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# Faculty Working Papers

## UNBIASED DECISION RULE FOR THE CHOICE OF REGRESSION MODELS

Takamitsu Sawa and Kei Takeuchi

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FACULTY WORKING PAPERS

College of Commerce and Business Administration

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May 19, 1977

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# UNBIASED DECISION RULE FOR THE CHOICE OF REGRESSION MODELS

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Unbiased Decision Rule for the Choice of Regression Models\*

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Takamitsu Sawa\*\* and Kei Takeuchi\*\*\*

May 11, 1977

#### Prepared Under

NATIONAL SCIENCE FOUNDATION GRANT SOC 76-22232

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\*\*Department of Economics, University of Illinois and Kyoto University. \*\*\*Faculty of Economics, University of 'Tokyo.



#### Abs tract

The unbiased decision rule, based on the conventional F-statistic, is proposed for the choice of the most adequate model from a given set of nested alternative regression models. Mallows' (1973) idea is adapted to measure the adequacy of each model. The biases of several customarily used criteria for the choice of regression models, including the AIC, Mallows'  $C_p$  and  $\overline{R}$ , are discussed. The critical point for the unbiased decision is numerically computed and tabulated. Also, the approximate formula for the unbiased critical point is derived.

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#### 1. Introduction

There has been a vast amount of literature dealing with procedures of selecting the most adequate regression model from a given set of alternatives. This fact illustrates that the choice of the most appropriate subset of regressors is one of the most difficult as well as bothersome problems in practical regression analysis. To compare several alternative models, the most frequently used as well as most primitive criterion may be the residual sum of squares

(1.1) 
$$
Q_p = \tilde{Y} \left[ I - \tilde{X} (X^{\dagger} X)^{-1} X^{\dagger} \right] Y = \sum_{i=1}^{n} (Y_i - \hat{Y}_i)^2
$$

for a regression model:  $E(Y) = XB$ ,  $V(Y) = \sigma^2 I$ , or an equivalent expression, the multiple correlation coefficient

(1.2) 
$$
R = \left[1 - \frac{Q_p}{\sum_{\substack{\Sigma \\ i=1}} (Y_i - \overline{Y})^2} \right]^{1/2}
$$

where Y is an n-dimensional vector random variable; X is an n x p matrix of fixed constants;  $\sigma^2$  is a scalar unknown;  $\beta$  is a p x 1 vector of unknowns; I is an n x n identity matrix;  $Y_i^r$ s are components of  $Y$ ;  $\overline{Y}$ is the mean of  $Y_i^s$ s;  $\hat{Y}_i^s$ s are interpolated values. These criteria have an apparent shortcoming in that they do not weigh the costs of successive increases in the parameter space against the improvements in model fit. To overcome this, we usually make an adjustment such as

(1.3) 
$$
\overline{R}^2 = 1 - (n - 1) (1 - R^2)/(n - p).
$$

R is commonly called the multiple correlation coefficient adjusted for the degrees of freedom. As a descriptive measure of the goodness of

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fit,  $\overline{R}$  has a sound intuitive appeal. So far, however, no persuasive reasons have been given to justify the use of R. That is, it is not clear why R should be preferred to any other possible adjustments to R.

Mallows (1973) proposed another criterion called the  $C_p$  statistic

(1.4) 
$$
C_p = Q_p + 2p \omega^2
$$

where the first term on the right hand side is the residual sum of squares, p is the number of regressors, and  $\hat{\omega}^2$  is an appropriately chosen unbiased estimate for the true variance of the  $Y_i$ 's. In fact it is an open question how to obtain  $\hat{\omega}^2$ , but it should be noted that  $\hat{\omega}^2$  is independent of p and common factor in  $C_n$  to all alternative models. The true distribution of Y is assumed to be N  $(\mu,\omega^2$  I). The C statistic has been derived as an unbiased estimate for the mean P squared error

(1.5) 
$$
W_p = E ||\n\begin{vmatrix} y^0 - \hat{y} \end{vmatrix}||^2 = \sum_{i=1}^n E (Y_i^0 - \hat{Y}_i)^2
$$

of the least squares prediction  $\hat{Y} = X (X^{\dagger}X)^{-1} X^{\dagger}Y$  for  $Y_0$  which is distributed as N  $(\mu, \omega^2 I)$  independently of Y.

