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ESTIMATION OF THE LOCATION PARAMETERS

BY

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Abstract. The paper concerns the estimation of univariable (multivariate) linear regression parameters based on the independent normally distributed random variables (vectors) with unknown variance (p. d. covariance matrix).

1. Univariate linear regression parameters. Let x_i (i = 1, 2, ..., n) be independent $N(\mu_i, \sigma^2)$, where if $\mu' = (\mu_1, ..., \mu_n)$, then

(1.1)
$$\mu = A\beta,$$

A being a known $(n \times m)$ -matrix of rank m, and β and σ^2 are unknown parameters.

The best linear unbiased estimate of β is

(1.2)
$$\hat{\beta} = (A'A)^{-1} A'x, \quad x' = (x_1, x_2, \dots, x_n),$$

and

(1.3)
$$\widehat{\beta} \sim N(\beta, \sigma^2 (A'A)^{-1}).$$

Other types of estimates for β are obtained using Bayes arguments.

Suppose we have a prior knowledge on β and assume that the prior distribution of β is $N(\beta_0, \sigma^2 A)$ when β_0 is known, and σ^2 and A may be known or not. Suppose σ^2 and A are known. Then the distribution of β , given x, is

$$N((\Lambda^{-1} + A'A)^{-1}(\Lambda^{-1}\beta_0 + A'x), \sigma^2(\Lambda^{-1} + A'A)^{-1}).$$

Hence Bayes estimate of β is given by

(1.4)
$$\beta_b = (I + \Lambda A' A)^{-1} \beta_0 + ((A' A)^{-1} \Lambda^{-1} + I)^{-1} \hat{\beta} = \beta_0 + W \hat{\delta},$$

where $\hat{\delta} = \hat{\beta} - \beta_0, \ \delta = \beta - \beta_0$ and $W = (I + (\Lambda A' A)^{-1})^{-1}$

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 $E\beta_h = \beta_0 + W\delta$

We have

(1.5) :

and

(1.6) $M_b = E(\beta_b - \beta)(\beta_b - \beta)' = \sigma^2 W(A'A)^{-1} W' + (I - W) \delta \delta' (I - W)'.$

Is it possible to find W so that $T = \sigma^2 (A'A)^{-1} - M_b$ is positive semidefinite? This will be possible if we consider W depending on σ^2 and δ . It is possible to write T as

(1.7)
$$T = \sigma^2 T_0 - (W - v) (\sigma^2 (A' A)^{-1} + \delta \delta') (W - v)',$$

where

$$T_0 = (A'A)^{-1} - \sigma^{-2} \delta \delta' \{1 - \delta' (\sigma^2 (A'A)^{-1} + \delta \delta')^{-1} \delta\}$$

and

$$v = \delta \delta' \left(\sigma^2 \left(A' A \right)^{-1} + \delta \delta' \right)^{-1}$$

Since

$$\left(\sigma^{2}\left(A^{\prime}A\right)^{-1}+\delta\delta^{\prime}\right)^{-1}=\left[A^{\prime}A-A^{\prime}A\delta\delta^{\prime}A^{\prime}A/(\sigma^{2}+\delta^{\prime}A^{\prime}A\delta)\right]/\sigma^{2},$$

the above expressions can be written as

(1.8)
$$T_0 = (A'A)^{-1} - \delta \delta' / (\sigma^2 + \delta' A' A \delta) = (I - \nu)(A'A)^{-1}$$

and

(1.9)
$$\mathbf{v} = \delta \delta' \, A' \, A / (\sigma^2 + \delta' \, A' \, A \delta).$$

It is easy to verify that T_0 is positive definite. Hence the best choice of W depends on δ and σ^2 , and it is given by W = v. This estimate cannot be utilized and hence substituting σ^2 and δ by s^2 and $\hat{\delta}$, respectively, where

$$s^{2} = x' [I - A(A'A)^{-1} A'] x/(n-m) = (x'x - \hat{\beta}' A'A\hat{\beta})/(n-m).$$

