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A NOTE ON CONFIDENCE INTERVALS IN REGRESSION PROBLEMS

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This note deals with the construction of confidence intervals for arbitrary real functions of multiple regression coefficients.

Consider the usual model

$$y_\alpha = \sum_i \beta_i x_{i\alpha} + \epsilon_\alpha \qquad \begin{array}{l} i = 1, \cdots, k \\ \alpha = 1, \cdots, N \end{array} \tag{1}$$

in which the ϵ_α are independently and normally distributed with mean zero, and common variance σ^2.

It is customary to construct confidence intervals for the β_i, using Student's t distribution. Alternatively, a joint confidence region can be constructed for the β_i using critical values of the F distribution. In both cases the usual statistic s^2, based on $N - k$ degrees of freedom, is used as an estimate of σ^2.

Durand [1] has discussed the use of the joint confidence region of the β_i, an ellipsoid in a k-dimensional space, for the construction of confidence intervals for linear functions, $Q = \sum_i h_i\beta_i$ of the regression coefficients. He points out that the chosen confidence coefficient (corresponding to the ellipsoid) is a lower bound for the joint confidence of any set of intervals thus derived.

Our first objective is to generalize this procedure by removing the restriction of linearity. Let

$$z = f(\beta_1, \beta_2, \cdots, \beta_k) \tag{2}$$

be any real function of the coefficients β_i. The form of the function is arbitrary but known.

For any arbitrarily selected value of z, say z_0, equation (2) represents a

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hypersurface in the k-dimensional parameter space of the β_i. Denote by $M[z]$ the set of all values of z_0 for which the corresponding hypersurfaces "cut" the ellipsoid, i.e., for which the equation:

$$z_0 = f(\beta_1, \beta_2, \cdots, \beta_k)$$

and the quadratic equation representing the ellipsoid have at least one common real solution in the β_i.

The set $M[z]$ is, in general, a closed interval, bounded by those two values of z for which the corresponding hypersurfaces are tangent to the ellipsoid. Furthermore, the event that the point corrresponding to the "true" values of the β_i is inside the ellipsoid implies that the z-value corresponding to these true values is an element of $M[z]$, but the converse is not necessarily true. Consequently, since the probability of the former event is equal to the confidence coefficient $1 - \alpha$, the probability of the latter event is at least $1 - \alpha$. If other functions $u = \varphi(\beta_1, \beta_2, \cdots, \beta_k)$, $v = \psi(\beta_1, \beta_2, \cdots, \beta_k)$, etc., are considered simultaneously with z, it follows that the confidence intervals constructed by the above procedure for z, u, v, $\cdots$ are all jointly valid with a joint confidence for which $1 - \alpha$ is a lower bound.

Our next objective is to discuss, in the light of the above procedure, a regression problem often encountered in practice.

Consider the straight line regression

$$y_\alpha = \beta_0 + \beta_1(x_\alpha - \bar{x}) + \epsilon_\alpha \qquad \alpha = 1, 2, \cdots, N \tag{3}$$

where $\bar{x} = (1/N)\sum_\alpha x_\alpha$. Having obtained least squares estimates for β_0 and β_1, say b_0 and b_1, consider p "future" observations of y and let it be required to find confidence intervals for the corresponding p values of x.

This problem involves, in addition to the random errors of the original N values of y, as reflected in the random fluctuations of the least squares estimates b_0 and b_1, also the random errors of the p "future" y values. Denote the "future" observations by $y_{N+1}, y_{N+2}, \cdots, y_{N+p}$, and their expected values by η_{N+1}, $\eta_{N+2}, \cdots, \eta_{N+p}$. Consider the $p + 2$ dimensional space with coordinates β_0, β_1, $\eta_{N+1}, \eta_{N+2}, \cdots, \eta_{N+p}$. The joint confidence ellipsoid for these $p + 2$ values, for any given confidence coefficient, will be centered on b_0, b_1, y_{N+1}, y_{N+2}, y_{N+p}, and can be found as follows by a generalization of a method used by Working and Hotelling [8]:

The quantity

$$\chi_1^2 = \frac{(\beta_0 - b_0)^2}{\sigma_{b_0}^2} + \frac{(\beta_1 - b_1)^2}{\sigma_{b_1}^2} + \frac{\sum_{i=1}^{p}(\eta_{N+i} - y_{N+i})^2}{\sigma^2} \tag{4}$$

has the chi-square distribution with $p + 2$ degrees of freedom. $\sigma_{b_0}^2$ and $\sigma_{b_1}^2$ are of course known functions of σ^2, $\sigma_{b_0}^2 = \sigma^2/N$ and $\sigma_{b_1}^2 = \sigma^2/\sum_{i=1}^{N}(x_i - \bar{x})^2$.

