Classical linear model*

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1. Model-free linear regression and ordinary least squares

1.1. Notations

We wish to explain or predict a variable y through k other $x_1, x_2, ..., x_k$. We T observations on each variable:

$$y = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_T \end{pmatrix} : \text{dependent variable (to explain)}$$

$$x_i = \begin{pmatrix} x_{1i} \\ x_{2i} \\ \vdots \\ x_{Ti} \end{pmatrix}, \quad i = 1, \dots, k : \text{explanatory variables.}$$

Usually, the explanatory variables are represented by the $T \times k$ matrix

$$X = [x_1, x_2, \dots, x_k] = \begin{bmatrix} x_{11} & x_{12} & \cdots & x_{1k} \\ x_{21} & x_{22} & \cdots & x_{2k} \\ \vdots & \vdots & & \vdots \\ x_{T1} & x_{T2} & \cdots & x_{Tk} \end{bmatrix} = \begin{bmatrix} X'_1 \\ X'_2 \\ \vdots \\ X'_T \end{bmatrix},$$

where X_t is a $k \times 1$ vector:

$$X'_{t} = (x_{t1}, x_{t2}, \dots, x_{tk}), \quad t = 1, \dots, T.$$

We wish to represent each observation y_t as a function of x_{t1}, \ldots, x_{tk} :

$$y_t = x_{t1}\beta_1 + x_{t2}\beta_2 + \dots + x_{tk}\beta_k + \varepsilon_t, \quad t = 1,\dots, T$$
 (1.1)

where ε_t is a "residual" which is left unexplained by the explanatory variables. This model can also be written in the following matrix form:

$$y = X\beta + \varepsilon \tag{1.2}$$

where $\varepsilon = (\varepsilon_1, \varepsilon_2, \dots, \varepsilon_T)'$.

1.2. The least squares problem

1.2.1 In general, we cannot obtain a "perfect fit" ($\varepsilon_t = 0$, t = 1, ..., T). In view of this, a natural approach (proposed by Gauss) consists in minimizing the sum of squared residuals:

$$\sum_{t=1}^{T} \varepsilon_t^2 = \sum_{t=1}^{T} \left[y_t - x_{t1} \beta_1 - \dots - x_{tk} \beta_k \right]^2$$
$$= (y - X\beta)' (y - X\beta) \equiv S(\beta) .$$

We consider the problem:

$$\min_{\beta} (y - X\beta)' (y - X\beta) .$$

Since

$$S(\beta) = (y' - \beta'X')(y - X\beta) = y'y - 2\beta'X'y + \beta'X'X\beta,$$

we have:

$$\frac{\partial S(\beta)}{\partial \beta} = -2X'y + 2X'X\beta.$$

To compute the above, we use the following result on differentiation with respect to a vector x:

$$\frac{\partial (x'a)}{\partial x} = a, (1.3)$$

$$\frac{\partial (x'Ax)}{\partial x} = (A+A')x. \tag{1.4}$$

For any point $\beta = \hat{\beta}$ such that $S(\beta)$ is a minimum, we must have:

$$\frac{\partial S(\beta)}{\partial \beta} \mid_{\beta = \hat{\beta}} = -2X'y + 2X'X\hat{\beta} = 0$$

hence

$$(X'X) \hat{\beta} = X'y$$
: normal equations.

1.2.2 When rank(X) = k, we must have rank(X'X) = k so that $(X'X)^{-1}$ exists. In this case, the normal equations have a unique solution:

$$\hat{\boldsymbol{\beta}} = (X'X)^{-1}X'y. \tag{1.5}$$

Once $\hat{oldsymbol{eta}}$ is known, we can compute the "fitted values" and the "residuals" of the model.

1.2.3 The model fitted values are

$$\hat{y} = X\hat{\beta} = X(X'X)^{-1}X'y = Py,$$

where

$$P = X(X'X)^{-1}X'$$
 (projection matrix)
 $P' = P, PP = P$ (symmetric idempotent matrix).

1.2.4 The model residuals are:

$$\hat{\varepsilon} = y - X\hat{\beta} = y - \hat{y} = y - Py = (I - P)y = My$$

where

$$PX = X, MX = 0, (1.6)$$

$$PM = P(I-P) = 0, MP = 0.$$
 (1.7)

1.2.5 Each column of M is orthogonal with each column of X:

$$X'M = 0,$$

$$x'_i M = 0, \quad i = 1, \dots, k.$$

Residuals and regressors are orthogonal:

$$X'\hat{\varepsilon} = X'My = 0$$

 $\Rightarrow x_i'\hat{\varepsilon} = 0, \quad i = 1, ..., k$
 $\Rightarrow i_T'\hat{\varepsilon} = \sum_{t=1}^T \hat{\varepsilon}_t = 0, \quad \text{if the matrix } X \text{ contains a constant.}$

where $\hat{\mathbf{\epsilon}} = (\hat{\mathbf{\epsilon}}_1, \hat{\mathbf{\epsilon}}_2, ..., \hat{\mathbf{\epsilon}}_T)'$ et $i_T = (1, 1, ..., 1)'$.

1.2.6 Fitted values and residuals are orthogonal:

$$\hat{\mathbf{y}}'\hat{\boldsymbol{\varepsilon}} = \mathbf{y}'PM\mathbf{y} = 0. \tag{1.8}$$

1.2.7 The vector *y* can be decomposed as the sum of two orthogonal vectors:

$$y = Py + (I - P)y = \hat{y} + \hat{\varepsilon}.$$
 (1.9)

1.2.8 For any vector β ,

$$S(\beta) \equiv (y - X\beta)'(y - X\beta) = (y - X\hat{\beta})'(y - X\hat{\beta}) + (\hat{\beta} - \beta)'X'X(\hat{\beta} - \beta)$$

$$\geq (y - X\hat{\beta})'(y - X\hat{\beta}) = S(\hat{\beta})$$

for

$$(y-X\beta)'(y-X\beta) = [y-X\hat{\beta}+X(\hat{\beta}-\beta)]'[y-X\hat{\beta}+X(\hat{\beta}-\beta)]$$

$$= \left[\hat{\varepsilon} + X \left(\hat{\beta} - \beta \right) \right]' \left[\hat{\varepsilon} + X \left(\hat{\beta} - \beta \right) \right]$$

$$= \hat{\varepsilon}' \hat{\varepsilon} + 2 \left(\hat{\beta} - \beta \right)' X' \hat{\varepsilon} + \left(\hat{\beta} - \beta \right)' X' X \left(\hat{\beta} - \beta \right)$$

$$= \hat{\varepsilon}' \hat{\varepsilon} + \left(\hat{\beta} - \beta \right)' X' X \left(\hat{\beta} - \beta \right) .$$

This directly verifies that $\beta = \hat{\beta}$ minimizes $S(\beta)$.

2. Classical linear model

In order to establish the statistical properties of $\hat{\beta}$, we need assumptions on X and ε . The following assumptions define the *classical linear model* (CLM).

2.1 Assumption $y = X\beta + \varepsilon$

where y is a $T \times 1$ vector of observations on a dependent variable,

X is a $T \times k$ matrix of observations on explanatory variables,

 β is a $k \times 1$ vector of fixed parameters,

 ε is a $T \times 1$ vector of random disturbances.

2.2 Assumption $E(\varepsilon) = 0$.

2.3 Assumption $E[\varepsilon \varepsilon'] = \sigma^2 I_T$.

2.4 Assumption *X* is fixed (non-stochastic).

2.5 Assumption $\operatorname{rank}(X) = k < T$.

From the assumption 2.1 - 2.4, we see that:

$$E(y) = E(y|X) = X\beta = \begin{pmatrix} X_1'\beta \\ \vdots \\ X_T'\beta \end{pmatrix}$$

$$= (x_1, x_2, \dots, x_k) \begin{pmatrix} \beta_1 \\ \beta_2 \\ \vdots \\ \beta_k \end{pmatrix}$$

$$= x_1\beta_1 + x_2\beta_2 + \dots + x_k\beta_k,$$

$$V(y) = V(y|X) = \sigma^2 I_T$$

$$= \begin{bmatrix} \sigma^2 & 0 & \cdots & 0 \\ 0 & \sigma^2 & \cdots & 0 \\ \vdots & \vdots & & \vdots \\ 0 & 0 & \cdots & \sigma^2 \end{bmatrix} = V(\varepsilon) .$$

If, furthermore, we add the assumption that ε follows a multinormal (or Gaussian) distribution, we get the normal classical linear model (NCLM).