Then, the new proposed estimate of β is

(1.10)
$$\hat{\beta}_b = \beta_0 + \frac{\hat{\delta}' A' A \hat{\delta}}{s^2 + \hat{\delta}' A' A \hat{\delta}} \hat{\delta}.$$

Sometimes it is better to use some other estimate of σ^2 instead of an unbiased estimate and, hence, we shall modify the estimate β_b given by (1.10) as

(1.11)
$$\hat{\beta}_{bl} = \beta_0 + \frac{\hat{\delta}' A' A \hat{\delta}}{cs^2 + \hat{\delta}' A' A \hat{\delta}} \hat{\delta},$$

where c is an appropriate constant. The estimator (1.4) is known as the *Ridge* estimator of β (see [5]), while the estimator (1.11) is known as the empirical Bayes estimator, which is a particular case of those proposed and studied by

Stein [8], Effron and Morris [2], etc. These estimators can be written as

(1.12)
$$\hat{\beta}_{bs} = \beta_0 + \left(1 - \frac{1}{u}r(u)\right)\hat{\delta},$$

where $u = (\hat{\delta}' A' A \hat{\delta})/(n-m)s^2$, and r(u) is a function of u.

Notice that (1.11) can be obtained from (1.12) by taking

(1.13)
$$r(u) = cu/(c + (n - m)u).$$

2. Multivariate linear regression parameters. Let $x_1, x_2, ..., x_n$ be independent *p*-dimensional observations and let $x_i \sim N(\mu_i, \Sigma)$. Suppose

$$\mu = \begin{bmatrix} \mu'_1 \\ \mu'_2 \\ \cdots \\ \mu'_n \end{bmatrix} = A\beta,$$

A being a known $(n \times m)$ -matrix of rank m. Here β and Σ are unknown parameters.

Let $X = (x_1, ..., x_n)'$. Then the maximum likelihood estimate of β is

$$\widehat{\beta} = (A'A)^{-1} A'X$$

and

(2.3)
$$\widehat{\beta}a \sim N(\beta a, a' \Sigma a(A' A)^{-1})$$

for any vector a.

To obtain other types of estimate for β , let us assume that $\beta a \sim N(\beta_0 a, a' \Sigma a A)$ for any vector a. Then the posterior distribution of βa , given X, is

$$N((\Lambda^{-1} + A'A)^{-1}(\Lambda^{-1}\beta_0 + A'X)a, a'\Sigma a(\Lambda^{-1} + A'A)^{-1})$$

for any vector a, and hence the Bayes estimate of β is

$$\beta_b = \beta_0 + W \hat{\delta}_s$$

where $\hat{\delta} \simeq \hat{\beta} - \beta_0$, $\delta = \beta - \beta_0$ and $W = (I_m + (\Lambda A' A)^{-1})^{-1}$.

Notice that, for all non-null vectors a, the distribution of $\beta_b a$ is

 $N((\beta_0 + W\delta)a, a' \Sigma a W (A' A)^{-1} W').$

Now, if $\beta' = (\beta_1, \beta_2, ..., \beta_m)$, then we write $\beta'_* = (\beta'_1, \beta'_2, ..., \beta'_m)$. In this notation, $\hat{\beta}_* \sim N(\beta_*, (A'A)^{-1} \otimes \Sigma)$ and $\beta_{b*} \sim N((\beta_0 + W\delta)_*, W(A'A)^{-1} W' \otimes \Sigma)$, where $P \otimes Q$ is the Kronecker product of P and Q and it is defined by $P \otimes Q = (p_{ij}Q)$ with $P = (p_{ij})$. Then the mean square error for β_b is

$$M_{b} = E(\beta_{b*} - \beta_{*})(\beta_{b*} - \beta_{*})' = W(A'A)^{-1}W' \otimes \Sigma + [(I - W)\delta]_{*}[(I - W)\delta]'_{*}.$$

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Is it possible to find W so that $T = (A'A)^{-1} \otimes \Sigma - M_b$ is positive semidefinite?