On the other hand, we have

$$\chi_2^2 = \frac{(N - 2)s^2}{\sigma^2} \tag{5}$$

a quantity distributed as chi-square with $(N - 2)$ degrees of freedom.

Since χ_1^2 and χ_2^2 are mutually independent, it follows from (4) and (5) that a joint confidence region, with coefficient $1 - \alpha$ for β_0, β_1, and the expected values of $y_{N+1}, \cdots, y_{N+p}$ is given by

$$\text{(6)} \qquad \frac{(\beta_0 - b_0)^2}{1/N} + \frac{(\beta_1 - b_1)^2}{1/\sum(x - \bar{x})^2} + \sum_{i=1}^{p} (\eta_{N+i} - y_{N+i})^2 = (p + 2)F_\alpha s^2$$

where F_α is the critical value of the F distribution with $p + 2$ and $N - 2$ degrees of freedom, at the α level of significance.

Consider now the function

$$x' = \bar{x} + \frac{\eta' - \beta_0}{\beta_1}$$

where η' is the expected value of one of the p "future" observations, and x' the corresponding true x-value. By the method previously outlined, confidence limits for x' are obtained by determining the two values of x' for which the hyperplane

$$\text{(7)} \qquad \eta' - \beta_0 = \beta_1(x' - \bar{x})$$

is tangent to the ellipsoid, provided that the set of values of x' for which the hyperplane (7) intersects the ellipsoid is a closed interval.

Denoting these limits by x_L' and x_U', it is found that the quantities $u_L = x_L' - \bar{x}$ and $u_U = x_U' - \bar{x}$ are the roots of the equation

$$\text{(8)} \quad \left(b_1^2 - \frac{K^2}{\sum(x - \bar{x})^2}\right) u^2 - 2b_1(y' - b_0)u + \left[(y' - b_0)^2 - \frac{N + 1}{N} K^2\right] = 0$$

where $K^2 = (p + 2)F_\alpha s^2$.

The condition for equation (8) to have distinct real roots is

$$\text{(9)} \qquad \frac{(y' - b_0)^2}{\sum(x - \bar{x})^2} + \frac{N + 1}{N}\left[b_1^2 - \frac{K^2}{\sum(x - \bar{x})^2}\right] > 0$$

Condition (9) is necessary but not sufficient for obtaining a confidence interval for x'. This is apparent from the fact that when x' is made $\pm\infty$, equation (7) represents the hyperplane $\beta_1 = 0$. Consequently, if the hyperplane $\beta_1 = 0$ intersects the ellipsoid, the parameter x' will have a discontinuity when (7) becomes $\beta_1 = 0$, and the roots x_L' and x_U', though distinct and real, will then not be the limits of a confidence interval for x'.

The condition for $\beta_1 = 0$ not to intersect the ellipsoid is

$$\text{(10)} \qquad b_1^2 \sum(x - \bar{x})^2 > K^2$$

It can be proved that condition (10), which implies (9), is both necessary and sufficient in order that the roots of (8) yield the limits of a confidence interval for x'.

If equation (10) is satisfied, the procedure leading to equation (8) can also be carried out for the remaining $p - 1$ "future" measurements, y'', y''', etc. In this manner one will obtain a set of confidence intervals (x_L', x_U'), (x_L'', x_U''),

(x_L''', x_U'''), etc., all of which are jointly valid with a confidence coefficient for which $1-\alpha$ is a lower bound. Furthermore, this lower bound will still apply if confidence intervals are also derived for any number of real functions of β_0, β_1 and the p values $\eta_{N+1}, \eta_{N+2}, \cdots, \eta_{N+p}$.

