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Ridge Estimation in Functional Measurement Error Models

A. R. Rasekh

Department of Statistics, Ahwaz University, Ahwaz, Iran

Abstract. We propose a ridge estimator as an alternative estimator in the presence of collinearity among the elements of unobservable values in functional measurement error models. Modifications of the estimator are also considered and properties derived which are analogous to those known in ordinary linear models. Our simulation results show that the modified ridge estimate will have shorter length, mean square errors and standard errors, than other estimates of the coefficients of the model.

Keywords: biased estimators, collinearity, functional relationship, parametric bootstrap, ridge parameter, variance reduction.

1. Introduction

Collinearity is troublesome and the effects of its presence on different aspects of linear models is well known (see for instance, Belsley, 1991). When there is collinearity among the predictor variables in ordinary linear model, alternative estimation procedures have been proposed which are generally biased. Among these procedures ridge estimators have received particularly attention. Hoerl and Kennard (1970, a, b) have introduced the ridge estimators and a large number of papers on the subject have been written since then. Recently, the ridge estimation techniques have been extended to generalized linear models. One can refer to Schaefer et al. (1984) and Nyquist (1991) for different versions of the extended ridge techniques in generalized linear models. Gamboa and Gunst (1992) have considered collinearity in measurement error models and defined collinearity in terms of a relationship between elements of unobservable values. Apart from this work, little attention has been given to the effects of collinearity on different aspects of the estimates of parameters of functional

measurement error models, nor to ridge estimation procedure as an alternative in the present of collinearity. Therefore, we concentrate here on functional measurement error models and consider collinearity and ridge estimates in this context. The functional measurement error model can be defined as follows:

$$\begin{aligned} Y_i &= y_i + e_i \\ X_i &= x_i + u_i \quad i = 1, \dots, n \\ y_i &= \beta'x_i. \end{aligned}$$

In this model x_i is a $p \times 1$ vector and y_i is a scalar of unobservable fixed values which can be observed through the $p \times 1$ random vector X_i and the random variable Y_i , respectively. The $p \times 1$ parameter vector β is unknown and to be estimated based on observations. We define $\varepsilon'_i = (e_i, u'_i)$, $i = 1, \dots, n$, as the errors of the model which are independent and we assume they have normal distribution with zero mean and

covariance matrix $\Sigma_{\varepsilon\varepsilon} = \begin{bmatrix} \sigma_{ee} & \Sigma_{eu} \\ \Sigma_{ue} & \Sigma_{uu} \end{bmatrix}$.

Generally we would anticipate that replicate observations are available on this model and so an estimate of the $\Sigma_{\varepsilon\varepsilon}$ exists and is given by $S_{\varepsilon\varepsilon} = \begin{bmatrix} S_{ee} & S_{eu} \\ S_{ue} & S_{uu} \end{bmatrix}$, but since the replicates do not directly affect the central themes of the work below, we have simplified the notation by referring only to single observations (see example in section 3). If we define $Z'_i = (Y_i, X'_i)$, $i = 1, \dots, n$, then the consistent estimate of β is

$$\hat{\beta} = (M_{XX} - \tilde{\tau}S_{uu})^{-1}(M_{XY} - \tilde{\tau}S_{ue}) \quad (1)$$

in which S_{uu} and S_{ue} are estimates of Σ_{uu} and Σ_{ue} , respectively, and

$$M_{ZZ} = n^{-1} \sum_{i=1}^n Z_i Z'_i = \begin{bmatrix} M_{YY} & M_{YX} \\ M_{XY} & M_{XX} \end{bmatrix}$$

$\tilde{\tau}$ is the smallest eigenvalue of M_{ZZ} in the metric of $S_{\varepsilon\varepsilon}$ and is derived from the

equation $|M_{ZZ} - \tau S_{\varepsilon\varepsilon}| = 0$ (see for instance, Cheng and Van Ness, 1999). Let

