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RIDGE ESTIMATION IN LINEAR REGRESSION

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ABSTRACT

Consider the linear regression model $Y = X\theta + \varepsilon$. Recently, a class of estimators, variously known as ridge estimators, has been proposed as an alternative to the least squares estimators in the case of collinearity, that is, when the design matrix $X'X$ is nearly singular. The ridge estimator is given by $\hat{\theta} = (X'X + KI)^{-1} X'Y$, where K is a constant to be determined. An optimal choice of the value of K is not known. This paper examines the risk (mean squared error) of the ridge estimator under the constraint $\theta'\theta \leq c$ and determines optimal values of K for which the risk is smaller than the risk of the least squares estimators where c is a constant.

Key words and phrases: Regression, Ridge Analysis, Multicollinearity, Mean Squared Error

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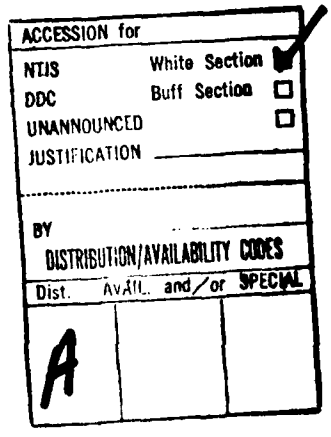

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RIDGE ESTIMATION IN LINEAR REGRESSION

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1. Introduction. In applications of multiple linear regression, the explanatory variables under consideration are often interrelated. The relation is technically called multicollinearity or near multicollinearity. The ordinary least squares estimate of the regression coefficients tends to become "unstable" in the presence of multicollinearity. More precisely, the variance of some of the regression coefficients becomes large. Hoerl (1959), (1962) and Hoerl and Kennard (1970,a), (1970,b) have suggested a class of estimators known as ridge estimators as an alternative to the least squares estimation in the presence of multicollinearity. The new method of estimation is called ridge analysis.

Ridge analysis has drawn considerable interest in recent years. The technique has been developed and new results have been obtained by several authors, e.g., Hawkins (1975), Hemmerle (1975), Sidik (1975). Newhouse and Oman (1975) have conducted a series of Monte Carlo experiments to compare the performance of ridge analysis with the least squares.

The ridge analysis is an ad hoc procedure which gives a biased estimator. We compare the ridge estimator with the least squares estimator with respect to the mean squared error. Hoerl and Kennard (1970,a) have claimed in their paper that for a certain choice of a parameter (K) the ridge estimator is uniformly superior to the least squares estimator. This is not true. It appears that the limitation of any optimal property of the ridge estimator and its relation to other known estimators is not often clearly comprehended by many applied statisticians engaged in regression analysis. The object of this paper is to expose the essential features of ridge analysis.

In the following section we show a basis for the choice of the ridge estimator, its biased character and compare it with an unbiased estimator. Furthermore, we obtain conditions under which the ridge estimator has smaller mean squared error than the least squared estimator.

2. Ridge analysis. Consider the linear regression model

$$Y = X\theta + \varepsilon$$

where Y is $n \times 1$ vector of observations, X is $n \times p$ design matrix, θ is $p \times 1$ vector of unknown parameters ε is $n \times 1$ vector of the observational errors. It is assumed that the components of ε are uncorrelated, and have a common variance equal to σ^2, say. Also, $E(\varepsilon) = 0$. Let prime denote the transpose of a vector or matrix. The least squares estimate of θ is obtained by minimizing $(Y-X\theta)'(Y-X\theta)$ with respect to θ, and is given by

(2.1) $$\hat{\theta} = (X'X)^{-1} X'Y.$$

It is assumed that the columns of X are linearly independent and therefore the rank of the design matrix X'X is equal to p.

