

NOTE ON THE NON-EXISTENCE OF A MAXIMUM  
LIKELIHOOD ESTIMATE<sup>1</sup>

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1. Summary

It is shown that in a regression model with intraclass correlation  $\rho$ , maximum likelihood estimates and minimum variance unbiased linear estimates of the regression coefficients are unaffected by the value of  $\rho$  when  $\rho$  is given, and that the former do not exist when  $\rho$  is not specified. The usual confidence intervals for the regression slopes remain valid, but there are difficulties in giving a confidence interval for the intercept.

2. Introduction and Statement of Result

In Halperin (1951) the following situation is examined. Writing

$$\underline{y} = (y_1, \dots, y_n), \quad \underline{1} = (1, \dots, 1), \quad \underline{x}_p = (x_{p1}, \dots, x_{pn})$$

with  $p=1, 2, \dots, k$  and  $0 < k < n-1$ , let  $\underline{y}$  be multivariate non-singular normal with mean  $\mu \underline{1}$  if  $k=0$  and

$$\mu \underline{1} + \sum_{p=1}^k C_p \underline{x}_p$$

otherwise, and with covariance matrix

$$R_n = \sigma^2 \begin{bmatrix} 1 & \rho & \cdots & \rho \\ \rho & 1 & \cdots & \rho \\ \vdots & \vdots & \ddots & \vdots \\ \rho & \rho & \cdots & 1 \end{bmatrix}.$$

Here the  $\underline{x}_p$  are fixed and known, linearly independent vectors with  $\underline{x}_p \underline{1}' = 0$ ; and  $\mu, C = (C_1, \dots, C_k), \sigma^2 > 0$  and  $\rho$  are unknown. It is stated in Halperin (1951, p. 574) that "the maximum likelihood equations for the estimation of [the] parameters . . . are of such a formidable character that an explicit solution does not appear possible."

It is shown here that no solution exists due to the fact that the likelihood does not possess a maximum. Nevertheless, if we write

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$\underline{\mu}^0$  and  $\underline{C}^0$  for the maximum likelihood estimates of  $\underline{\mu}$  and  $\underline{C}$  for the case in which  $\rho$  is known to be 0 :

$$\underline{\mu}^0 = \underline{n}^{-1} \underline{y} \underline{1}', \quad \underline{C}^0 = \underline{y} \underline{x}' (\underline{x} \underline{x}')^{-1}, \quad (\underline{x}' = [\underline{x}'_1, \dots, \underline{x}'_k])$$

it turns out that  $\underline{\mu}^0$  and  $\underline{C}^0$  also maximize the likelihood for *any given*  $\rho$ . In fact,  $(\underline{\mu}^0, \underline{C}^0)$  is also a minimum variance unbiased linear estimate of  $(\underline{\mu}, \underline{C})$  for any given  $\rho$ , namely that element in the class of unbiased estimates of  $(\underline{\mu}, \underline{C})$  linear in  $\underline{y}$  which has the smallest generalized variance and has the smallest variance for the estimate of any estimable linear function of  $(\underline{\mu}, \underline{C})$ , no matter what be the form of the distribution of  $\underline{y}$  or the values of its first and second moments.

If  $\rho$  is known to be non-negative but otherwise unknown, the likelihood equations still do not possess a solution, but the maximum of the likelihood is attained at  $\rho=0$  and so the estimate does not converge stochastically to the true value when  $\rho \neq 0$ .

### 3. Proofs

Let  $\underline{E} = [\underline{1}', \dots, \underline{1}']$ . Then  $\underline{R}_n = \sigma^2 \rho \underline{E} + \sigma^2 (1 - \rho) \underline{I}$  and  $\sigma^2 (1 - \rho) (1 + m\rho) \underline{R}_n^{-1} = -\rho \underline{E} + (1 + m\rho) \underline{I}$ , ( $m = n - 1$ ).

That the minimum variance unbiased linear estimates of  $\underline{\mu}$  and  $\underline{C}$  for any given  $\rho$  are  $\underline{\mu}^0$  and  $\underline{C}^0$  now follows by substitution in the formulae for such estimates (Aitken (1934-5)) for the case of a general covariance matrix of the residuals which is fully specified up to a scale factor.