$\Gamma_{xx} = \lim_{n \rightarrow \infty} n^{-1} \sum_{i=1}^n x_i x_i'$ be the second order moment matrix of the model and assume

that Γ_{xx} is a positive definite matrix. We can show that $\hat{\Gamma}_{xx} = (M_{XX} - \tilde{\tau} S_{uu})$ is a consistent estimate of Γ_{xx} (see Fuller, 1987, p. 128) and so another representation for $\hat{\beta}$ is $\hat{\beta} = \hat{\Gamma}_{xx}^{-1} (M_{XY} - \tilde{\tau} S_{ue})$. Furthermore, an asymptotic covariance matrix of $\hat{\beta}$ is

$$\Sigma_{\beta\beta} = \Gamma_{xx}^{-1} \{ (\Sigma_{uu} + \Gamma_{xx}) \sigma_{vv} - \Sigma_{uv} \Sigma_{vu} \} \Gamma_{xx}^{-1} \quad (2)$$

in which $\sigma_{vv} = \sigma_{ee} + \beta' \Sigma_{uu} \beta - 2\beta' \Sigma_{ue}$ and $\Sigma_{uv} = \Sigma_{eu} - \beta' \Sigma_{uu}$.

Gamboa and Gunst (1992) defined collinearity in terms of a relationship between elements of the unobservable x_i values using the second order moment matrix Γ_{xx} . They derived asymptotic justification of using the estimator of Γ_{xx} as a basis for diagnosis of collinearity in measurement errors models.

In section 2 we concentrate on ridge estimates in the context of functional measurement error models and we derive the ridge estimate of β . In section 3 we look at an example using a set of data relating to Egyptian pottery. Finally, section 4 contains a parametric bootstrap simulation study, with the aim of comparing $\hat{\beta}$ and two different versions of the ridge estimates.

2. Ridge estimation

In ordinary and generalized linear models the idea of ridge estimation is to fix the length of the regression coefficient vector β to say H , and to minimize the sum of squares errors subject to this constraint. We examine this argument in order to derive a ridge estimate of the parameter β in our functional measurement error models. Our argument is as the one used in generalized linear models, using Newton-Raphson

iteration.

According to Sprent (1966) an estimate of the parameter β can be derived using the following normalized sum of squares equation

$$Q(\beta) = \sigma_{vv}^{-1} \sum_{i=1}^n (Y_i - \beta'X_i)^2. \quad (3)$$

Fuller (1987, p. 125) shows that under the assumption of normality, maximization of the likelihood function with respect to β is equivalent to minimization of the normalized sum of squares equation.

To derive a ridge estimate of the parameter β , using Newton-Raphson minimization procedure, we can minimize the restricted sum of squares equation

$$Q^k(\beta) = \sigma_{vv}^{-1} \sum_{i=1}^n (Y_i - \beta'X_i)^2 - \frac{kn}{2} (\beta'\beta - H)$$

in which $-2^{-1}k$ is the Lagrange multiplier. The first derivative of $Q^k(\beta)$ with respect to β is

$$\begin{aligned} U^k(\beta) &= \sigma_{vv}^{-1} \sum_{i=1}^n v_i \ddot{x}_i - nk\beta \\ &= U(\beta) - nk\beta \end{aligned} \quad (4)$$

where $\ddot{x}_i = X_i - \sigma_{vv}^{-1} \sum_{uv} v_{uv} v_i$, $v_i = Y_i - \beta'X_i$ and $U(\beta) = \sigma_{vv}^{-1} \sum_{i=1}^n v_i \ddot{x}_i$. Furthermore,

the derivative of $U^k(\beta)$ with respect to β is $\frac{\partial U^k(\beta)}{\partial \beta} = -\sigma_{vv}^{-1} \sum_{i=1}^n \ddot{x}_i \ddot{x}_i' - nkI$. If we

denote the negative of the derivative of $U^k(\beta)$ and the derivative of $U(\beta)$ by $\Omega^k(\beta)$ and $\Omega(\beta)$, respectively, then we have

$$\Omega^k(\beta) = \Omega(\beta) + nkI. \quad (5)$$

If we denote the restricted estimate of β from (4) (which is a function of the k) by $\tilde{\beta}(k)$, then an approximation to this estimate can be obtained by carrying out a Taylor

series expansion of the first derivative $U^k(\beta)$ about the real parameter value β_0 . This procedure yields

$$U^k\{\tilde{\beta}(k)\} = U^k(\beta_0) - \{\tilde{\beta}(k) - \beta_0\}' \Omega^k(\beta_0).$$

Using relations (4), (5) and the fact that $U^k\{\tilde{\beta}(k)\} = 0$, the first order approximation of $\tilde{\beta}(k)$ is

$$\begin{aligned} \tilde{\beta}(k) &= \{\Omega^k(\beta_0)\}^{-1} \{U^k(\beta_0) + \Omega^k(\beta_0)\beta_0\} \\ &= \{\Omega(\beta_0) + nkI\}^{-1} \{U(\beta_0) + \Omega(\beta_0)\beta_0\}. \end{aligned}$$