2.6 Assumption ε follows a multinormal distribution.

3. Linear unbiased estimation

From the assumptions 2.1 - 2.5, we can make the following observations.

3.1 $\hat{\beta}$ is linear with respect to y.

PROOF $\hat{\beta}$ has the form $\hat{\beta} = Ay$, where $A = (X'X)^{-1}X'$ is a non-stochastic matrix.

3.2
$$\hat{\beta} = (X'X)^{-1}X'(X\beta + \varepsilon) = \beta + (X'X)^{-1}X'\varepsilon$$
.

3.3 $\hat{\beta}$ is an unbiased estimator of β .

PROOF
$$E(\hat{\beta}) = \beta + (X'X)^{-1}X'E(\varepsilon) = \beta$$
.

3.4
$$V(\hat{\beta}) = \sigma^2 (X'X)^{-1}$$
.

PROOF

$$\begin{split} \mathsf{V}(\hat{\beta}) &= \mathsf{E}\big[\big(\hat{\beta} - \beta\big)\big(\hat{\beta} - \beta\big)'\big] \\ &= \mathsf{E}\big[\big(X'X\big)^{-1}X'\varepsilon\varepsilon'X\big(X'X\big)^{-1}\big] \\ &= \big(X'X\big)^{-1}X'\mathsf{E}\big(\varepsilon\varepsilon'\big)X\big(X'X\big)^{-1} \\ &= \sigma^2\big(X'X\big)^{-1} \end{split}$$

where the last identity follows from Assumption 2.3.

3.5 Theorem Gauss-Markov theorem. $\hat{\beta}$ is the best estimator of β in the class of linear linear unbiased estimators (BLUE) of β , i.e. $V(\tilde{\beta}) - V(\hat{\beta})$ is a positive semidefinite matrix for any linear unbiased estimator (LUE) $\tilde{\beta}$ of β . In particular, if $\tilde{\beta} = Cy$ and $D = C - (X'X)^{-1}X'$, then

$$V(\tilde{\boldsymbol{\beta}}) = V(\hat{\boldsymbol{\beta}}) + \sigma^2 DD'$$
.

PROOF Since $\tilde{\beta}$ is unbiased and

$$C = D + (X'X)^{-1}X',$$

we have:

$$\begin{split} \mathsf{E}\big(\tilde{\boldsymbol{\beta}}\big) &= \mathsf{E}\left\{\left[D + \big(X'X\big)^{-1}X'\right](X\boldsymbol{\beta} + \boldsymbol{\varepsilon})\right\} \\ &= DX\boldsymbol{\beta} + \boldsymbol{\beta} \\ &= \boldsymbol{\beta} \;, \end{split}$$

hence

$$DX = 0$$
 and $CX = I_k$.

Consequently,

$$\tilde{\beta} = Cy = CX\beta + C\varepsilon = \beta + C\varepsilon$$

and

$$\tilde{\beta} - \beta = C\varepsilon$$
,

hence

$$\begin{split} \mathsf{V}\big(\tilde{\boldsymbol{\beta}}\big) &= \mathsf{E}\big[\big(\tilde{\boldsymbol{\beta}} - \boldsymbol{\beta}\big)\big(\tilde{\boldsymbol{\beta}} - \boldsymbol{\beta}\big)'\big] = \mathsf{E}\left[\boldsymbol{C}\boldsymbol{\varepsilon}\boldsymbol{\varepsilon}'\boldsymbol{C}'\right] = \sigma^2\boldsymbol{C}\boldsymbol{C}' \\ &= \sigma^2\big[\boldsymbol{D} + \big(\boldsymbol{X}'\boldsymbol{X}\big)^{-1}\boldsymbol{X}'\big]\big[\boldsymbol{D}' + \boldsymbol{X}\big(\boldsymbol{X}'\boldsymbol{X}\big)^{-1}\big] \\ &= \sigma^2\big[\boldsymbol{D}\boldsymbol{D}' + \big(\boldsymbol{X}'\boldsymbol{X}\big)^{-1}\big] = \sigma^2\boldsymbol{D}\boldsymbol{D}' + \sigma^2\left(\boldsymbol{X}'\boldsymbol{X}\right)^{-1} \\ &= \sigma^2\boldsymbol{D}\boldsymbol{D}' + \mathsf{V}\big(\hat{\boldsymbol{\beta}}\big) \end{split}$$

and

$$V(\tilde{\beta}) - V(\hat{\beta}) = \sigma^2 DD' \tag{3.1}$$

is a positive semidefinite matrix.

3.6 Corollary Let w be a $k \times 1$ vector of constants. Then,

$$V(w'\tilde{\boldsymbol{\beta}}) \geq V(w'\hat{\boldsymbol{\beta}})$$

for any linear unbiased estimator $\tilde{\beta}$ of β .

PROOF Since $E(\tilde{\beta}) = E(\hat{\beta}) = \beta$, we have:

$$\begin{split} \mathsf{E}\left(w'\tilde{\pmb{\beta}}\right) &= \mathsf{E}\left(w'\hat{\pmb{\beta}}\right) = w'\pmb{\beta}\,, \\ \mathsf{V}\left(w'\tilde{\pmb{\beta}}\right) &= w'\mathsf{V}\left(\tilde{\pmb{\beta}}\right)w = w'\left[\sigma^2DD' + \mathsf{V}\left(\hat{\pmb{\beta}}\right)\right]w \\ &= \sigma^2w'DD'w + w'\mathsf{V}\left(\hat{\pmb{\beta}}\right)w \end{split}$$

$$= \sigma^2 w' D D' w + V \left(w' \hat{\beta} \right) \ge V \left(w' \hat{\beta} \right) ,$$

for $w'DD'w \ge 0$.

In particular, we must have:

$$V(\tilde{\beta}_i) \ge V(\hat{\beta}_i)$$
, $i = 1, ...k$.

3.7 Theorem GENERALIZED GAUSS-MARKOV THEOREM. Let L be a $r \times k$ fixed matrix and $\gamma = L\beta$. Then $\hat{\gamma} = L\hat{\beta}$ is the BLUE γ , i.e. $V(\tilde{\gamma}) - V(\hat{\gamma})$ is a positive semidefinite matrix for any linear unbiased estimator $\tilde{\gamma}$ of γ . In particular, if $\tilde{\gamma} = Cy$ and $D = C - L(X'X)^{-1}X'$, then

$$V(\tilde{\gamma}) = V(\hat{\gamma}) + \sigma^2 DD'$$

and

$$\mathsf{C}\left(\tilde{\gamma}-\hat{\gamma},\hat{\gamma}\right)=0\;.$$

PROOF Since $\tilde{\gamma}$ is unbiased and

$$C = D + L(X'X)^{-1}X'$$

we have

$$E(\tilde{\gamma}) = E\{(D+L(X'X)^{-1}X'](X\beta+\varepsilon)\}$$

$$= DX\beta+L\beta=DX\beta+\gamma$$

$$= \gamma,$$

hence

$$DX = 0$$
 and $CX = L$.

Consequently,

$$\tilde{\gamma} = Cy = CX\beta + C\varepsilon$$

$$= L\beta + C\varepsilon = \gamma + C\varepsilon$$

and

$$\begin{split} \mathsf{V}\left(\tilde{\gamma}\right) &= \mathsf{E}\left[\left(\tilde{\gamma} - \gamma\right)\left(\tilde{\gamma} - \gamma\right)'\right] = \mathsf{E}\left[C\varepsilon\varepsilon'C'\right] = \sigma^2CC' \\ &= \sigma^2\left[D + L\left(X'X\right)^{-1}X'\right]\left[D' + X\left(X'X\right)^{-1}L'\right] \\ &= \sigma^2\left[DD' + L\left(X'X\right)^{-1}L'\right] \\ &= \sigma^2DD' + \sigma^2L\left(X'X\right)^{-1}L' = \sigma^2DD' + \mathsf{V}\left(L\hat{\beta}\right) \\ &= \sigma^2DD' + \mathsf{V}\left(\hat{\gamma}\right)\,, \end{split}$$

so

$$V(\tilde{\gamma}) - V(\hat{\gamma}) = \sigma^2 DD' \tag{3.2}$$

is a positive semidefinite matrix, and

$$C(\tilde{\gamma}, \hat{\gamma}) = E[C\varepsilon\varepsilon'X(X'X)^{-1}L']$$

$$= \sigma^{2}CX(X'X)^{-1}L' = \sigma^{2}L(X'X)^{-1}L' = V(\hat{\gamma}),$$

$$C(\tilde{\gamma} - \hat{\gamma}, \hat{\gamma}) = C(\tilde{\gamma}, \hat{\gamma}) - C(\hat{\gamma}, \hat{\gamma}) = V(\hat{\gamma}) - V(\hat{\gamma}) = 0.$$
(3.3)

3.8 Corollary QUADRATIC GAUSS-MARKOV OPTIMALITY. Let Q be a $r \times r$ positive semidefinite fixed matrix and L a $r \times k$ fixed matrix, $\gamma = L\beta$ and $\hat{\gamma} = L\hat{\beta}$. Then

$$\mathsf{E} \big[\big(\tilde{\gamma} - \gamma \big)' Q \big(\tilde{\gamma} - \gamma \big) \big] \ge \mathsf{E} \big[\big(\hat{\gamma} - \gamma \big)' Q \big(\hat{\gamma} - \gamma \big) \big]$$

for any linear unbiased estimator $\tilde{\gamma}$ of γ .