Based on a different and more profound reasoning, Akaike (1974) suggested a procedure for model identification, which is called the Akaike Information Criterion (AIC) . It is defined as minus twice the maximized likelihood function plus twice the number of parameters in the likelihood function. This assumes that the likelihood function is well defined by each of the alternative models. Given a set of alternative models, we choose the one that gives the smallest AIC. The decision rule based on the AIC is termed the minimum AIC (MAIC)

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 $\label{eq:2.1} \frac{1}{2} \int_{\mathbb{R}^3} \left| \frac{d\mu}{\mu} \right|^2 \, d\mu = \$ the contract of the contract of the  $\frac{1}{2} \left( \frac{1}{2} \right)^{2}$  ,  $\frac{1}{2} \left( \frac{1}{2} \right)^{2}$ 

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procedure. This procedure has an advantage of being applicable to any statistical problem as long as each of the alternative models well defines the likelihood function. If we apply the MAIC procedure to a linear normal regression model, we arrive at the asymptotically equivalent decision rule as Mallows'  $C_n$ .

One of the present authors (Sawa (1976)) has recently developed another information criterion for the choice of regression models. The criterion is called the BIG and has been derived, following Akaike (1973), from the Kullback-Leibler measure of the mean information for discrimination between two alternative models. However, the difference between the AIC and the BIG is quite pronounced for the sample size typically dealt with in practical data analysis. Primarily it stems from the difference existing between Akaike 's and Sawa's views on the true model. $\frac{1}{x}$ 

The purpose of the present paper is to propose another criterion for the choice of regression models. The proposed decision rule is called the unbiased decision rule; unbiased in the sense that it leads us to the correct decision with probability higher than .5.

If the alternative models are nested, all the decision rules described above, are reduced to a decision based on a magnitude of the observed F statistic. Therefore, they can be compared in terms of implied critical points for the preliminary F test of the null hypothesis that a subset of coefficients be zero. Some readers may feel that it is useless to study the preliminary test any more because the resultant estimator has been proved to be inadmissible. To avoid this

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criticism In advance, we point out that what we are proposing is not an estimation procedure but a procedure for model identification. More precisely, in the present context we aim to develop a procedure for identifying the most adequate model from a given set of alternatives rather than estimating unknown parameters involved in a given true model

#### 2. Unbiased Critical Point

We begin by postulating a linear normal regression model

$$
(2.1) \qquad \underline{Y} \sim N \left(\underline{X}\beta, \sigma^2 \underline{I}\right)
$$

for an n-dimensional vector random variable Y, the true distribution of which is

$$
(2.2) \t y \sim N (\mu, \omega^2 I),
$$

where X is an n x p full rank matrix of known constants;  $\beta$  is a p x 1 vector of unknown parameters; I is an n x n identity matrix;  $\mu$  is an n x 1 vector of unknowns;  $\omega^2$  and  $\sigma^2$  are unknown positive constants.

The regression model  $(2.1)$  assumes that the mean vector  $\mu$  belongs to a linear subspace spanned by the columns of X. The least squares estimate  $\hat{\beta} = (X'X)^{-1}X'Y$  has a normal distribution with mean  $\beta_0 =$  $(X'X)^{-1}X'\mu$  and variance  $\omega^2 (X'X)^{-1}$ .<sup>2</sup>/

Let us consider two nested alternative regression models (2.3)  $M_1: Y \sim N (X_1 \beta_1, \sigma_1^2 I)$ (2.4)  $M_2: Y \sim N (X_1 \beta_1 + X_2 \beta_2, \sigma_2^2 I)$ 

where  $X^{\dagger}_1$  and  $X^{\dagger}_2$  are, respectively, n x p and n x q matrices. Without loss of generality we may assume that  $X_1$  and  $X_2$  are orthogonal. The

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regression coefficients  $\beta_1$  and  $\beta_2$  are

$$
(2.5) \qquad \beta_1 = (x_1^{\prime} x_1)^{-1} x_1^{\prime} \mu, \ \beta_2 = (x_2^{\prime} x_2)^{-1} x_2^{\prime} \mu.
$$