Minus twice the logarithm of the likelihood of  $\underline{y}$  is, apart from a constant,

$$(1) \quad n \log \sigma^2 + m \log (1 - \rho) + \log (1 + m\rho) + \frac{(1 + m\rho) \underline{u} \underline{u}' - \rho (\underline{u} \underline{1}')^2}{\sigma^2 (1 - \rho) (1 + m\rho)},$$

where  $\underline{u} = \underline{y} - \underline{E} \underline{y}$ . Here we have substituted  $(\underline{u} \underline{1}')^2 - \underline{u} \underline{u}'$  for the sum of the cross-products of the elements of  $\underline{u}$ .

From this it is seen that the distribution of  $\underline{y}$  is non-singular if and only if  $\sigma^2$  is positive and

$$(2) \quad -\frac{1}{m} < \rho < 1.$$

The partial derivative of (1) with respect to  $\mu$  is  $\underline{\underline{u}}_1'/\sigma^2(1+m\rho)$ ; since  $\sigma^2 > 0$  and  $m\rho > -1$ , this can vanish only if  $\underline{\underline{u}}_1' = 0$ . For the partial derivative of (1) with respect to  $C$  we find (after setting  $\underline{\underline{u}}_1' = 0$ )  $\underline{\underline{u}}x'/\sigma^2(1-\rho)$ ; since  $\sigma^2 > 0$  and  $\rho < 1$ , this can vanish only if  $\underline{\underline{u}}x' = 0$ . But  $\underline{\underline{u}}_1' = 0$  and  $\underline{\underline{u}}x' = 0$  together constitute the usual normal equations for  $\mu^0$  and  $C^0$ .

Upon substituting  $\underline{\underline{u}}_1' = 0$ , the partial derivative of (1) with respect to  $\sigma^2$  is  $n/\sigma^2 - \underline{\underline{u}}\underline{\underline{u}}'/\sigma^4(1-\rho)$ , which can vanish only if  $\sigma^2(1-\rho) = \underline{\underline{u}}\underline{\underline{u}}'/n$ . Substituting this and  $\underline{\underline{u}}_1' = 0$  in (1) we obtain, apart from a constant,

$$(3) \quad -\log(1-\rho) + \log(1+m\rho).$$

As a function of  $\rho$  this is steadily increasing over the range (2) and tends to infinite values at the ends of the range. Consequently, the likelihood does not possess a maximum in (2).

If the range of  $\rho$  is restricted *a priori* to non-negative values, the maximum of the likelihood is attained at  $\rho = 0$ . Even so, since the derivative,  $n(1-\rho)^{-1}(1+m\rho)^{-1}$ , of (3) is positive, the likelihood equations fail to have a solution even in this case.

#### 4. Confidence Intervals

The expected value of the sum  $V$  of squares of residuals is  $\sigma^2(1-\rho)(n-k-1)$ . Let  $\underline{\underline{D}}$  be a  $k \times s$  matrix of rank  $s$  and  $\underline{\underline{C}}\underline{\underline{D}}$  represent  $s$  estimable linear combinations of  $C_1, \dots, C_k$ . It is readily shown (see Halperin (1951) and Walsh (1947) for special cases) that if

$$W = (\underline{\underline{C}}^0 - \underline{\underline{C}})\underline{\underline{D}}[\underline{\underline{D}}'(\underline{\underline{u}}\underline{\underline{u}}')^{-1}\underline{\underline{D}}]^{-1}\underline{\underline{D}}'(\underline{\underline{C}}^0 - \underline{\underline{C}})'$$

$W/\sigma^2(1-\rho)$  and  $V/\sigma^2(1-\rho)$  are independently distributed like  $\chi^2$  with  $s$  and  $n-k-1$  degrees of freedom. It follows that the usual confidence intervals for any linearly independent set of estimable linear combinations of  $C_1, \dots, C_k$  (and so for any subset) using the  $F$  distribution are valid.

Now, writing

$$\Theta = \frac{1-\rho}{1+m\rho},$$

we can also show (Walsh (1947)) that

$$(n\Theta)^{\frac{1}{2}}(\mu^0 - \mu)/\sigma(1-\rho)^{\frac{1}{2}}$$

is a standard normal variate distributed independently of  $W$  and  $V$ , so that the usual confidence interval for  $\mu$  or combinations of  $\mu$  and components of  $\underline{\underline{C}}$  (such as a prediction of  $\underline{\underline{y}}$  for given  $\underline{\underline{x}}$ ) are not valid.

Sometimes, however, it is possible (Konijn (1962)) to obtain a crude estimate of  $\Theta$ , in which case approximate confidence intervals may be obtained.

#### *References*

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