PROOF Let $\tilde{\gamma} = C\gamma$ and $D = C - L(X'X)^{-1}X'$. Then

$$\begin{split} \mathsf{E}\big[\big(\tilde{\gamma}-\gamma\big)'Q\big(\tilde{\gamma}-\gamma\big)\big] &= \mathsf{E}\big[\mathrm{tr}\,Q\,(\tilde{\gamma}-\gamma)\,(\tilde{\gamma}-\gamma)'\big] \\ &= \mathsf{tr}\,Q\mathsf{E}\big[\big(\tilde{\gamma}-\gamma\big)\,(\tilde{\gamma}-\gamma)'\big] \\ &= \mathsf{tr}\,Q\,\big[\sigma^2DD'+\mathsf{V}\,(\hat{\gamma})\big] \\ &= \sigma^2\mathsf{tr}\,\big(QDD'\big)+\mathsf{tr}\,\big[Q\mathsf{V}\,(\hat{\gamma})\big] \\ &= \sigma^2\mathsf{tr}\,\big(D'QD\big)+\mathsf{tr}\,Q\mathsf{E}\big[\big(\hat{\gamma}-\gamma\big)\,(\hat{\gamma}-\gamma)'\big] \\ &= \sigma^2\mathsf{tr}\,\big(D'QD\big)+\mathsf{E}\big[\mathsf{tr}\,(\hat{\gamma}-\gamma)'\,Q\,(\hat{\gamma}-\gamma)\big] \\ &= \sigma^2\mathsf{tr}\,\big(D'QD\big)+\mathsf{E}\big[\big(\hat{\gamma}-\gamma\big)'\,Q\,(\hat{\gamma}-\gamma\big)\big] \\ &\geq \mathsf{E}\big[\big(\hat{\gamma}-\gamma\big)'\,Q\,(\hat{\gamma}-\gamma\big)\big] \end{split}$$

since Q is p.s.d. $\Rightarrow D'QD$ is p.s.d. $\Rightarrow \operatorname{tr} D'QD \geq 0$.

3.9 Corollary For any LUE of $\tilde{\gamma}$ of $\gamma = L\beta$,

$$\operatorname{tr} V(\tilde{\gamma}) \geq \operatorname{tr} V(\hat{\gamma})$$
.

PROOF

$$\operatorname{tr} \mathsf{V}\left(\tilde{\gamma}\right) \ = \ \operatorname{tr} \mathsf{E} \left[\left(\tilde{\gamma} - \gamma\right) \left(\tilde{\gamma} - \gamma\right)' \right] = \mathsf{E} \left[\operatorname{tr} \left(\tilde{\gamma} - \gamma\right) \left(\tilde{\gamma} - \gamma\right)' \right]$$

$$= \ \mathsf{E}\big[\left(\tilde{\gamma} - \gamma\right)'(\tilde{\gamma} - \gamma)\big] \ge \mathsf{E}\big[\left(\hat{\gamma} - \gamma\right)'(\hat{\gamma} - \gamma)\big] = \operatorname{tr}\mathsf{V}\left(\hat{\gamma}\right)$$

by Corollary 3.8 with Q = I.

3.10 Lemma PROPERTIES OF MATRIX DOMINANCE. If A = B + C where B is a p.d. matrix and C is a p.s.d. matrix, then

- (a) A is p.d.,
- (b) $|B| \leq |A|$,
- (c) $B^{-1} A^{-1}$ is p.s.d.

3.11 Corollary Let L be an $r \times k$ fixed matrix, $\gamma = L\beta$ and $\hat{\gamma} = L\hat{\beta}$. Then

$$|V(\tilde{\gamma})| \ge |V(\hat{\gamma})|$$

for any LUE $\tilde{\gamma}$ of γ .

PROOF Since $\hat{\gamma}$ is the BLUE of γ (by the generalized Gauss-Markov theorem), we have:

$$V(\tilde{\gamma}) = V(\hat{\gamma}) + C \tag{3.4}$$

where *C* is p.s.d. If $|V(\hat{\gamma})| = 0$, then $|V(\hat{\gamma})| \le |V(\tilde{\gamma})|$, for car $|V(\tilde{\gamma})| \ge 0$. If $|V(\hat{\gamma})| > 0$, then $V(\hat{\gamma})$ is p.d. This entails that $V(\tilde{\gamma})$ is also p.d. and $|V(\hat{\gamma})| \le |V(\tilde{\gamma})|$.

3.12 $\hat{y} = X\beta + P\varepsilon$, $\hat{\varepsilon} = My = M\varepsilon$.

PROOF

$$\hat{y} = Py = P[X\beta + \varepsilon] = X\beta + P\varepsilon$$
, car $PX = X$,
 $\hat{\varepsilon} = My = M[X\beta + \varepsilon] = M\varepsilon$, car $MX = 0$.

3.13 $E(\hat{y}) = X\beta$, $E(\hat{\varepsilon}) = 0$.

PROOF

$$\begin{split} \mathsf{E}\left(\hat{\gamma}\right) &= \mathsf{E}\left[X\boldsymbol{\beta} + P\boldsymbol{\varepsilon}\right] = X\boldsymbol{\beta} + P\mathsf{E}\left(\boldsymbol{\varepsilon}\right) = X\boldsymbol{\beta} \;, \\ \mathsf{E}\left(\hat{\boldsymbol{\varepsilon}}\right) &= \mathsf{E}\left(\boldsymbol{y} - \hat{\boldsymbol{y}}\right) = X\boldsymbol{\beta} - X\boldsymbol{\beta} = 0 \;. \end{split}$$

3.14
$$V(\hat{y}) = \sigma^2 P$$
, $V(\hat{\varepsilon}) = \sigma^2 M$.

PROOF

$$\begin{split} \mathsf{V}\left(\hat{y}\right) &=& \mathsf{V}\left(X\hat{\boldsymbol{\beta}}\right) = X \mathsf{V}\left(\hat{\boldsymbol{\beta}}\right) X' = \sigma^2 X \left(X'X\right)^{-1} X' = \sigma^2 P \;, \\ \mathsf{V}\left(\hat{\boldsymbol{\epsilon}}\right) &=& \mathsf{V}\left(My\right) = M \mathsf{V}\left(y\right) M' = \sigma^2 M \;. \end{split}$$

3.15 \hat{y} is the best linear unbiased estimator of $X\beta$.

PROOF This follows directly on taking L = X in the generalized Gauss-Markov theorem.

3.16 $\hat{\varepsilon}$ is the best linear unbiased estimator (BLUE) of ε , in the sense that $E(\hat{\varepsilon} - \varepsilon) = 0$ and

$$V(\tilde{\epsilon} - \epsilon) - V(\hat{\epsilon} - \epsilon)$$
 is a p.s.d. matrix

for for LUE $\tilde{\epsilon}$ of ϵ .

PROOF Since $\tilde{\varepsilon}$ is a LUE of ε , we must have:

$$\tilde{\varepsilon} = Ay$$
 and $\mathsf{E}(\tilde{\varepsilon} - \varepsilon) = 0$.

Consequently,

$$E(\tilde{\varepsilon}) = E(Ay)$$

$$= E[A(X\beta + \varepsilon)] = AX\beta = 0, \forall \beta,$$

which entails that

$$AX = 0$$
,
$$\tilde{\varepsilon} = A(X\beta + \varepsilon) = A\varepsilon$$
.