Mallows' statistic for each of the models is given by

(2.6) 
$$
c_p = Q_p + 2 p \hat{\omega}^2
$$

for M<sub>1</sub> and

(2.7) 
$$
C_{p+q} = Q_{p+q} + 2 (p+q) \omega^2
$$

for  $M_2$ , where  $Q_p$  and  $Q_{p+q}$  are the residual sums of squares for  $M_1$  and  $M_p$ , respectively;  $\hat{\omega}^2$  is a certain unbiased estimate of  $\omega^2$ . Without additional information, a reasonable estimate of  $\omega^2$  would be the unbiased rstimate  $Q_{p+q}/(n-p-q)$  of  $\sigma_2^2$ . Then Mallows' decision rule, based on whether  $C_p < C_{p+q}$  or  $C_p > C_{p+q}$ , is equivalent to a decision based on whether F is less than or greater than two, where

(2.8) 
$$
F = \frac{(Q_p - Q_{p+q})/q}{Q_{p+q}/(n-p-q)}
$$

is the conventionally used F statistic to test the null-hypothesis that  $M_1$  is true. Hence Mallows' C<sub>p</sub> decision rule is equivalent to a preliminary F test with a constant critical point 2 irrespective of the degrees of freedom.

If the simpler model  $M_1$  is "true", F has a central F distribution with q and n-p-q degrees of freedom; if the more complex model  $M_2$  is true, it has a singly noncentral F distribution, with noncentrallty parameter.

$$
(2.9) \qquad \lambda_1 = \mu^* \underline{x}_2 \left( \underline{x}_2^* \underline{x}_2 \right)^{-1} \underline{x}_2^* \mu / \omega^2
$$

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and q and n-p-q degrees of freedom. If the true distribution of Y is N (µ, $\omega^2$  I) and hence M<sub>1</sub> and M<sub>2</sub> are both incorrect, F has a doubly noncentral  $F$  distribution with q and n-p-q d.f. and noncentrality parameters  $\lambda_1$  and

(2.10) 
$$
\lambda_2 = \mu' \left[ I - X \left( X'X \right)^{-1} X' \right] \mu / \omega^2
$$

where  $X = (X_1, X_2)$ .

The MAIC procedure leads us to a preliminary F test with a varying critical point: that is, we choose  $M_1$  if

(2.11) 
$$
F \leq [\exp(\frac{2q}{n}) - 1] \frac{(n-p-q)}{q}
$$

and choose  $M_2$  otherwise. The AIC critical point, given in  $(2.11)$ , varies with n, p, and q. It approaches <sup>2</sup> from below as n becomes large.

Sawa's (1977) MBIC procedure is somewhat more complicated. It implies the following decision rule: choose  $M_1$  if

 $(2.12)$  n log W - 2 (p+2) W + 2 W<sup>2</sup> + 2 (p+q+1) < 0 or vice versa, where

(2.13) 
$$
W = \frac{Q_{p+q}}{Q_p} = [1 + \frac{q}{n-p-q} F]^{-1}
$$

Although the BIC critical point cannot be explicitly written as a function of n, p, and q,  $(2.12)$  is equivalent to the inequality that F is less than some constant depending on n, p, and q. Asymptotically, the critical point approaches 2, and hence the BIC is equivalent to the  $AIC.$ <sup>3/</sup>

It is also straightforward to see that the decision based on  $\overline{R}$ is also equivalent to the preliminary F test with a constant critical point equalling one.

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In what follows we confine our discussion to a class of decision rules based on the F statistic: choose M<sub>1</sub> if F  $\leq$  c and choose M<sub>2</sub> if F <sup>&</sup>gt; c, where c is nonnegative and varies with n, p, and q.

Following Mallows (1973) , we choose

$$
(2.14) \quad W_p = E \left[ \left| \frac{y}{z_0} - \frac{\hat{y}}{z} \right| \right]^2
$$

as a risk function of the model  $M_1$ , where  $Y_0$  is an n-dimensional random vector, independent of Y but distributed with the same mean y and variance-covariance matrix  $\omega^2 I$  as Y, and  $\hat{Y} = X (X'X)^{-1} X'Y$ . By virtue of the independence assumed between Y and Y<sub>0</sub>, we have

(2.15) 
$$
W_p = \mu' \left[ \frac{\pi}{2} - \frac{x_1}{2!} (\frac{x_1^* x_1}{2!} - \frac{1}{2!} \frac{x_1^*}{2!}) \right] \mu + (n + p) \omega^2
$$
  
 $= [\lambda_1 + \lambda_2 + (n + p)] \omega^2$ 

Similarly, the risk function of the model  $M^2$  is

(2.16) 
$$
W_{p+q} = \mu' \left[ I - X \left( X'X \right)^{-1} X' \right] \mu + (n+p+q) \omega^2
$$

$$
= \left[ \lambda_q + (n+p+q) \right] \omega^2
$$

If  $\hat{\omega}^2$  is an unbiased estimate of  $\omega^2$  independent of Y, then we can unbiasedly estimate  $W_p$  and  $W_{p+q}$  by  $C_p$  and  $C_{p+q}$ , because E  $(Q_p)$  =  $(\lambda_1 + \lambda_2 + n - p)$  w<sup>2</sup> and E  $(Q_{p+q}) = (\lambda_2 + n - p - q)$  w<sup>2</sup>.