On the other hand, using unrestricted sum of squares equation (3), a first order estimate of β , say $\hat{\beta}$, is

$$\hat{\beta} = \beta_0 + \Omega^{-1}(\beta_0)U(\beta_0). \quad (6)$$

Hence a first order ridge estimate $\tilde{\beta}(k)$ is

$$\tilde{\beta}(k) = \{\Omega(\beta_0) + nkI\}^{-1} \Omega(\beta_0)\hat{\beta}. \quad (7)$$

Replacing β_0 by its estimate $\hat{\beta}$, from the definition of $\Omega(\beta)$ we have

$$\Omega(\hat{\beta}) = \hat{\sigma}_{vv}^{-1} \sum_{i=1}^n \hat{x}_i \hat{x}_i' \quad (8)$$

in which $\hat{x}_i = X_i - \hat{\sigma}_{vv}^{-1} \hat{\Sigma}_{uv} \hat{v}_i$ and $\hat{v}_i = Y_i - \hat{\beta}' X_i$. Substituting (8) in (7) we have

$$\tilde{\beta}(k) = (\hat{\sigma}_{vv}^{-1} \sum_{i=1}^n \hat{x}_i \hat{x}_i' + nkI)^{-1} \hat{\sigma}_{vv}^{-1} \sum_{i=1}^n \hat{x}_i \hat{x}_i' \hat{\beta}.$$

If we define $\tilde{\Gamma} = n^{-1} \sum_{i=1}^n \hat{x}_i \hat{x}_i'$, then we have

$$\tilde{\beta}(k) = (\hat{\sigma}_{vv}^{-1} \tilde{\Gamma}_{xx} + kI)^{-1} \hat{\sigma}_{vv}^{-1} \tilde{\Gamma}_{xx} \hat{\beta}. \quad (9)$$

Finally, using $\hat{\beta}$ from (1) instead of the first order estimate (6) in (9), the ridge estimate of β is obtained. It is obvious that for k equal to zero, the ridge estimate

$\tilde{\beta}(k)$ is exactly the same as the estimate $\hat{\beta}$. One problem with the ridge estimate $\tilde{\beta}(k)$ is that $\tilde{\Gamma}_{xx}$ is not a consistent estimate of Γ_{xx} . In fact we can show that $\tilde{\Gamma}_{xx} = \Gamma_{xx} + \Sigma_{\eta\eta} + o_p(1)$ in which $\Sigma_{\eta\eta} = \Sigma_{uu} - \sigma_{vv}^{-1} \Sigma_{uv} \Sigma_{vu}$. An alternative definition of the ridge estimate can be suggested using the consistent estimate $\hat{\Gamma}_{xx} = M_{XX} - \tilde{\tau} \Sigma_{uu}$ instead of $\tilde{\Gamma}_{xx}$ in (9). Using $\hat{\Gamma}_{xx}$, a different version of the ridge estimate is given as

$$\hat{\beta}(k) = (\hat{\sigma}_{vv}^{-1} \hat{\Gamma}_{xx} + kI)^{-1} \hat{\sigma}_{vv}^{-1} \hat{\Gamma}_{xx} \hat{\beta}.$$

In the literature k has been referred to as the ridge parameter. The choice of this parameter in ordinary linear model is still unresolved and because of this problem several approaches have been developed to guide the data analyst in selection of the ridge parameter values. Some of the approaches give cut-off points that are based on the different functions of the estimate of β , while the other approaches suggest a plotting scheme using mean square errors or elements of the ridge estimators versus different values of the k and looking for the best value of the k . We suggest using this latter technique for selecting the ridge parameter in functional measurement error models.

The ridge estimate $\hat{\beta}(k)$ has some properties, which are analogous with those for the ridge estimate in ordinary linear models. Instead of an analytical illustration, in section 4, we consider these properties using a parametric bootstrap simulation study.