Let

$$B = A - M$$
 where $M = I - X(X'X)^{-1}X'$.

Then

$$AX = [B+M]X = BX = 0$$
, since $MX = 0$,

hence

$$V(\tilde{\varepsilon} - \varepsilon) = V[A\varepsilon - \varepsilon]$$

$$= V[(B+M)\varepsilon - \varepsilon] = V[(B+M-I)\varepsilon]$$

$$= E[(B+M-I)\varepsilon\varepsilon'(B'+M-I)]$$

$$= \sigma^{2}[B-X(X'X)^{-1}X'][B'-X(X'X)^{-1}X']$$

$$= \sigma^{2}[BB'+X(X'X)^{-1}X'],$$

and

$$\begin{split} \mathsf{V}\left(\hat{\boldsymbol{\varepsilon}} - \boldsymbol{\varepsilon}\right) &= \mathsf{E}\left[\left(M - I\right)\boldsymbol{\varepsilon}\boldsymbol{\varepsilon}'\left(M - I\right)\right] \\ &= \sigma^{2}\left(I - M\right) = \sigma^{2}X\left(X'X\right)^{-1}X'\,, \end{split}$$

so that

$$V\left(\tilde{\boldsymbol{\varepsilon}}-\boldsymbol{\varepsilon}\right)=\sigma^{2}\textit{BB}'+V\left(\hat{\boldsymbol{\varepsilon}}-\boldsymbol{\varepsilon}\right)\;.\label{eq:epsilon}$$

Thus

$$V(\tilde{\varepsilon} - \varepsilon) - V(\hat{\varepsilon} - \varepsilon) = \sigma^2 B B'$$

a p.s.d. matrix.

3.17 $C(\hat{\boldsymbol{\beta}}, \hat{\boldsymbol{\varepsilon}}) = C(\hat{\boldsymbol{\beta}}, y - X\hat{\boldsymbol{\beta}}) = 0.$

PROOF

$$\begin{split} \mathsf{C}\big(\hat{\beta}\,,\hat{\varepsilon}\big) &=& \mathsf{E}\big[\big(\hat{\beta}-\beta\big)\hat{\varepsilon}'\big] = \mathsf{E}[\,\big(X'X\big)^{-1}X'\varepsilon\varepsilon'M] \\ &=& \sigma^2\,\big(X'X\big)^{-1}X'M = 0 \;. \end{split}$$

3.18 $C(\hat{y}, \hat{\varepsilon}) = 0.$

PROOF

$$\begin{array}{lcl} \mathsf{C}\left(\hat{y},\hat{\pmb{\varepsilon}}\right) & = & \mathsf{E}\left[\left(X\hat{\pmb{\beta}} - X\pmb{\beta}\right)\hat{\pmb{\varepsilon}}'\right] \\ & = & X\,\mathsf{E}\left[\left(\hat{\pmb{\beta}} - \pmb{\beta}\right)\hat{\pmb{\varepsilon}}'\right] = X\,\mathsf{C}\left(\hat{\pmb{\beta}},\hat{\pmb{\varepsilon}}\right) = 0\;. \end{array}$$

3.19 Estimation of σ^2 . Since $\sigma^2 = E(\varepsilon_t^2)$, t = 1, ..., T, it is natural to consider the residuals of the regression which can be viewed as estimations of the error terms ε_t :

$$\hat{\varepsilon} = y - X\hat{\beta} = My = M(X\beta + \varepsilon) = M\varepsilon$$
,

$$\sum_{t=1}^{T} \hat{\varepsilon}_{t}^{2} = \hat{\varepsilon}' \hat{\varepsilon} = \varepsilon' M' M \varepsilon = \varepsilon' M \varepsilon ,$$

hence

$$\begin{split} \mathsf{E}\left[\hat{\varepsilon}'\hat{\varepsilon}\right] &= \mathsf{E}\left[\varepsilon' M \varepsilon\right] = \mathsf{E}\left[\operatorname{tr}\left(\varepsilon' M \varepsilon\right)\right] \\ &= \mathsf{E}\left[\operatorname{tr}\left(M \varepsilon \varepsilon'\right)\right] = \operatorname{tr}\left[M \mathsf{E}\left(\varepsilon \varepsilon'\right)\right] \\ &= \sigma^2 \operatorname{tr} M \,, \end{split}$$

where

$$\operatorname{tr} M = \operatorname{tr} \left[I_T - X \left(X'X \right)^{-1} X' \right] = \operatorname{tr} I_T - \operatorname{tr} \left[X \left(X'X \right)^{-1} X' \right]$$

$$= \operatorname{tr} I_T - \operatorname{tr} \left[X'X \left(X'X \right)^{-1} \right] = \operatorname{tr} I_T - \operatorname{tr} I_k$$

$$= T - k.$$

Thus,

$$\begin{split} \mathsf{E}\big(\hat{\varepsilon}'\hat{\varepsilon}\big) &=& \sigma^2 \left(T-k\right) \\ \mathsf{E}\left[\frac{\hat{\varepsilon}'\hat{\varepsilon}}{T-k}\right] &=& \sigma^2 \; . \end{split}$$

3.20 The statistic

$$s^{2} = \hat{\varepsilon}'\hat{\varepsilon}/(T-k) = y'My/(T-k)$$

is an unbiased estimator of σ^2 , and $s^2(X'X)^{-1}$ is an unbiased estimator of $V\left(\hat{\beta}\right) = \sigma^2(X'X)^{-1}$:

$$\begin{array}{rcl} \mathsf{E}\left(s^2\right) & = & \sigma^2\,, \\ \mathsf{E}\left[s^2\left(X'X\right)^{-1}\right] & = & \sigma^2\left(X'X\right)^{-1}\,. \end{array}$$

4. Prediction

In the previous section, we studied how one can estimate β in the linear regression model. Suppose now we know the matrix X_0 of explanatory variables for m additional periods (or observations). We wish to predict the corresponding values of y:

$$y_0 = X_0 \beta + \varepsilon_0$$

where

$$\mathsf{E}\left(arepsilon_{0}\right)=0\;,\mathsf{V}\left(arepsilon_{0}\right)=\sigma^{2}\mathit{I}_{m}\;,\mathsf{E}\left(arepsilonarepsilon_{0}^{\prime}\right)=0\;.$$

The natural "predictor" in this case is:

$$\hat{y}_0 = X_0 \hat{\beta} = X_0 (X'X)^{-1} X'y.$$
(4.1)

We can then show the following properties.

4.1 \hat{y}_0 is an unbiased estimator of $X_0\beta$:

$$\mathsf{E}(\hat{y}_0) = X_0 \beta = \mathsf{E}(y_0), \quad \mathsf{E}(\hat{y}_0 - y_0) = 0.$$

4.2
$$V(\hat{y}_0) = V(X_0\hat{\beta}) = X_0V(\hat{\beta})X'_0 = \sigma^2X_0(X'X)^{-1}X'_0.$$

4.3
$$C(y_0, \hat{y}_0) = 0.$$

PROOF

$$\begin{split} \mathsf{C}\left(y_{0},\hat{y}_{0}\right) &= \mathsf{E}\left[\left(y_{0}-X_{0}\beta\right)\left(X_{0}\hat{\beta}-X_{0}\beta\right)'\right] \\ &= \mathsf{E}\left[\varepsilon_{0}\left(\hat{\beta}-\beta\right)'X_{0}'\right] = \mathsf{E}\left[\varepsilon_{0}\varepsilon'X\left(X'X\right)^{-1}X_{0}'\right] = 0\;. \end{split}$$

4.4 \hat{y}_0 is best linear unbiased estimator of $X_0\beta$, in the sense that $V(\tilde{y}_0) - V(\hat{y}_0)$ is a p.s.d. matrix for any linear unbiased estimator \tilde{y}_0 of $X_0\beta$. In particular, if $\tilde{y}_0 = Cy$ and $D = C - X_0(X'X)^{-1}X'$, then

$$V(\tilde{y}_0) = V(\hat{y}_0) + \sigma^2 DD'.$$

PROOF This follows directly from the generalized Gauss-Markov theorem.

The "prediction errors" are given by:

$$\hat{e}_0 = y_0 - \hat{y}_0 = y_0 - X_0 \hat{\beta}$$

= $X_0 \beta + \varepsilon_0 - X_0 \hat{\beta} = \varepsilon_0 + X_0 (\beta - \hat{\beta})$.