Let $B' = (b_1, b_2, \dots, b_m)$ and $B_* = (b'_1, b'_2, \dots, b'_m)'$. Then, if T is positive semi-definite,

$$(B_*)' TB_* = \operatorname{tr} \Sigma B \{ (A'A)^{-1} - W(A'A)^{-1} W' \} B' - \left(\operatorname{tr} (I - W) \delta B \right)^2$$

should be nonnegative for all non-null matrices B. Let us transform:

$$B \to \Sigma^{-1/2} B_1 (A' A)^{1/2},$$

$$W \to (A' A)^{-1/2} W_1 (A' A)^{1/2},$$

$$\delta \to (A' A)^{-1/2} \delta_1 \Sigma^{1/2}.$$

Then

$$(B_{\star})' TB_{\star} = \operatorname{tr} B_1' B_1 (I - W_1 W_1') - [\operatorname{tr} (I - W_1) \delta_1 B_1]^2$$

Now, if we choose $W_1 = \delta_1 \delta'_1 (I + \delta_1 \delta'_1)^{-1}$ or

$$W_{1} = \delta \Sigma^{-1} \delta' [(A'A)^{-1} + \delta \Sigma^{-1} \delta']^{-1},$$

then at least it can be verified that T is positive definite for p = 1 and 2. It would be nice if this were true for any p.

Since δ and Σ are unknown quantities, we can substitute $\hat{\delta}$ and cS for their estimates, where $S = X [I - A(A'A)^{-1}A'] X'/(n-m)$. Then we can propose for β the estimate

(2.5)
$$\hat{\beta}_{be} = \beta_0 + \delta (cS + \hat{\delta}' A' A \hat{\delta})^{-1} (\hat{\delta}' A' A \hat{\delta}),$$

which is a generalization of (1.11). Formula (2.5) can be rewritten as

(2.6)
$$\widehat{\beta}_{be} = \beta_0 + (\widehat{\delta}S^{-1}\,\widehat{\delta}') \left((A'A)^{-1}\,c + \widehat{\delta}S^{-1}\,\widehat{\delta}' \right)^{-1} \widehat{\delta},$$

which is a generalization of Thompson's estimator [9, 10]. As in the univariate situation, we define

$$\beta_{bS} = \beta_0 + W \hat{\delta},$$

where W is a function of $\hat{\delta}S^{-1}\hat{\delta}'$.

3. Other types of estimates.

(a) Univariate. Let us base our estimate of β (of Section 1), based on the empirical testing, on $H_0(\beta = \beta_0)$ VS $H(\beta \neq \beta_0)$. Hence the proposed estimate of β is

$$\hat{\beta}_{em} = \begin{cases} \beta_0 + f_1(u)\hat{\delta} & \text{if } u \leq c, \\ f_2\left(\frac{\hat{\beta}' A' A\hat{\beta}}{(n-m)s^2}\right)\hat{\beta} & \text{otherwise,} \end{cases}$$

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where $u = \hat{\delta}' A' A \hat{\delta}/(n-m) s^2$ and c is a constant. Here f_1 and f_2 are some appropriate functions. Alam [1] used $f_1(u) = u/(1+u)$ and $f_2(w) = 1$, while Upadhyaya and Srivastava [11] used $f_1(u) = 1 - a \exp(-bu)$ and $f_2(w) = 1$. They obtained mean square errors.

(b) Multivariate. In the model of Section 2 we can propose

$$\hat{\beta}_{em} = \begin{cases} \beta_0 + F_1(\hat{\delta}S^{-1}\hat{\delta}')\hat{\delta} & \text{if } \operatorname{tr}(\hat{\delta}S^{-1}\hat{\delta}'A'A) \leq c_a \text{ or} \\ & |\hat{\delta}'A'A\hat{\delta}|/|S + \hat{\delta}'A'A\hat{\delta}| \geq c, \\ F_2(\hat{\beta}S^{-1}\hat{\beta}')\hat{\beta} & \text{otherwise,} \end{cases}$$

where F_1 and F_2 are matrix functions of $\hat{\delta}S^{-1}\hat{\delta}'$ and $\hat{\beta}S^{-1}\hat{\beta}'$, respectively.