We have $E[\hat{\theta}] = \theta$. That is, $\hat{\theta}$ is an unbiased estimator of θ. Let $\lambda_1, \ldots, \lambda_p$ denote the characteristic roots of X'X. The mean squared error of $\hat{\theta}$ ($MSE\hat{\theta}$) is given by

(2.2) $$E(\hat{\theta}-\theta)'(\hat{\theta}-\theta) = \sigma^2 \text{ trace } (X'X)^{-1}$$
$$= \sigma^2 \sum_{i=1}^{p} \frac{1}{\lambda_i} .$$

If the explanatory variables are nearly multicollinear then the matrix X'X is illconditioned, that is, one (or more) of the characteristic roots of X'X is small. In that case MSE θ becomes large, as it is seen from (2.2). We can avoid MSE θ becoming large by inflating the characteristic roots. That is, substituting $\tilde{\theta}$ for θ, given by

(2.3) $$\tilde{\theta} = (X'X+KI)^{-1} X'Y$$

where I is $p \times p$ identity matrix and K is a positive number. The estimator $\tilde{\theta}$ is the ridge estimator, proposed by Hoerl and Kennard as an alternative to the least squares estimator.

We have

(2.4) $$E\tilde{\theta} = (X'X+KI)^{-1}(X'X)\theta$$

Therefore, $\tilde{\theta}$ is a biased estimator of $\hat{\theta}$ unless K = 0, in which case $\tilde{\theta} = \hat{\theta}$. Let P be an orthogonal matrix diagonalizing X'X, that is

$$PX'XP' = D$$

where D is a diagonal matrix with the ith diagonal element equal to λ_i. Let $\alpha = (\alpha_1, \ldots, \alpha_p)' = P\theta$. The mean squared error is given after simplification by

(2.5) $$E(\tilde{\theta}-\theta)'(\tilde{\theta}-\theta) = \sigma^2 \sum_{i=1}^{p} \frac{\lambda_i}{(\lambda_i+K)^2} + K^2 \sum \frac{\alpha_i^2}{(\lambda_i+K)^2} .$$

From (2.2) and (2.5) we see that for any given K > 0

$$MSE\,\tilde{\theta} > MSE\,\hat{\theta}$$

for sufficiently large values of $\theta'\theta$. Therefore, the ridge estimator can be compared to the least squares estimator only if θ is constrained. Suppose it is known apriori that $\theta'\theta \leq c$ where c is a positive number. This condition would be

realized in many practical situations. Since $\theta'\theta = \alpha'\alpha$, we have $\alpha_i^2 \leq c$, $i = 1, \ldots, p$. Hence from (2.5) we get

$$\text{(2.6)} \qquad \text{MSE } \tilde{\theta} \leq \sigma^2 \sum_{i=1}^{p} \frac{\lambda_i}{(\lambda_i+K)^2} + K^2 c \sum_{i=1}^{p} \frac{1}{(\lambda_i+K)^2} \quad .$$

Theorems 2.1, 2.2, and 2.3 below give certain results on the choice of K in order that the ridge estimator has smaller mean squared error than the least squares estimator.

Theorem 2.1. If $\theta'\theta \leq c$ then MSE $\tilde{\theta}$ < MSE $\hat{\theta}$ for $0 < K \leq \frac{2\sigma^2}{c}$.

Proof: From (2.6) we have for $K \leq \frac{2\sigma^2}{c}$

$$\text{MSE } \tilde{\theta} \leq \sigma^2 \sum_{i=1}^{p} \frac{\lambda_i}{(\lambda_i+K)^2} + \frac{2K}{(\lambda_i+K)^2}$$

$$= \sigma^2 \sum_{i=1}^{p} \frac{\lambda_i+2K}{(\lambda_i+K)^2}$$

$$< \sigma^2 \sum_{i=1}^{k} \frac{1}{\lambda_i}$$

$$= \text{MSE } \hat{\theta} \quad .$$

Theorem 2.2. If $\theta'\theta < \frac{\sigma^2}{p} \sum_{i=1}^{p} \frac{1}{\lambda_i}$ then MSE $\tilde{\theta}$ < MSE $\hat{\theta}$ for $K > 0$.