4.5 \hat{y}_0 is a linear unbiased predictor (LUP) of y_0 :

$$\mathsf{E}\left[\hat{e}_{0}\right]=0\;.$$

PROOF $\hat{y}_0 = X_0 \hat{\beta}$ and

$$\mathsf{E}\left[\hat{e}_{0}\right] = \mathsf{E}\left[y_{0} - \hat{y}_{0}\right] = X_{0}\beta - X_{0}\beta = 0 \; .$$

4.6
$$V(\hat{e}_0) = \sigma^2 \left[I_m + X_0 (X'X)^{-1} X_0' \right].$$

PROOF

$$\begin{aligned}
\mathsf{V}(y_{0} - \hat{y}_{0}) &= \mathsf{V}(y_{0}) + \mathsf{V}(\hat{y}_{0}) - \mathsf{C}(y_{0}, \hat{y}_{0}) - \mathsf{C}(\hat{y}_{0}, y_{0}) \\
&= \sigma^{2} I_{m} + \sigma^{2} X_{0} \left(X'X\right)^{-1} X'_{0} \\
&= \sigma^{2} \left[I_{m} + X_{0} \left(X'X\right)^{-1} X'_{0}\right].
\end{aligned}$$

4.7 Theorem \hat{y}_0 is the best linear unbiased predictor (BLUP) of y_0 , in the sense that $V(y_0 - \tilde{y}_0) - V(y_0 - \hat{y}_0)$ is a p.s.d. matrix for any LUP \tilde{y}_0 of y_0 . In particular, if $\tilde{y}_0 = Cy$ and $D = C - X_0(X'X)^{-1}X'$, then

$$V(y_0 - \tilde{y}_0) = V(y_0 - \hat{y}_0) + \sigma^2 DD'$$
.

PROOF

$$V(y_0 - \tilde{y}_0) = V(y_0) + V(\tilde{y}_0) - C(y_0, \tilde{y}_0) - C(\tilde{y}_0, y_0)$$

where

$$\mathsf{C}\left(y_{0},\tilde{y}_{0}\right)=\mathsf{E}\left[\varepsilon_{0}\varepsilon'C'\right]=0$$

for, by the generalized Gauss-Markov theorem,

$$\mathsf{E}\left[\tilde{y}_{0}\right] = X_{0}\beta \Rightarrow CX = X_{0} \Rightarrow \tilde{y}_{0} = C\left(X\beta + \varepsilon\right) = X_{0}\beta + C\varepsilon$$
.

Further, $V(\tilde{y}_0) = V(\hat{y}_0) + \sigma^2 DD'$ and $V(y_0) = \sigma^2 I_m$. Consequently,

$$V(y_{0} - \tilde{y}_{0}) = \sigma^{2}I_{m} + V(\hat{y}_{0}) + \sigma^{2}DD'$$

$$= \left[\sigma^{2}I_{m} + \sigma^{2}X_{0}(X'X)^{-1}X'_{0}\right] + \sigma^{2}DD'$$

$$= V(y_{0} - \hat{y}_{0}) + \sigma^{2}DD'.$$

5. Estimation with Gaussian errors

If we wish to build confidence intervals and perform hypothesis tests, we need a more complete specification of the error distribution. The standard hypothesis for this is to assume that the errors follow a Gaussian distribution.

5.1 Assumption $\varepsilon \sim N_T \left[0, \sigma^2 I_T \right]$.

This means that the errors ε_t are i.i.d. $N\left[0,\sigma^2\right]$. We can now completely establish the distribution of the least squares estimator.

5.2
$$y \sim N[X\beta, \sigma^2 I_T]$$
, since $y = X\beta + \varepsilon$.

5.3
$$\hat{\beta} \sim N\left[\beta, \sigma^2 (X'X)^{-1}\right]$$
, since $\hat{\beta} = (X'X)^{-1} X'y$.

The probability density function of *y* is given by:

$$L(y; X\beta, \sigma^2 I_T) = \frac{1}{(2\pi\sigma^2)^{T/2}} \exp\left\{-\frac{1}{2} \frac{(y - X\beta)'(y - X\beta)}{\sigma^2}\right\}.$$

5.4 $\hat{\beta} = (X'X)^{-1}X'y$ and $\hat{\sigma}^2 = \hat{\varepsilon}'\hat{\varepsilon}/T$ are the maximum likelihood estimators of β and σ^2 respectively.

PROOF To maximize L is equivalent to maximizing ln(L). Since

$$\begin{split} \ln(L) &= -\frac{T}{2}\ln(2\pi) - \frac{T}{2}\ln(\sigma^2) - \frac{1}{2\sigma^2}(y - X\beta)'(y - X\beta) \\ &= -\frac{T}{2}\ln(2\pi) - \frac{T}{2}\ln(\sigma^2) - \frac{1}{2\sigma^2}\left[y'y - 2y'X\beta + \beta'X'X\beta\right] \;, \end{split}$$

the first-order conditions (which are necessary) for a maximum is:

$$\begin{split} \frac{\partial \left(\ln(L) \right)}{\partial \beta} &= -\frac{1}{2\sigma^2} \left[-2X'y + 2 \left(X'X \right) \beta \right] = 0 \;, \\ \frac{\partial \left(\ln(L) \right)}{\partial \sigma^2} &= -\frac{T}{2} \frac{1}{\sigma^2} + \frac{1}{2\sigma^4} \left(y - X\beta \right)' \left(y - X\beta \right) = 0 \;, \end{split}$$

hence

$$(X'X)\hat{\beta} = X'y, \hat{\beta} = (X'X)^{-1}X'y,$$

 $\hat{\sigma}^2 = (y-X\hat{\beta})'(y-X\hat{\beta})/T.$

Further the second-order derivative of ln(L) is:

$$\frac{\partial \left(\ln(L)\right)}{\partial \beta' \partial \beta} = -\frac{1}{\sigma^2} \left(X'X\right) \tag{5.1}$$

which is negative semidefinite as required for a maximum.

5.5
$$\hat{y} = X\hat{\boldsymbol{\beta}} \sim N_T \left[X\boldsymbol{\beta}, \sigma^2 P \right].$$

- **5.6** $\hat{\varepsilon} = M\varepsilon \sim N_T \left[0, \sigma^2 M\right]$.
- **5.7** $\hat{\varepsilon}$ and $\hat{\beta}$ are independent, because $\hat{\varepsilon}$ et $\hat{\beta}$ are multinormal and $C(\hat{\beta},\hat{\varepsilon})=0$.
- **5.8** $\hat{\varepsilon}$ and \hat{y} are independent, because $\hat{\varepsilon}$ and \hat{y} are multinormal and $C(\hat{y}, \hat{\varepsilon}) = 0$.
- **5.9 Lemma** DISTRIBUTION OF AN IDEMPOTENT QUADRATIC FORM IN I.I.D. GAUSSIAN VARIABLES. Let Q be a $T \times T$ symmetric idempotent matrix of rank $q \leq T$. If $\varepsilon \sim N_T \left[0, \sigma^2 I_T \right]$, then

$$\varepsilon' Q \varepsilon / \sigma^2 \sim \chi^2(q)$$
.

PROOF Since Q is a symmetric idempotent matrix, there is a $T \times T$ orthogonal matrix C, i.e. $CC' = C'C = I_T$, such that

$$CQC' = \begin{pmatrix} I_q & 0 \\ 0 & 0 \end{pmatrix}$$
,

hence

$$\varepsilon'Q\varepsilon = \varepsilon'C'CQC'C\varepsilon = (C\varepsilon)'(CQC')(C\varepsilon)$$
.

Further,

$$\begin{array}{ll} \varepsilon & \sim & N\left[0,\sigma^2I_T\right] \Rightarrow C\varepsilon \sim N\left[0,\sigma^2CI_TC'\right] \\ \Rightarrow & C\varepsilon \sim N\left[0,\sigma^2I_T\right] \ . \end{array}$$

Let $v = C\varepsilon = (v_1, v_2, \dots, v_T)'$. Then

$$v_1, v_2, \dots, v_T$$
 are i.i.d. $N\left[0, \sigma^2\right]$

and

$$\varepsilon' Q \varepsilon = v' (CQC') v
= (v_1, v_2, ..., v_T) \begin{pmatrix} I_q & 0 \\ 0 & 0 \end{pmatrix} \begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ v_T \end{bmatrix}
= v_1^2 + v_2^2 + \dots + v_q^2 + 0 . v_{q+1}^2 \dots + 0 . v_T^2
= \sum_{t=1}^q v_t^2 .$$

This entails

$$\frac{\varepsilon' Q \varepsilon}{\sigma^2} = \sum_{t=1}^q \left(\frac{v_t}{\sigma}\right)^2 ,$$

where
$$\frac{v_t}{\sigma} \stackrel{ind}{\sim} N[0,1]$$
, $t = 1,...,T$,

and

$$\varepsilon' Q \varepsilon / \sigma^2 \sim \chi^2(q)$$
.