Based on the Mallows' risk, we say that the simpler model  $M^1$  is better than  $M_2$  if  $W_p < W_{p+q}$  and <u>vice versa</u>. That is, we choose  $M_1$  if  $(2.17)$   $\lambda_1 \leq q$ 

and choose  $M_{\gamma}$  if  $\mathbf{Z}$  and  $\mathbf{Z}$  are the set of  $\mathbf{Z}$  and  $\mathbf{Z}$  are the set of  $\mathbf{Z}$ 

 $(2.18)$   $\lambda_1 > q$ 

Now we are in a position to define the unbiasedness of a decision rule.



Definition: A decision rule based on the F statistic with critical point c is said to be unbiased if (2.19) Pr  $(F < c | \lambda_1 \leq q) \geq .5$ and (2.20) Pr (F > c |  $\lambda_1$  > q) > .5.

If either of the above conditions is not fulfilled, the decision rule is said to be biased.

Noting that  $\lambda_1$  is the noncentrality parameter of the numerator of  $\perp$ F and also that the F distribution is continuous, we realize that the above conditions are equivalent to a single equality

(2.21) 
$$
\Pr
$$
 (F < c |  $\lambda_1 = q$ ) = .5

which implies that the probability of selecting  $M_1$  (or  $M_2$ ) is .5 when  $N_1$  and  $N_2$  ard indifferent.

Ine unbi-used critical point c satisfying  $(2.21)$  depends on the noncentrality parameter  $\lambda_2$  of the denominator as well as the degrees of freidem. The parameter  $\lambda_0$  measures the discrepancy of  $M_0$  from the Ithe diseribution. Since there is no way of estimating  $\lambda_2$ , we confine ourselves to the case when  $\lambda_2 = 0$ , i.e., when the more complicated model  $M<sub>2</sub>$  is true. The unbiased critical points are computed and tabulated in Table 2.1 for various values of q and n p-q. To solve the equation (2.21) we mad? use of the algorithm developed by Mudholkar, et al. (1976) for Gram-Charlier series approximation of the noncentral F distribution. The approximation is accurate enough for the present purpose. To compare the result with the conventional preliminary F test with a fixed significance level ve computed the probability of F exceeding the unbiased critical point under the null-hypothesis that  $M_1$  is true. The results are tabulated in Table 2.2.

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The following points are observed from these tables. First, the unbiased critical point Increases with q and decreases with the degrees of freedom. The MAIC and Mallows' procedures are biased toward the simpler model; i.e., they are favorable to the model with less parameters unless we have the extremely small degrees of freedom associated with the large number of additional parameters. Secondly, the implied significance level varies over a fairly wide range. This may imply that a decision rule with fixed level of significance may not be recommended as far as unbiasedness is concerned. Thirdly, the decision rule based on  $\overline{R}$  is nearly unbiased when  $q = 1$ . Therefore, a decision rule based on  $\overline{R}$  has a desirable property of unbiasedness if the decision is concerned with one additional variable.

#### 3. Approximate Formula

In this section we will derive the approximate formula for the unbiased critical point. Our decision has been based on the statistic F defined by (2.8), the distribution of which is the doubly noncentral F with q and  $\nu$  (= n-p-q) degrees of freedom and noncentrality parameters  $\lambda_1$  and  $\lambda_2$ . If we apply Patnaik's (1949) central  $\chi^2$  approximation to each of the noncentral  $\chi^2$  variates, we may approximate

(3.1) 
$$
\frac{1+\rho_2}{1+\rho_1} \mathbf{F}, \text{ where } \rho_1 = \frac{\lambda_1}{q} \text{ and } \rho_2 = \frac{\lambda_2}{v}
$$

by a central F distribution with degrees of freedom

(3.2) 
$$
v_1 = \frac{q(1 + 2\rho_1)}{(1 + \rho_1)^2}, v_2 = \frac{v(1 + 2\rho_2)}{(1 + \rho_2)^2}.
$$