3. Example

In this section we consider an example using a set of data which we refer to as the Egyptian pottery data. Briefly, this data set arises from an extensive archaeological survey of pottery production and distribution in the ancient Egyptian city of Al-Amarna. The data consist of measurements of chemical contents (mineral elements) made on many samples of pottery using two different techniques, *NAA* and *ICP* (see

Smith et al, 1988 for description of techniques). The set of pottery has been collected from different locations around the city and each pottery has its own "fabric code". Archaeologists believe that observations from pottery with the same fabric code and from the same provenance can essentially be regarded as replicated observations. Our preliminary analysis using multivariate analysis of variance (not reported here) also confirmed this idea. Consequently, the data set has been divided into $n = 27$ groups and in each group there are replicated observations. Due to limitation of space the original data set is not given here, but it is available from the author on request. Among all mineral elements our interest is in the relation between Na measured with NAA versus six elements Na, Al, K, V, Cr and Mn measured with ICP . Thus, we fitted a functional measurement error model to this data set.

Table 1. Eigenvalues, condition indexes and variance decomposition proportion of the matrix $\hat{\Gamma}_{xx}$ in the scaled form.

Eigenvalue	Condition index	Variance decomposition proportions					
		$\hat{\beta}_1$	$\hat{\beta}_2$	$\hat{\beta}_3$	$\hat{\beta}_4$	$\hat{\beta}_5$	$\hat{\beta}_6$
5.461	1.000	0.004	0.000	0.001	0.000	0.008	0.000
0.351	3.944	0.025	0.001	0.004	0.000	0.847	0.000
0.115	6.897	0.868	0.004	0.010	0.005	0.041	0.008
0.039	11.883	0.020	0.129	0.047	0.001	0.018	0.190
0.031	13.273	0.015	0.064	0.822	0.028	0.016	0.000
0.004	38.295	0.067	0.802	0.116	0.966	0.069	0.801

We considered the eigenstructure of the matrix $\hat{\Gamma}_{xx}$ in the scaled form (see Gamboa and Gunst, 1992) as basis for the collinearity diagnostic in this case. The eigenvalues and condition indexes (see Belsley, 1991) of this matrix are presented in the first two columns of table 1. In practice, some cut-off points for comparing the magnitude of calculated condition indexes have been suggested. Belsley (1991) suggests using the value 30 as a cut-off point for the existence moderate collinearity.

Comparing the calculated condition indexes given in this table we can see that there is one collinearity among the elements of unobservable x_i values.

In order to specify the variables that are involved in collinearity, we considered the variance decomposition proportion method, using the asymptotic covariance matrix of $\hat{\beta}$, given in (2), in the scaled form. One can refer to Belsley (1991) for full description of this method in ordinary linear model and to Rasekh (1996) for adaptation of this technique in functional measurement error models.

The numerical results of the variance decomposition proportion in the ordered form according to the condition indexes are given in columns 3 to 8 of table 1. The elements in each column indicate the proportion of each condition index for the variance of each element of $\hat{\beta}$. A glance at results of this table verifies that the condition index of the last row, which is the largest one, plays a large role in the variance decomposition proportions of the columns 2, 4 and 6, indicating involvement of the 2nd, 4th and 6th elements of the unobservable x_i values in a collinear relation. In order to derive the ridge estimate of β we standardized the elements of the observable random vectors (Y_i, X_i') , $i = 1, \dots, n$, so that they will have the unit length. Therefore, the parameters of the model will also be in the scaled form. We computed several $\hat{\beta}(k)$ for different values of the k in the interval $(0, 1)$ and with increment 0.01. Then we plotted elements of the $\hat{\beta}(k)$ versus different k values.

Figure 1 exhibits the ridge trace of the elements of $\hat{\beta}(k)$ versus different values of k . In this figure ridge estimates $\hat{\beta}_4(k)$ and $\hat{\beta}_5(k)$ have small values and are around the zero line. Increasing k has the great effect on the coefficient estimate $\hat{\beta}_6(k)$ of the 6th element of unobservable x_i values (Mn element) which is involve in collinearity. It drops quickly in magnitude while the coefficient estimates for the noncollinear x_i values change relatively little as k is increased. Visual inspection of the ridge trace

suggests that a small value of k , one in the interval (0.10, 0.20), produces a stabilisation of the ridge trace. In fact from this figure we can see that all estimators are reasonably stable in this interval and so a choice of k equals to 0.15 is reasonable.