5.10

$$\frac{S(\hat{\beta})}{\sigma^2} = \frac{\hat{\varepsilon}'\hat{\varepsilon}}{\sigma^2} \sim \chi^2(T-k) .$$

PROOF This follows directly on applying Lemma 5.9 with Q=M and the fact that ${\rm tr}\,(M)=T-k$.

5.11 Let R be a $q \times k$ fixed matrix. Then,

$$R\hat{\boldsymbol{\beta}} \sim N_q \left[R\boldsymbol{\beta}, \sigma^2 R \left(X'X \right)^{-1} R' \right]$$
 (5.2)

Further $R\hat{\beta}$ and s^2 are independent.

PROOF $\hat{\beta} \sim N\left[\beta, \sigma^2(X'X)^{-1}\right]$ entails $R\hat{\beta} \sim N\left[R\beta, \sigma^2R(X'X)^{-1}R'\right]$. Since $\hat{\beta}$ and $\hat{\epsilon}$ are independent, $R\hat{\beta}$ and $\hat{\epsilon}'\hat{\epsilon}$ are also independent, so that $R\hat{\beta}$ and $s^2 = \hat{\epsilon}'\hat{\epsilon}/(T-k)$ are independent.

5.12 Let R be a $q \times k$ fixed matrix of rank $q, r = R\beta$ and

$$S(R, \hat{\boldsymbol{\beta}}) = [R\hat{\boldsymbol{\beta}} - r]' \left[R \left(X'X \right)^{-1} R' \right]^{-1} [R\hat{\boldsymbol{\beta}} - r] .$$

Then

$$S(R,\hat{\boldsymbol{\beta}})/\sigma^2 \sim \chi^2(q)$$
 (5.3)

Further, $S(R, \hat{\beta})$ and s^2 are independent.

PROOF

$$R\hat{\boldsymbol{\beta}} - r = R\left(\hat{\boldsymbol{\beta}} - \boldsymbol{\beta}\right)$$

and

$$R\left(\hat{\boldsymbol{\beta}}-\boldsymbol{\beta}\right) \sim N_q\left[0,\sigma^2R\left(X'X\right)^{-1}R'\right] \ .$$

Thus,

$$S(R, \hat{\beta})/\sigma^2 = \left[R\left(\hat{\beta} - \beta\right)\right]' \left[\sigma^2 R\left(X'X\right)^{-1} R'\right]^{-1} \left[R\left(\hat{\beta} - \beta\right)\right]$$

 $\sim \chi^2(q)$.

6. Confidence and prediction intervals

6.1. Confidence interval for the error variance

In the normal classical linear model, we have:

$$\hat{\epsilon}'\hat{\epsilon}/\sigma^2 = (T-k)s^2/\sigma^2 \sim \chi^2(T-k)$$
.

Thus, we can find a and b such that

$$\begin{split} \mathsf{P}\left[\chi^2\left(T-k\right) > b\right] &= \frac{\alpha}{2}\,,\\ \mathsf{P}\left[\chi^2\left(T-k\right) < a\right] &= \frac{\alpha}{2}\,,\\ \mathsf{P}\left[a \leq \chi^2\left(T-k\right) \leq b\right] &= 1 - \left(\frac{\alpha}{2} + \frac{\alpha}{2}\right) = 1 - \alpha\,, \end{split}$$

which entails that

$$\begin{split} \mathsf{P}\left[a &\leq \frac{(T-k)\,s^2}{\sigma^2} \leq b\right] = 1 - \alpha \\ \mathsf{P}\left[\frac{1}{b} \leq \frac{\sigma^2}{(T-k)\,s^2} \leq \frac{1}{a}\right] = 1 - \alpha \\ \mathsf{P}\left[\frac{(T-k)\,s^2}{b} \leq \sigma^2 \leq \frac{(T-k)\,s^2}{a}\right] = 1 - \alpha \;. \end{split}$$

It is important to note this is not the smallest confidence interval for σ^2 .

6.2. Confidence interval for a linear combination of regression coefficients

Consider now the linear combination $w'\beta$. Then

$$w'\hat{\boldsymbol{\beta}} - w'\boldsymbol{\beta} \sim N\left[0, \sigma^2 w'\left(X'X\right)^{-1}w\right]$$

hence

$$\frac{w'\hat{\beta} - w'\beta}{\sigma\Lambda} \sim N[0,1]$$

where $\Delta = \sqrt{w'(X'X)^{-1}w}$. Since σ is unknown, consider:

$$t = \frac{w'\hat{\beta} - w'\beta}{s\Delta}$$

$$= \frac{w'\hat{\beta} - w'\beta}{\Delta\sigma\sqrt{\frac{s^2}{\sigma^2}}} = \frac{w'\hat{\beta} - w'\beta}{\sigma\Delta} / \sqrt{\frac{(T-k)s^2}{\sigma^2(T-k)}}$$

$$= Y/\sqrt{\frac{X}{T-k}}$$

where *X* and *Y* are independent, $Y \sim N[0,1]$ and $X \sim \chi^2(T-k)$. Thus, *t* follows a Student *t* distribution with T-k degrees of freedom:

$$t \sim t (T - k)$$

hence

$$P\left[-t_{\alpha/2} \le t\left(T - k\right) \le t_{\alpha/2}\right] = 1 - \alpha$$

where $P\left[t\left(T-k\right)>t_{lpha/2}\right]=lpha/2$ and

$$P\left[w'\hat{\beta} - t_{\alpha/2}s\Delta \le w'\beta \le w'\hat{\beta} + t_{\alpha/2}s\Delta\right] = 1 - \alpha$$
.

6.3. Confidence region for a regression coefficient vector

We now wish to build a confidence region for a vector $R\beta$ of linear combinations of the elements of β , where $R: q \times k$ and has rank q. Then

$$S(R,\hat{\boldsymbol{\beta}})/\sigma^2 = (R\hat{\boldsymbol{\beta}} - R\boldsymbol{\beta})'(R(X'X)^{-1}R')^{-1}(R\hat{\boldsymbol{\beta}} - R\boldsymbol{\beta})/\sigma^2 \sim \chi^2(q) .$$

Since σ is unknown, let us consider:

$$F = S(R, \hat{\beta})/qs^2 = \frac{S(R, \hat{\beta})/q\sigma^2}{(T-k)s^2/\sigma^2(T-k)} = \frac{X_1/q}{X_2/(T-k)}$$

where X_1 and X_2 are independent,

$$X_1 = S(R, \hat{\beta}) / \sigma^2 \sim \chi^2(q) ,$$

 $X_2 = (T - k) s^2 / \sigma^2 \sim \chi^2(T - k) .$

Thus F follows a Fisher distribution with (q, T - k) degrees of freedom:

$$F \sim F(q, T - k)$$
.

If we define F_{α} by

$$P[F(q,T-k) > F_{\alpha}] = \alpha ,$$

the set of all vectors $R\beta$ such that $F \leq F_{\alpha}$:

$$(R\hat{\boldsymbol{\beta}} - R\boldsymbol{\beta})' [R(X'X)^{-1}R']^{-1} (R\hat{\boldsymbol{\beta}} - R\boldsymbol{\beta})/qs^2 \le F_{\alpha}$$
.

is a confidence region with level $1 - \alpha$ for $R\beta$. This set is a an ellipsoid (*confidence ellipsoid*).