4. Bias and mean square error.

(a) Univariate. First of all we shall consider the estimate $\hat{\beta}_{be} = \beta_0 + f(u)\hat{\delta}$, where f(u) is a function of $u = (\hat{\delta}' A' A\hat{\delta})/(n-m)s^2$. We observe that $\hat{\delta}$ and $(n-m)s^2$ are here independently distributed, $\hat{\delta} \sim N(\delta, \sigma^2(A'A)^{-1})$ and $(n-m)s^2/\sigma^2 \sim \chi^2_{n-m}$. Let $w = (\hat{\delta}' A' A\hat{\delta})/\sigma^2$ and $v = (n-m)s^2/\sigma^2$. The problem is to find

(4.1)
$$E(\hat{\delta}|w, v)$$
 and $E(\hat{\delta}\hat{\delta}'|w, v)$.

To obtain these results, we observe that the density of $\hat{\delta}$ is

(4.2)
$$(2\pi)^{-m/2} \sigma^{-m} |A'A|^{1/2} \exp\left(-\frac{1}{2\sigma^2}(\hat{\delta}-\delta)'A'A(\hat{\delta}-\delta)\right)$$

and the density of w is

(4.3)
$$g(w|m, \lambda) = e^{-\lambda/2} \sum_{j=0}^{\infty} \frac{(\lambda/2)^j}{j!} \frac{w^{(m+2j-2)/2} e^{-w/2}}{2^{(m+2j)/2} \Gamma(m/2+j)}$$
 for $0 < w < \infty$

or

(4.3a)
$$g(w|m, \lambda) = g(w|m, 0) a(w|m, \lambda),$$

where $\lambda = \delta' A' A \delta / \sigma^2$ and g(w|m, 0) is obtained from (4.3) by putting $\lambda = 0$. Hence, the density of $\hat{\delta}$, given w, is

(4.4)
$$w^{1-m/2}(\pi\sigma^2)^{-m/2}|A'A|^{1/2}\Gamma(m/2)\{a(w|m,\lambda)\}^{-1}\exp\left(\frac{1}{\sigma^2}\delta'A'A\hat{\delta}\right).$$

Let $z = (A'A)^{1/2} \hat{\delta} / \sigma \sqrt{w}$ and $\mu = (A'A)^{1/2} \delta / \sigma \sqrt{\lambda}$. Then (4.4) can be rewritten as

(4.5)
$$\{a(w|m, \lambda)\}^{-1} \exp(\sqrt{w\lambda} \mu' z) [dz],$$

where $z' z = \mu' \mu = 1$ and [dz] is a unit invariant Haar over O(1, m)

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 $= \{z: z'z = 1\}$. The distribution given by (4.5) is known as Fisher – von Mises distribution and studied by various authors (e.g. [4, 6, 12]).

Let C be an orthogonal matrix the first row vector of which is μ . Then Cz = y gives [dz] = [dy], and the density of y, given w, is

(4.6)
$$\{a(w|m, \lambda)\}^{-1} \exp(\sqrt{w\lambda} y_1) [dy],$$

where

(4.7)
$$[dy] = \frac{\Gamma(m/2)}{\pi^{m/2}} \frac{dy}{|y_i|} \quad \text{over } y'y = 1.$$

By (4.6) and (4.7) it is easy to show that y_1 and $\{y_i/\sqrt{1-y_1^2}$ for $i = 2, 3, ..., m\}$ are independently distributed, the distribution of y_1 , given w, is

(4.8)
$$h(\dot{y_1}) = \left\{ B\left(\frac{1}{2}, \frac{m-1}{2}\right) a(w|m, \lambda) \right\}^{-1} \exp(\sqrt{w\lambda} y_1) (1-y_1^2)^{(m-3)/2}$$

for $y_1^2 \le 1$,

and the joint density of $l_i = y_i/\sqrt{1-y_1^2}$ for i = 2, 3, ..., m is similar to (4.7) by replacing m by m-1. Hence

(4.9)
$$El_i = 0, El_i l_j = 0$$
 for $i \neq j = 2, 3, ..., m$

and

(4.10)
$$El_i^2 = (m-1)^{-1}$$
 for $i = 2, 3, ..., m$.