Proof: Let D(K) denote the quantity on the right hand side of (2.6). Differentiating D(K) with respect to K we have

$$\text{(2.7)} \qquad \partial D(K)/\partial K = \sum_{i=1}^{p} \frac{2\lambda_i (cK-\sigma^2)}{(\lambda_i+K)^2} \quad .$$

The right hand side of (2.7) is equal to zero for $K = \frac{\sigma^2}{c}$ and is $<(>)\ 0$ for $K <(>) \frac{\sigma^2}{c}$. Therefore, D(K) is first decreasing then increasing as K varies from 0 to ∞. Now

$$D(0) = \sigma^2 \sum_{i=1}^{p} \frac{1}{\lambda_i}$$

$$= \text{MSE } \hat{\theta}$$

$$D(\infty) = pc \quad .$$

Hence

$$D(c) \leq \max(pc, \text{MSE } \tilde{\theta})$$

$$= \text{MSE } \hat{\theta} \text{ for } c \leq \frac{\sigma^2}{p} \sum_{i=1}^{p} \frac{1}{\lambda_i} .$$

Since $D(K)$ is an upper bound on the value of MSE $\hat{\theta}$, the theorem follows. []

From a Bayesian point of view suppose that the components of θ are independently and identically distributed with means ξ and variance τ^2.

Theorem 2.3. If the components of θ are independently and identically distributed with mean ξ and variance τ^2 then the average mean squared error of the ridge estimator is minimized for $k = \sigma^2/(\xi^2+\tau^2)$.

Proof: Let E denote expectation with respect to the given prior distribution of θ. We have

$$E(\text{MSE } \tilde{\theta}) = \sigma^2 \sum_{i=1}^{p} \frac{\lambda_i}{(\lambda_i+K)^2} + K^2 \sum_{i=1}^{p} \frac{\xi^2+\tau^2}{(\lambda_i+k^2)} . \tag{2.8}$$

As in the proof of Theorem 2.2 we find that the right hand side of (2.8) is minimized for $K = \sigma^2/(\xi^2+\tau^2)$. []

We have seen above that the ridge estimator is preferred to the least squares estimator in certain situations when the parameter θ is constrained. The following theorem gives a basis for the choice of the ridge estimator under the given constraint.

Theorem 2.4. The value of θ minimizing $R(\theta) = (Y-X\theta)'(Y-X\theta)$, given $\theta'\theta \leq c$ is equal to $\tilde{\theta}$ where K is chosen such that $\tilde{\theta}'\tilde{\theta} = c$.

Proof: By direct computation we get

$$\tilde{\theta}'\tilde{\theta} = (PX'Y)'(D+KI)^{-2}(PX'Y) . \tag{2.9}$$

It is seen from (2.9) that $\tilde{\theta}'\tilde{\theta}$ is decreasing in K. Therefore, the value of K, given by $\tilde{\theta}'\tilde{\theta} = c$ is uniquely determined.

We have

$$\begin{aligned} R(\tilde{\theta}) &= (Y-X\tilde{\theta})'(Y-X\tilde{\theta}) \\ &= (Y-X\hat{\theta})'(Y-X\hat{\theta}) + (X'Y)'[(X'X+KI)^{-1}-(X'X)^{-1}] \\ &\quad X'X[(X'X+KI)^{-1}-(X'X)^{-1}](X'Y) \\ &= (Y-X\hat{\theta})'(Y-X\hat{\theta}) + (PX'Y)'\, D^*\, (PX'Y) \end{aligned} \tag{2.10}$$

where D^* is a $p \times p$ diagonal matrix whose ith diagonal element is equal to

$$\frac{k^2}{\lambda_i^2(k+\lambda_i)^2} .$$

From (2.10) we see that $R(\tilde{\theta})$ is increasing in k.

Consider the problem of minimizing $R(\theta)$ with respect to θ under the constraint $\theta'\theta = c$. By the Langrangian method the minimizing value of θ is given by

$$\lambda\theta - X'(Y-X\theta) = 0$$

or

$$\theta = (X'X+\lambda I)^{-1}X'Y$$

where λ is determined such that $\theta'\theta = c$. That is, the minimizing value of θ is the ridge estimator $\tilde{\theta}$, where k is determined such that $\tilde{\theta}'\tilde{\theta} = c$.