6.4. Prediction intervals

 $y_0 = x_0' \boldsymbol{\beta} + \boldsymbol{\varepsilon}_0$

where

$$\left(\frac{\varepsilon}{\varepsilon_0}\right) \sim N\left[0, \sigma^2 I_{T+1}\right].$$

Further

$$\hat{y}_{0} = x'_{0}\hat{\beta}, \quad \hat{\beta} = (X'X)^{-1}X'y,
\hat{y}_{0} - y_{0} = x'_{0}(\hat{\beta} - \beta) - \varepsilon_{0} \sim N\{0, \sigma^{2}[1 + x'_{0}(X'X)^{-1}x_{0}]\}.$$

hence

$$\frac{\hat{y}_0 - y_0}{\sigma \Delta_1} \sim N[0, 1] ,$$

where $\Delta_1 = \left[1 + x_0' \left(X'X\right)^{-1} x_0\right]^{1/2}$, and

$$\frac{\hat{y}_0 - y_0}{s\Delta_1} \sim t \left(T - k \right)$$

where $t_{\alpha/2}$ satisfies

$$\mathsf{P}\left[\hat{y}_0 - t_{\alpha/2} s \Delta_1 \le y_0 \le \hat{y}_0 + t_{\alpha/2} s \Delta_1\right] = 1 - \alpha \ .$$

6.5. Confidence regions for several predictions

We now consider the problem of predicting a vector of observations y_0 generated according to the same model independently of y:

$$y_0 = X_0 \boldsymbol{\beta} + \boldsymbol{\varepsilon}_0 ,$$

$$\begin{pmatrix} \boldsymbol{\varepsilon} \\ \boldsymbol{\varepsilon}_0 \end{pmatrix} \sim N \left[0, \boldsymbol{\sigma}^2 I_{T+m} \right] ,$$

where X_0 is known but y_0 is not observed. For predicting y_0 , let us define:

$$\hat{y}_0 = X_0 \hat{\beta},
\hat{e}_0 = y_0 - \hat{y}_0 = \varepsilon_0 - X_0 (\hat{\beta} - \beta),$$

where

$$\begin{split} \mathsf{E} \left(\hat{e}_{0} \right) &= 0, \\ \mathsf{V} \left(\hat{e}_{0} \right) &= \sigma^{2} \left[I_{m} + X_{0} \left(X'X \right)^{-1} X_{0}' \right] = \sigma^{2} D_{0}, \\ \hat{e}_{0} &\sim N \left[0, \sigma^{2} \left[I_{m} + X_{0} \left(X'X \right)^{-1} X_{0}' \right] \right]. \end{split}$$

Consequently,

$$\hat{e}'_0 V (\hat{e}_0)^{-1} \hat{e}_0 \sim \chi^2(m) ,$$

 $\hat{e}'_0 D_0^{-1} \hat{e}_0 / \sigma^2 \sim \chi^2(m) .$

Since σ^2 is unknown, we replace it by s^2 :

$$(T-k)s^2/\sigma^2 \sim \chi^2(T-k)$$
.

Further, since s^2 is independent of y_0 and $\hat{y}_0 = X\hat{\beta}$, s^2 is independent of \hat{e}_0 ,

$$F = \frac{\hat{e}'_0 D_0^{-1} \hat{e}_0}{ms^2} = \frac{\hat{e}'_0 D_0^{-1} \hat{e}_0 / \sigma^2 m}{(T - k) s^2 / \sigma^2 (T - k)} \sim F(m, T - k),$$

$$F = (y_0 - \hat{y}_0)' \left[I_m + X_0 \left(X' X \right)^{-1} X_0' \right]^{-1} (y_0 - \hat{y}_0) / ms^2 \sim F(m, T - k).$$

Then the set of vectors y_0 such that

$$F \leq F_{\alpha}(m, T-k)$$

is a confidence region for y_0 with level $1 - \alpha$.

7. Hypothesis tests

7.0.1 Let us now consider the problem of testing an hypothesis of the form

$$H_0: w'\beta = w_0 \tag{7.1}$$

where w be a $k \times 1$ vector of constants. To test H_0 , it is natural to consider the difference:

$$w'\hat{\boldsymbol{\beta}} - w_0 = w'\left(\hat{\boldsymbol{\beta}} - \boldsymbol{\beta}\right) \sim N\left[0, \sigma^2 w'\left(X'X\right)^{-1}w\right].$$

Under the assumptions of the Gaussian classical linear model, we then have:

$$\frac{w'\hat{\beta} - w_0}{\sigma\Delta} \sim N[0,1], \Delta = \left[w'\left(X'X\right)^{-1}w\right]^{1/2},$$

$$t = \frac{w'\hat{\beta} - w_0}{s\Delta} \sim t(T - k).$$

This suggests the following tests of H_0 :

reject
$$H_0$$
 at level α against $w'\beta - w_0 \neq 0$ when $|t| \geq t_{\alpha/2}$ (two-sided test) (7.2)

reject
$$H_0$$
 at level α against $w'\beta - w_0 > 0$ when $t \ge t_\alpha$ (one-sided test) (7.3)

reject
$$H_0$$
 at level α against $w'\beta - w_0 < 0$ when $t \le -t_\alpha$ (one-sided test). (7.4)

An important special case of the above problem consists in testing the value of any given component of β :

$$H_0(\beta_{io}): \beta_i = \beta_{io}$$

where β_i is an element of β .

Let us now consider the more general hypothesis which consists in testing the value of a general vector linear transformation of β :

$$H_0: R\beta = r = \begin{bmatrix} w'_1 \\ w'_2 \\ \vdots \\ w'_q \end{bmatrix} \beta = \begin{bmatrix} w'_1\beta \\ w'_2\beta \\ \vdots \\ w'_q\beta \end{bmatrix}$$

$$(7.5)$$

where *R* is a $q \times k$ fixed matrix with full row rank [rank(R) = q].

7.0.2 Wald-type test. A natural approach then consists in estimating $R\beta$ by $R\hat{\beta}$, and then to examine the difference $R\hat{\beta} - r$. Under H_0 ,

$$R\hat{\boldsymbol{\beta}} \sim N[r, \Sigma_R]$$
 , where $\Sigma_R = \sigma^2 R \left(X'X \right)^{-1} R'$.

We need a concept of distance between $R\hat{\beta}$ and r. By (5.3),

$$W = (R\hat{\beta} - r)'\Sigma_R^{-1}(R\hat{\beta} - r) \sim \chi^2(q)$$
 under H_0 .

We tend to reject H_0 when W is too large $(W \ge c$. However, σ^2 and Σ_R are unknown. It is then natural tom replace σ^2 by the estimate s^2 , and Σ_R by

$$\hat{\Sigma}_R = s^2 R \left(X' X \right)^{-1} R' .$$

This yields a Wald-type criterion:

$$\begin{split} \hat{W} &= (R\hat{\beta} - r)'\hat{\Sigma}_{R}^{-1}(R\hat{\beta} - r) \\ &= (R\hat{\beta} - r)'\left[s^{2}R\left(X'X\right)^{-1}R'\right]^{-1}(R\hat{\beta} - r) \\ &= (R\hat{\beta} - r)'\left[R\left(X'X\right)^{-1}R'\right]^{-1}(R\hat{\beta} - r)/s^{2} \\ &= S(R, \hat{\beta})/s^{2} \; . \end{split}$$

Since

$$F = \hat{W}/q = S(R, \hat{\beta})/qs^2 \sim F(q, T - k)$$
,

we reject H_0 at level α when

$$F > F_{\alpha}(q, T - k). \tag{7.6}$$

7.0.3 Likelihood ratio test. Another approach to testing H_0 consists in looking for a likelihood ratio test. This test is based on focusing on the likelihood function:

$$L(y;X\beta,\sigma^2I_T) = \frac{1}{(2\pi\sigma^2)^{T/2}} \exp\left\{-\frac{1}{2} \frac{(y-X\beta)'(y-X\beta)}{\sigma^2}\right\}. \tag{7.7}$$

Let

$$L(\hat{\Omega}) = \max_{\beta, \sigma^2} L = \max_{(\beta, \sigma^2) \in \Omega} L \tag{7.8}$$

i.e. we find values of β and σ^2 which maximize "the probability of the observed sample", and

$$L(\hat{\omega}) = \max_{\beta, \sigma^2} L = \max_{(\beta, \sigma^2) \in \omega} L$$

$$R\beta = r$$
(7.9)

i.e. we find values of β and σ^2 which maximize "the probability of the observed sample" and satisfy H_0 , where

$$\Omega = \left\{ \left(\beta, \sigma^2 \right) : -\infty < \beta_i < +\infty, \ i = 1, \dots, k, \ 0 < \sigma^2 < +\infty \right\},$$

$$\omega = \left\{ \left(\beta, \sigma^2 \right) \in \Omega : R\beta = r \right\}.$$

We see easily that

$$0 \le L(\hat{\boldsymbol{\omega}}) \le L(\hat{\boldsymbol{\Omega}})$$
,

hence

$$0 \le \frac{L(\hat{\Omega})}{L(\hat{\Omega})} \le 1$$
, $\frac{L(\hat{\Omega})}{L(\hat{\Omega})} \ge 1$.