Thus

$$E(y_1|w) = \int_{-1}^{1} y_1 h(y_1) dy_1$$

and, since $\int y_1 (1-y_1^2)^{(m-3)/2} dy_1 = -(m-1)^{-1} (1-y_1^2)^{(m-1)/2}$, we get

(4.11)
$$E(y_1|w) = (\sqrt{w\lambda/(m-1)} E(1-y_1^2))$$

$$= (\sqrt{w\lambda/m}) a(w|m+2, \lambda)/a(w|m, \lambda),$$

(4.11a)
$$E(y_i|w) = E(l_i(l-y_1^2)^{1/2}|w) = 0$$
 for $i = 2, 3, ..., m$,

(4.12)
$$E(y_i^2|w) = 1 - E\{(1 - y_1^2)|w\}$$

 $= 1 - ((m-1)/m) a(w|m+2, \lambda)/a(w|m, \lambda),$

(4.12a)
$$E(y_i y_1 | w) = E\{y_1 (1 - y_1^2)^{1/2} l_i | w\} = 0 \quad \text{for } i \neq 1,$$

(4.12b)
$$E(y_i y_j | w) = E\{l_i l_j (1 - y_1^2) | w\} = 0$$
 for $i \neq j = 2, 3, ..., m$,
and

(4.12c) $E(y_i^2|w) = E\{l_i^2(1-y_1^2)|w\} = (m-1)a(w|m+2, \lambda)/a(w|m, \lambda).$

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Hence

(4.13)
$$E(y|w) = e_1(\sqrt{w\lambda/m}) a(w|m+2, \lambda)/a(w|m, \lambda)$$

and

(4.14)
$$E(yy'|w) = e_1 e'_1 (1-b) + m^{-1} bI,$$

where $e'_1 = (1, 0, ..., 0)$ and $b = a(w|m+2, \lambda)/a(w|m, \lambda)$.

Now we are in a position to give expressions for $E(\hat{\delta}|w)$ and $E(\hat{\delta}\hat{\delta}'|w)$ as

(4.15)
$$E(\hat{\delta}|w) = \sigma \sqrt{w} (A'A)^{-1/2} C' E(y|w)$$
$$= \delta (w/m) a(w|m+2, \lambda)/a(w|m, \lambda),$$

and

(4.16)
$$E(\hat{\delta}\hat{\delta}'|w) = \sigma^2 (A'A)^{-1} (w/m) b + w(1-b) \delta\delta'/\lambda.$$

Using the density (4.3) and (4.3a) of w, we note that

(4.17) $g(w|m+2, \lambda) = g(w|m, \lambda)(w/m) a(w|m+2, \lambda)/a(w|m, \lambda)$ and hence

(4.18)
$$E\hat{\beta}_{be} = \beta_0 + Ef(w/v)\,\hat{\delta} = \beta_0 + \delta Ef(w^*/v)$$

and

(4.19)
$$E(\hat{\beta}_{be} - \beta)(\hat{\beta}_{be} - \beta)' = \sigma^{2} (A'A)^{-1} E\{f(w^{*}/v)\}^{2} - 2\delta\delta' Ef(w^{*}/v) + (\delta\delta'/\lambda) [E\{f(w/v)\}^{2}w - mE\{f(w^{*}/v)\}^{2}] + \delta\delta',$$

where w^* is distributed as noncentral χ^2 with m+2 degrees of freedom and noncentral parameter λ , while w is distributed as noncentral χ^2 with m degrees of freedom and noncentral parameter λ . Thus, the mean square error matrix is

(4.19a)
$$M_b = E(\hat{\beta}_{be} - \beta)(\hat{\beta}_{be} - \beta)' = a_1 \sigma^2 (A' A)^{-1} + a_2 \delta \delta',$$

where $a_1 = E \{f(w^*/v)\}^2 = E(f(F^*))^2$ and $a_2 = 1 - m(a_1/\lambda) - 2E(f(F^*)) + \lambda^{-1} E \{f(w/v)\}^2 w$ and $F^* = w^*/v$.