We have shown above $\tilde{\theta}_k'\tilde{\theta}_k$ is decreasing in k and that $R(\tilde{\theta})$ is increasing in k. It follows that $\tilde{\theta}$ which minimizes $R(\theta)$ under the constraint $\theta'\theta = c$, minimizes $R(\theta)$ also under the constraint $\theta'\theta \leq c$. □

Remark: We have a comparison between the least squares estimation and ridge estimation. The ridge estimator is given by minimizing $R(\theta)$ under a certain constraint on the value of $\theta'\theta$, whereas the least squares estimator is given by minimizing $R(\theta)$ without that constraint.

Throughout the foregoing discussion we have assumed that the quantity k arising in the definition of the ridge estimator $\tilde{\theta}$, is a scalar constant. By letting k depend on the observation Y suitably, we might be able to obtain an estimator which has a smaller MSE than the least squares estimator for all values of θ. Hoerl and Kennard (1970,a) have suggested an iterative method of choosing such a value of K. However, they did not show that the final estimator had a smaller MSE than the least squares estimator. On the other hand, (see Alam (1974)) any estimator of the form

$$\phi((Y'X(X'X)^{-1}X'Y)/\sigma^2)\ \hat{\theta}$$

has smaller MSE than $\hat{\theta}$ where $\phi(Z)$ is a function, such that, $Z(1-\phi(Z))$ is non-decreasing in Z and $0 \leq Z(1-\phi(Z)) \leq 2\alpha p - 4$ and

$$\alpha = \left(\frac{1}{p}\sum_{i=1}^{p}\frac{1}{\lambda_i}\right)\min(\lambda_1, \ldots, \lambda_p) .$$

See also, Sclove (1968) and Stein (1960).

References

[1] Alam, K. (1974). Minimax estimators of the mean of a multivariate normal distribution. Tech. Report, Mathematical Sciences, Clemson University.

[2] Hawkins, D. M. (1975). Relations Between Ridge Regression and Eigenanalysis of the Augmented Correlation Matrix. Technometrics, Vol. 17, pp. 477-80.

[3] Hemmerle, W. J. (1975). An Explicit Solution for Generalized Ridge Regression. Technometrics, Vol. 17, pp. 309-14.

[4] Hoerl, A. E. (1959). Optimum Solution of Many Variable Equations. Chemical Engineering Progress 55, pp. 69-78.

[5] Hoerl, A. E. (1962). Applications of Ridge Analysis to regression problems. Chemical Engineering Progress 58, pp. 54-59.

[6] Hoerl, A. E. and Kennard, R. W. (1970). Biased Estimation for Nonorthogonal Problems. Technometrics, Vol. 12, pp. 55-67.

[7] Hoerl, A. E. and Kennard, R. W. (1970). Ridge Regression: Application to non-orthogonal problems. Technometrics, Vol. 12, pp. 69-82.

[8] Newhouse, J. P. and Oman, S. D. (1971). An evaluation of ridge estimators. Rand Technical Report R-716-PR.

[9] Sclove, S. L. (1968). Improved estimators for coefficients in linear regression. J. Amer. Statisti. Assoc. 63, 597-606.

[10] Sidik, S. M. (1975). Comparison of Some Biased Estimation Methods (Including Ordinary Subset Regression) in the Linear Model. Nasa Technical Report TN D-7932.

[11] Stein, C. M. (1960). Multiple regression. Contributions to probability and statisitics. Essays in honour of Harold Hotelling, Olkin, I (ed.), Stanford University Press, 423-43.

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Consider the linear regression model $Y = X\theta + \varepsilon$. Recently, a class of estimators, variously known as ridge estimators, has been proposed as an alternative to the least squares estimators in the case of collinearity, that is, when the design matrix $X'X$ is nearly singular. The ridge estimator is given by $\hat{\theta} = (X'X + KI)^{-1} X'Y$, where K is a constant to be determined. An optimal choice of the value of K is not known. This paper examines the risk (mean squared error) of the ridge estimator under the constraint $\theta'\theta \leq c$ and determines optimal values of K for which

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the risk is samller than the risk of the least squares estimators where c is a constant.