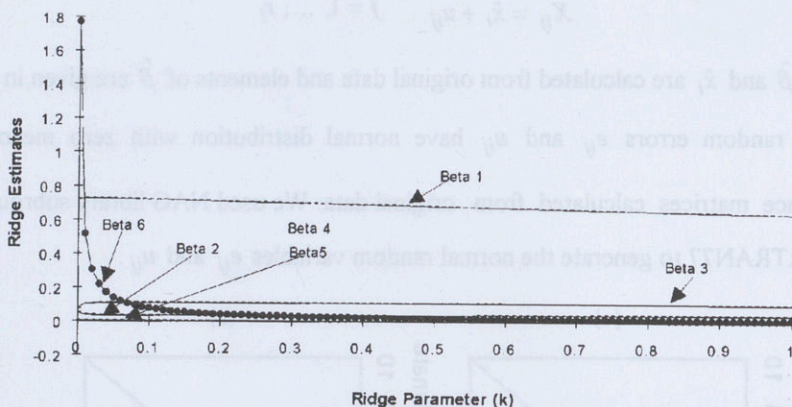


Figure 1. Plot of elements of the ridge estimate versus different values of k^* .

4. Parametric bootstrap study

In ordinary and generalized linear models many simulation studies have been constructed with the aim of comparing different aspects of various biased estimation procedures with each other and with subset selection procedures. One can refer to recent works by Breiman (1995), Frank and Friedman (1993) and Hoerl, Schuenemeyer and Hoerl (1986). However, in functional measurement error models the task of collinearity diagnostic and biased estimation procedures has only started. Therefore, in this section we will be restricted to a relatively smaller simulation study including only the estimate $\hat{\beta}$ and two versions of the ridge estimate of β . The aim of this study is to get a picture of these estimates using a parametric bootstrap simulation with 5000 replicates. The bootstrap study is based on the Egyptian pottery data set, which has been used in the previous section. We generated data with the following specifications:

The group number is $n = 27$ and the numbers of replications in each group, r_i , is

the same as those for the original data. In each step of the bootstrap replications we generated data for the model

$$\begin{aligned} Y_{ij} &= \hat{\beta}'\hat{x}_i + e_{ij} & i = 1, \dots, 27 \\ X_{ij} &= \hat{x}_i + u_{ij} & j = 1, \dots, r_i \end{aligned}$$

where $\hat{\beta}$ and \hat{x}_i are calculated from original data and elements of $\hat{\beta}$ are given in table 1. The random errors e_{ij} and u_{ij} have normal distribution with zero mean and covariance matrices calculated from original data. We used NAG library subroutines for FORTRAN77 to generate the normal random variables e_{ij} and u_{ij} .

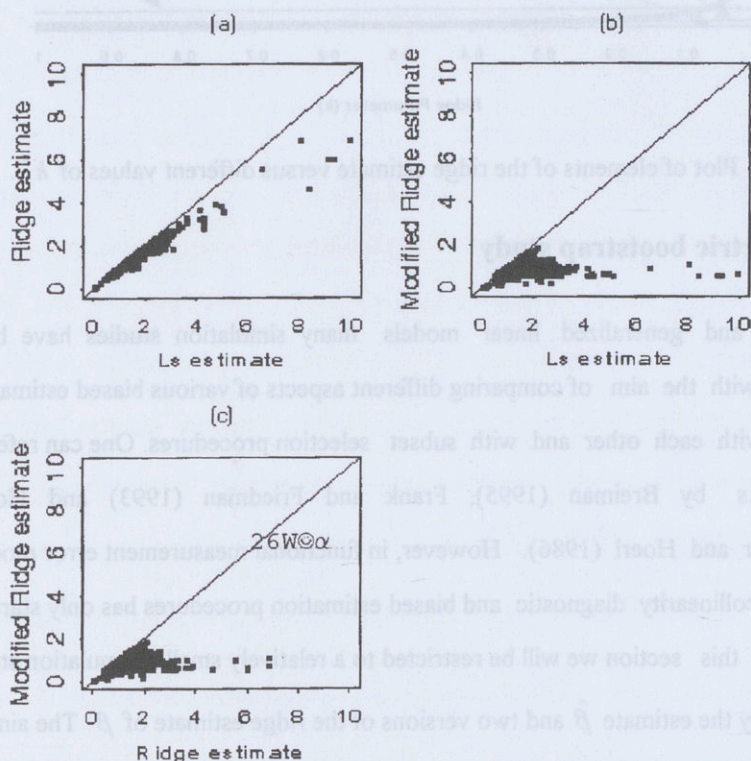


Figure 2. Plot of the bootstrap replicates of (a) $\hat{\beta}'(k)\hat{\beta}(k)$ against $\hat{\beta}'\hat{\beta}$, (b) $\tilde{\beta}'(k)\tilde{\beta}(k)$ against $\hat{\beta}'\hat{\beta}$ and (c) $\hat{\beta}'(k)\hat{\beta}(k)$ against $\tilde{\beta}'(k)\tilde{\beta}(k)$.