Now we have an approximate equality

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 $\label{eq:2} \mathcal{L}=\left\{ \left\langle \left\langle \mathbf{r}_{1},\mathbf{r}_{2},\mathbf{r}_{3},\mathbf{r}_{4},\mathbf{r}_{5},\mathbf{r}_{6}\right\rangle \right\rangle \mathbf{r}_{1},\mathbf{r}_{2},\mathbf{r}_{3},\mathbf{r}_{4}\right\} ,$ and the control of the control of the company of the second company of the company of  $\mathcal{O}(\mathcal{O}_\mathcal{O})$  . The contract of the contract of the contract of  $\mathcal{O}(\mathcal{O}_\mathcal{O})$ 

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$$
(3.3) \qquad P(F \le c) \sim P[U = (\frac{\chi_1^2}{\nu_1})^{1/3} - c^{1/3} (\frac{1 + \rho_2}{1 + \rho_1})^{1/3} (\frac{\chi_2^2}{\nu_2})^{1/3} < 0].
$$

where  $\chi_1^2$  and  $\chi_2^2$  are independent  $\chi^2$  variate  $\rho$  with  $v_1$  and  $v_2$  degrees of freedom, respectively. The cubic root of the  $\chi^2$  variate is approximately normally distributed, and hence we approximate the distribution of U by the normal distribution. The approximate mean of U is given by

$$
(3.4) \qquad \mu_{\mathbf{U}} \simeq (1 - \frac{2}{9\nu_{1}}) - c^{1/3} \left( \frac{1 + \rho_{2}}{1 + \rho_{1}} \right)^{1/3} (1 - \frac{2}{9\nu_{2}})
$$

where the error of approximation is of order  $0(\nu_{1}^{-2})$  and  $0(\nu_{2}^{-2})$ . Since the median of the normal distribution is identical with the mean, the right hand side of (3.3) is approximately equal to 0.5 when  $\mu_{11} = 0$ , I.e.

(3.5) 
$$
c = \left(\frac{1 - 2/(9v_1)}{1 - 2/(9v_2)}\right)^3
$$

$$
= \frac{2}{1 + \rho_2} \left\{\frac{1 - 1/(6q)}{1 - 2(1 + 2\rho_2) / [9v(1 + \rho_2)^2]} \right\}^3
$$

The value of c given by (3.5) is monotone decreasing in  $\rho_2$ , and when  $p_{\eta} = 0$  it is equal to

$$
c = 2 \left\{ \frac{1 - 1/(6q)}{1 - 2/(9\nu)} \right\},
$$

which may be regarded as the approximate formula for the unbiased critical points tabulated in Table 2.1.

## 4. Conclusion

Various decision rules have been developed and used for the model selection in practical regression analysis. Some of them are based on intuitive reasoning, while others on sophisticated theoretical frameworks.  $\mathcal{L}^{\text{max}}$ 

In any case, as long as alternative models are nested, all the decision rules, considered in this paper, reduce to a decision based on the magnitude of the conventionally used F statistic. The difference among them is, therefore, described in terms of "implied" critical points.

To compare various decision rules we have introduced a certain criterion of optimality, which is termed the unbiasedness of a decision rule. The critical point for the F test that leads us to the unbiased decision has been calculated for various combinations of the degrees of freedom and the number of variables. It turned out that the decision rules which are customarily used are more or less biased; that is, the MAIC and Mallows' rules are biased toward the simpler model, whereas the minimum  $\bar{R}$  rule is rather biased toward the more complex model.

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Unbiased Critical Point

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Table

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## Footnotes

- 1. See Sawa (1976).
- 2. In Sawa (1976)  $\beta_0$  is denoted by the pseudo-true value of  $\beta$ .
- 3. For a small sample typically dealt with in practical data analysis, the difference between the AIC and BIC critical points Is far from negligible.

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 $\label{eq:2.1} \mathbf{u} = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 1 \end{bmatrix}, \qquad \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 1 \end{bmatrix}$ 

 $\label{eq:3.1} \frac{1}{\sqrt{2\pi}}\frac{d\Phi}{d\Phi} = \frac{1}{2\pi}\frac{d\Phi}{d\Phi}$ 

 $\mathcal{L}_{\text{max}}$  and  $\mathcal{L}_{\text{max}}$  and  $\mathcal{L}_{\text{max}}$ 

 $\sim 100$  km s  $^{-1}$ 