For the various particular functions f_{i} (4.19) or (4.19a) can be calculated explicitly. This is left to the reader.

(b) Multivariate. The estimate of β can be written in two different forms according to m > p or m < p. For m < p we write

(4.20)
$$\hat{\beta}_{lbe} = \beta_{l0} + G(\hat{\delta}_1 V^{-1} \hat{\delta}_1') \hat{\delta}_1,$$

and for m > p

(4.21)
$$\hat{\beta}_{lbe} = \beta_{l0} + \hat{\delta}_1 G_0 (V^{-1} \hat{\delta}'_1 \hat{\delta}_1),$$

where $\hat{\beta}_{lbe} = \sqrt{A'A} \hat{\beta}_{lbe} \Sigma^{-1/2}, \beta_{l0} = \sqrt{A'A} \beta_0 \Sigma^{-1/2}, V = \Sigma^{-1/2} S \Sigma^{-1/2} (n-m)$ and $\hat{\delta}_1 = \sqrt{A'A} \hat{\delta} \Sigma^{-1/2}$.

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The distribution of V is Wishart with n-m degrees of freedom, $\hat{\delta}_1 \sim N_{m,p}(\delta_1, I_m, I_p)$ and they are independent.

It is extremely difficult to obtain the mean and mean square matrix for the elements of $\hat{\beta}_{lbe}$ defined in (4.20) and (4.21). We shall only consider the situation where m = 1 and p > 1. For this purpose the estimate given in (4.20) can be written as

(4.21a)
$$\widehat{\beta}_{lbe} = \beta_{l0} + g(\widehat{\delta}_1 V^{-1} \widehat{\delta}_1') \widehat{\delta}_1,$$

where $\hat{\delta}_1$, β_{l0} and $\hat{\beta}_{lbe}$ are row vectors and g is a scalar function $\hat{\delta}_1 V^{-1} \hat{\delta}'_1$. Since $\hat{\delta}_1$ and V are independently distributed, we shall use the orthogonal transformation $CVC' = V_1$, where the first row of C is $\hat{\delta}_1/\sqrt{\hat{\delta}_1 \hat{\delta}'_1}$. Then $V_1^{-1} = CV^{-1}C'$ and if $V_1^{-1} = (v^{ij})$, $v^{11} = \hat{\delta}_1 V^{-1} \hat{\delta}'_1/\hat{\delta}_1 \hat{\delta}'_1$ and $1/v^{11} = v \sim \chi^2_{n-p}$, then (4.21a) can be rewritten as

(4.22)
$$\hat{\beta}_{lbe} = \beta_{l0} + g(\hat{\delta}_1 \, \hat{\delta}'_1 / v) \, \hat{\delta}_1,$$

which is exactly similar to the estimate considered in Section 4(a). Using (4.18), we get

(4.23)
$$E(\hat{\beta}_{lbe}) = \beta_{l0} + Eg(w^*/v)\delta_1,$$

where

$$w \sim \chi^2_{n-p}, w^* \sim \chi^2_{p+2}(\lambda), \ \lambda = \delta_1 \,\delta_1' \text{ and } \delta_1 = (A'A)^{1/2} \,\delta\Sigma^{-1/2}$$

Further, by (4.19a), we get

(4.24)
$$M = E(\hat{\beta}_{lbe} - \beta_1)'(\hat{\beta}_{lbe} - \beta_1) = a_1 I + a_2 \delta_1' \delta_1,$$

where $a_1 = E(g(w^*/v))^2$, $a_2 = 1 - p(a_1/\lambda) - 2Eg(w^*/v) + \lambda^{-1}E\{g(w/v)\}^2 w$, $w \sim \chi_p^2(\lambda)$, $w^* \sim \chi_{p+2}^2(\lambda)$ and $v \sim \chi_{n-p}^2$.

Other situations are left to the reader.

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