ii) continue ........

Hence

\[ \text{Var}(c^\tau X) = \text{Var}(c^\tau X - \zeta^\tau Z^\tau X + \zeta^\tau Z^\tau X) \]
\[ = \text{Var}(c^\tau X - \zeta^\tau Z^\tau X) + \text{Var}(\zeta^\tau Z^\tau X) \]
\[ + 2 \text{Cov}(\zeta^\tau Z^\tau X, c^\tau X - \zeta^\tau Z^\tau X) \]
\[ = \text{Var}(c^\tau X - \zeta^\tau Z^\tau X) + \text{Var}(l^\tau \hat{\beta}) \]
\[ \geq \text{Var}(l^\tau \hat{\beta}). \]