We reject H_0 when

$$LR(y) \equiv \frac{L(\hat{\Omega})}{L(\hat{\omega})} \ge \lambda_{\alpha}$$

where λ_{α} depends on the level of the test:

$$P[LR(y) \ge \lambda_{\alpha}] = \alpha$$
.

7.0.4 $L(\hat{\Omega})$ is achieved when $\beta = \hat{\beta}$ and $\sigma^2 = \hat{\sigma}^2$:

$$\begin{split} L(\hat{\Omega}) &= \frac{1}{\left(2\pi\hat{\sigma}^2\right)^{T/2}} \exp\left\{-\frac{1}{2} \frac{\left(y - X\hat{\beta}\right)' \left(y - X\hat{\beta}\right)}{\hat{\sigma}^2}\right\} = \frac{1}{\left(2\pi\hat{\sigma}^2\right)^{T/2}} \exp\left\{-\frac{T}{2}\right\} \\ &= \frac{e^{-T/2}}{\left[2\pi\hat{\sigma}^2\right]^{T/2}} = \frac{T^{T/2}e^{-T/2}}{\left(2\pi\right)^{T/2} \left[\left(y - X\hat{\beta}\right)' \left(y - X\hat{\beta}\right)\right]^{T/2}} \\ &= \frac{T^{T/2}e^{-T/2}}{\left(2\pi\right)^{T/2} S_{\Omega}^{T/2}} \,, \end{split}$$

where $S_{\Omega} = \left(y - X\hat{\beta}\right)' \left(y - X\hat{\beta}\right)$.

7.0.5 To find $L(\hat{\omega})$, it is equivalent to maximize

$$\ln(L) = -\frac{T}{2}\ln(2\pi) - \frac{T}{2}\ln(\sigma^2) - \frac{1}{2\sigma^2}(y - X\beta)'(y - X\beta)$$

under the constraint $R\beta = r$. Consider σ^2 as given. It is then sufficient to solve the problem:

$$\operatorname{Min}_{\beta} (y - X\beta)' (y - X\beta)$$

with restriction $r - R\beta = 0$. Ton do this, we consider the Lagrangian function:

$$\mathscr{L} = (y - X\beta)'(y - X\beta) - \lambda'[r - R\beta].$$

The optimum $\pmb{\beta} = \tilde{\pmb{\beta}}$ must satisfy the first-order conditions:

$$\frac{\partial \mathcal{L}}{\partial \beta} = -2X'y + 2(X'X)\tilde{\beta} + R'\lambda = 0$$
 (7.10)

$$\frac{\partial \mathcal{L}}{\partial \lambda} = r - R\tilde{\beta} = 0. \tag{7.11}$$

On multiplying by (7.10) by $R(X'X)^{-1}$, we get:

$$-2R\left(X'X\right)^{-1}X'y + 2R\tilde{\beta} + R\left(X'X\right)^{-1}R'\lambda = 0$$

$$R\left(X'X\right)^{-1}R'\lambda = 2R\left(X'X\right)^{-1}X'y - 2r = 2\left[R\hat{\beta} - r\right]$$

$$\lambda = 2\left[R\left(X'X\right)^{-1}R'\right]^{-1}\left[R\hat{\beta} - r\right].$$

By (7.10),

$$2(X'X)\tilde{\beta} = 2X'y - R'\lambda$$
 (7.12)
= $2X'y - 2R' \left[R(X'X)^{-1} R' \right]^{-1} \left[R\hat{\beta} - r \right]$ (7.13)

hence

$$\tilde{\beta} = (X'X)^{-1}X'y - (X'X)^{-1}R' \left[R(X'X)^{-1}R' \right]^{-1} \left[R\hat{\beta} - r \right]
= \hat{\beta} + (X'X)^{-1}R' \left[R(X'X)^{-1}R' \right]^{-1} \left[r - R\hat{\beta} \right].$$

We see that $\tilde{\beta}$ does not depend on σ^2 . Substituting $\tilde{\beta}$ in $\ln(L)$, we see that

$$\ln(L) = -\frac{T}{2}\ln(2\pi) - \frac{T}{2}\ln\sigma^2 - \frac{1}{2\sigma^2}S_{\omega}$$

where $S_{\omega} = \left(y - X\tilde{\boldsymbol{\beta}}\right)' \left(y - X\tilde{\boldsymbol{\beta}}\right)$, from which we get

$$\frac{\partial \ln(L)}{\partial \sigma^2} = -\frac{T}{2\sigma^2} + \frac{S_{\omega}}{2\sigma^4} = 0$$

at the optimum, hence

$$\tilde{\sigma}^2 = S_{\omega}/T = \left(y - X\tilde{\beta}\right)' \left(y - X\tilde{\beta}\right)/T ,$$

$$L(\hat{\omega}) = \frac{T^{T/2}e^{-T/2}}{\left(2\pi\right)^{T/2}S_{\omega}^{T/2}} ,$$

The likelihood ratio test is given by the critical region:

$$\frac{L(\hat{\Omega})}{L(\hat{\omega})} = \left(\frac{S_{\omega}}{S_{\Omega}}\right)^{T/2} \ge \lambda_{\alpha}$$

or, equivalently,

$$\frac{S_{\omega}}{S_{\Omega}} \ge \lambda_{\alpha}^{2/T}. \tag{7.14}$$

Since

$$S_{\omega} = (y - X\tilde{\beta})'(y - X\tilde{\beta})$$

$$= (y - X\hat{\beta})'(y - X\hat{\beta}) + (\hat{\beta} - \tilde{\beta})'(X'X)(\hat{\beta} - \tilde{\beta})$$

$$= S_{\Omega} + (\hat{\beta} - \tilde{\beta})'(X'X)(\hat{\beta} - \tilde{\beta}),$$

we also see that

$$S_{\omega} - S_{\Omega} = \left(r - R \hat{\beta} \right)' \left[R \left(X'X \right)^{-1} R' \right]^{-1} R \left(X'X \right)^{-1} \left(X'X \right) \left(X'X \right)^{-1}$$

$$R' \left[R \left(X'X \right)^{-1} R' \right]^{-1} \left[r - R \hat{\beta} \right]$$

$$= \left(r - R \hat{\beta} \right)' \left[R \left(X'X \right)^{-1} R' \right]^{-1} \left[r - R \hat{\beta} \right]$$

$$= \left(R \hat{\beta} - r \right)' \left[R \left(X'X \right)^{-1} R' \right]^{-1} \left(R \hat{\beta} - r \right) = S(R, \hat{\beta})$$

$$= \left(qs^{2} \right) F,$$

hence

$$F = \frac{S_{\omega} - S_{\Omega}}{qs^2} = \frac{\left(S_{\omega} - S_{\Omega}\right)/q}{S_{\Omega}/(T - k)}$$

and

$$\frac{S_{\omega}}{S_{\Omega}} = \frac{S_{\Omega} + (qs^2) F}{S_{\Omega}} = 1 + \frac{(qs^2) F}{(T - k) s^2} = 1 + \frac{q}{T - k} F \ge \lambda_{\alpha}^{2/T}$$

$$\iff F \ge \frac{T - k}{q} \left(\lambda_{\alpha}^{2/T} - 1\right) = F_{\alpha}.$$

The likelihood ratio test of H_0 : $R\beta = r$ has the critical region

$$F \equiv \frac{\left(S_{\omega} - S_{\Omega}\right)/q}{S_{\Omega}/(T - k)} \ge F_{\alpha} \left(q, T - k\right)$$

where

$$F \sim F(q, T - k)$$
.

This is an easy method for testing $H_0: R\beta = r$. Note also that:

$$LR = \left(\frac{S_{\omega}}{S_{\Omega}}\right)^{T/2} = \left(1 + \frac{q}{T - k}F\right)^{T/2},$$

$$F = \frac{T - k}{q}\left(LR^{2/T} - 1\right).$$

8. Estimator optimal properties with Gaussian errors

When errors are Gaussian, the OLS estimators $\hat{\beta}_i$, $i=1,\ldots,k$ and $s^2=\left(y-X\hat{\beta}\right)'\left(y-X\hat{\beta}\right)/(T-k)$ have minimum variance in the class of all unbiased estimators of β_i , $i=1,\ldots,k$, and σ^2 respectively [see Rao (1973, section 5a)].

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