We simulated 5000 data sets and in each step we calculated estimators $\hat{\beta}$, $\tilde{\beta}(k)$ and $\hat{\beta}(k)$ and their square length for the ridge parameter $k = 0.15$. Plots of the length

of different estimates versus each other are given in figure 2. In each step we also considered the appropriateness of the ridge specific value of $k = 0.15$ and found that generally this value was appropriate. Figures 2.a and 2.b show plots of the bootstrap replicate of $\tilde{\beta}'(k)\tilde{\beta}(k)$ and $\hat{\beta}'(k)\hat{\beta}(k)$ versus $\hat{\beta}'\hat{\beta}$, respectively. These figures indicate that different versions of the ridge estimates will produce estimates of the parameters with shorter length rather than $\hat{\beta}$. Figure 2.c is also a plot of the bootstrap replicates of $\hat{\beta}'(k)\hat{\beta}(k)$ versus $\tilde{\beta}'(k)\tilde{\beta}(k)$. From this plot we find that $\hat{\beta}(k)$ will produce shorter estimates than $\tilde{\beta}(k)$, specially when the estimated vector is long.

Table 2 exhibits elements of the estimate $\hat{\beta}$ and the mean values of bootstrap estimates $\tilde{\beta}(k)$ and $\hat{\beta}(k)$ for the value $k = 0.15$. The last row of this table also gives us the mean length of the different bootstrap estimates. From this table we can also see that the length of the estimator $\hat{\beta}(k)$ is shorter than any other estimator.

Table 2. $\hat{\beta}$ and mean values of bootstrap estimates of $\tilde{\beta}(k)$ and $\hat{\beta}(k)$ and mean values of their squared length.

Parameter	$\hat{\beta}$	Bootstrap $\tilde{\beta}(k)$	Bootstrap $\hat{\beta}(k)$
β_1	0.72114	0.75737	0.75742
β_2	0.04845	0.03713	0.03701
β_3	0.07625	0.09092	0.09241
β_4	-0.00286	-0.00201	-0.00200
β_5	0.00018	0.00045	0.00043
β_6	1.76933	0.06857	0.07815
$\beta'\beta$	3.65874	0.95801	0.73516

Further, table 3 presents the bootstrap estimate of standard errors (s.e.) of the elements of $\hat{\beta}$, $\tilde{\beta}(k)$ and $\hat{\beta}(k)$ and shows that standard errors of the elements of parameter estimator is slightly improved using the ridge technique, but comparing standard errors of different versions of the ridge estimates, we can see that $\hat{\beta}(k)$ is

favourable to $\tilde{\beta}(k)$ concerning standard errors properties.

Finally, we calculated the mean square errors of different estimators and compared the percent reductions in mean square errors of the ridge estimates with one for $\hat{\beta}$. The results are given in last rows of the table 3. Indications are that using $\hat{\beta}(k)$ the percent reduction is 10%, while using $\tilde{\beta}(k)$ the reduction is 2%. In general, it would appear that ridge estimate $\hat{\beta}(k)$ shows the greatest promise in reducing the standard errors and means square errors rather than $\hat{\beta}$ and $\tilde{\beta}(k)$.

Table 3. Bootstrap estimates of s.e. and MSE of $\hat{\beta}$, $\tilde{\beta}(k)$ and $\hat{\beta}(k)$.

Parameter	s.e. ($\hat{\beta}$)	s.e. ($\tilde{\beta}(k)$)	s.e. ($\hat{\beta}(k)$)
β_1	0.06002	0.05957	0.05950
β_2	0.01647	0.01633	0.01573
β_3	0.08418	0.08315	0.07350
β_4	0.00084	0.00083	0.00070
β_5	0.00061	0.00060	0.00054
β_6	0.63321	0.59944	0.36899
Percent reduction in MSE		2%	10%

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A.M.S. Subject classification: 26D15, 62F03

1. Introduction:

Nous avons déjà étudié des exemples de test statistiques non standard portant sur des caractères gaussiens (voir [5]) ou de Bernoulli (voir [6]) puis nous