Equation (8) should be compared to the relation obtained by the use of Fieller's theorem [3, 4]. This theorem leads to a confidence interval for $x' - \bar{x}$ by considering it as the ratio of the two normally distributed variables $y' - b_0$ and b_1, whose variances are $(N + 1)\sigma^2/N$ and $\sigma^2/\sum(x - \bar{x})^2$ and whose covariance is zero. The confidence interval, with coefficient $1 - \alpha$, thus found is given by the roots of the equation

$$(11) \quad \left(b_1^2 - \frac{t_\alpha^2 s^2}{\sum(x - \bar{x})^2}\right)u^2 - 2b_1(y' - b_0)u + \left[(y' - b_0)^2 - \frac{N+1}{N} t_\alpha^2 s^2\right] = 0$$

where t_α is the critical value of Student's t, at the two-sided α level, and u is defined as above.

The only difference between equations (8) and (11) is the substitution of K^2 for t^2s^2, i.e., the substitution of $[(p + 2)F_\alpha]^{\frac{1}{2}}$ for t_α. This substitution results in a widening of the confidence interval, caused by the joint consideration of $p + 2$ parameters instead of the single parameter η', (or its corresponding x'). It is of interest to observe that the relation between $[(p + 2)F_\alpha]^{\frac{1}{2}}$ and t_α is precisely that found by Scheffé [6] in establishing simultaneous confidence statements for all means in an analysis of variance, as contrasted with individual confidence statements based on Student's t.

In deciding whether in a particular application, joint or single confidence intervals should be used, one may be guided by the following plausible rule. Joint confidence intervals are indicated in situations involving two or more quantities that are determined as so many phases of a single problem. On the other hand, quantities involved in unrelated problems, even though they are derived from the same basic data, should not be treated jointly in deriving confidence intervals. It appears advisable, in view of this rule, to partition all the quantities derived from a single set of data into groups such that the quantities within a group—inasmuch as they correspond to the same problem, are treated jointly for the derivation of confidence intervals; while the groups themselves are treated independently of each other.

Groups involving single predictions should be treated by Fieller's theorem, since there appears to be no justification, in such cases, for widening the confidence interval through inclusion of confidence statements about the slope and the intercept.

It is of interest to note that the confidence interval based on equation (8) may be obtained by drawing hyperbolic confidence limits [2] for the straight line represented by equation (3), in accordance with the relations

$$(12) \qquad y = b_0 + b_1(x - \bar{x}) \pm K\left[\frac{N+1}{N} + \frac{(x - \bar{x})^2}{\sum(x - \bar{x})^2}\right]^{1/2}$$

and by determining the x-interval defined by the intersection of the line $y = y'$

with the two branches of this hyperbola. It is readily seen that the condition that such an x-interval exists and be of finite length is equivalent to the condition that the two asymptotes of the hyperbola have slopes of equal sign. Since these slopes are $b_1 - K/[\sum(x - \bar{x})^2]^{\frac{1}{2}}$ and $b_1 + K/[\sum(x - \bar{x})^2]^{\frac{1}{2}}$, the condition in question is $b_1^2 - K^2/(\sum(x - \bar{x})^2) > 0$. This is condition (10) obtained previously by a different line of reasoning.

It may be observed, finally, that the inverse problem, viz, to determine uncertainty intervals for observed y values corresponding to given x values [2] is not a classical case of interval estimation, since it is concerned with bracketing a random variable, not a population parameter, by means of two statistics. Intervals of this type are discussed by Weiss [7].

Applications of the procedure outlined in this note to a problem in chemistry are discussed elsewhere [5].

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A NOTE ON INCOMPLETE BLOCK DESIGNS

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1. Introduction. Kempthorne [1] has shown the efficiency factor of an incomplete block design to be a quantity proportional to the harmonic mean of the nonzero latent roots of the matrix of coefficients of the reduced normal equations for the intra-block estimates of treatment effects. He has further stated that the geometric mean in a certain sense corresponds to the generalized variance but has not explicitly explained it. The present note is intended to clear this point and to prove that the design with highest efficiency factor (in any case, whether the harmonic mean or the geometric mean is taken as a measure of efficiency) is

(a) a balanced incomplete block design, if such a design exists; and

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