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Mean Square Error Performance of the Modified Jackknifed Ridge Predictors in the Linear Mixed Models

Özge Kuran[1*]

*[1]Dicle University Faculty of Science Department of Statistics, DİYARBAKIR

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Multicollinearity.

Abstract: The goal of this study is to introduce the modified jackknifed ridge prediction method in the linear mixed models. Then, the matrix mean square error (MMSE) comparisons are done. Finally, a real data analysis is given to observe the behavior of the modified jackknifed ridge predictors.

Lineer Karma Modellerde Modified Jackknifed Ridge Ön Tahmin Edicilerin Hata Kareler Ortalaması Performansı

Anahtar Kelimeler
Jackknifed ridge ön tahmin ediciler,
Lineer karma modeller,
Modified jackknifed ridge ön tahmin ediciler,
Çoklu iç ilişki.

Özet: Bu çalışmanın amacı, lineer karma modellerde modified jackknifed ridge ön tahmin metodunu tanımlamaktır. Daha sonra, matris hata kare ortalamasına (MMSE) göre karşılaştırmalar yapmaktır. Son olarak, modified jackknifed ridge ön tahmin edicilerin davranışlarını gözlemlemek amacıyla gerçek bir veri analizi çalışması verilmiştir.

*İlgili Yazar, email: ozge.kuran@dicle.edu.tr

1. Introduction

Linear mixed models (see [1]; [2]) have been broadly employed for longitudinal-repeated measurements data, clustered data and multilevel data. (see [3]; [4]; [5]; [6]).

Linear mixed models are the following form

$$y = X\beta + Zu + \varepsilon \tag{1}$$

where y is an $n \times 1$ vector of responses, X is an $n \times p$ known design matrix for the fixed effects, β is a $p \times 1$ parameter vector of fixed effects, Z is an $n \times q$ known design matrix for the random effects, u is a $q \times 1$ vector of random effects and ε is an $n \times 1$ vector of random errors. It is where G, W are known positive definite (pd) matrices. Then, $var(y) = \sigma^2 H$ where $H = ZGZ' + W$.

The estimator of β and the predictor of u are derived from [7] and [8] as

$$\hat{\beta} = (X'H^{-1}X)^{-1}X'H^{-1}y \tag{2}$$

$$\hat{u} = GZ'H^{-1}(y - X\hat{\beta})$$

where $\hat{\beta}$ is named as the best linear unbiased estimator (BLUE) and $\hat{u}$ is named as the best linear unbiased predictor (BLUP).

Multicollinearity is a widely occurring and potentially serious problem that can be defined as near-linear dependence among the variable of the design matrix of the fixed effects. On account of multicollinearity, some serious problems can be arised. For example, interpretation, in validation, and analysis of the model, like unreasonable sign, unstable estimates, high-standard errors, and so on. To overcome from these problems, some procedures were advanced.

The ridge estimator which is suggested by [9] in linear regression model is the most popular one. But, since ridge estimator may handle substantial amount of bias, [10] recommended the jackknifed estimator that had both smaller bias and mean square error than the ridge estimator under some conditions. Jackknifed styles of ridge estimator and some other distincts are investigated in the linear regression models; see [11], [12], [13], [14], [15], [16], [17], [18], [19], [20], [21], [22] and [23].

[24] and [25] were suggested the ridge estimator and predictor as

$$\hat{\beta}(k) = \left(X'H^{-1}X + kI_p\right)^{-1} X'H^{-1}y \tag{3}$$

$$\hat{u}(k) = GZ'H^{-1}(y - X\hat{\beta}(k))$$

where $k > 0$ is known as the biasing parameter.

Additionally, [26] defined the jackknifed ridge estimator and predictor as

$$\tilde{\beta}(k) = [I_p - k^2\left(X'H^{-1}X + kI_p\right)^{-2}]\hat{\beta} \tag{4}$$

$$\tilde{u}(k) = GZ'H^{-1}(y - X\tilde{\beta}(k))$$

where $\hat{\beta}$ is the BLUE given by Eq. (2).

In this article, modified jackknifed ridge estimator and predictor are introduced in linear mixed models. And then, our study can explain as follows. After new estimator and predictor are suggested, the matrix mean square error (MMSE) comparisons are made in Section 2. In Section 3, the estimation of the biasing parameters are investigated. Greenhouse gases data analysis is constructed in Section 4 and conclusions are given in Section 5.

2. Some Comparisons

In this section, before comparisons are done, the modified jackknifed ridge predictors in the linear mixed models are introduced by using [26]. The proposed predictors are designated as the modified jackknifed ridge estimator and the modified jackknifed ridge predictor, respectively, as

$$\tilde{\beta}_m(k) = \left[I_p - k^2\left(X'H^{-1}X + kI_p\right)^{-2}\right]\hat{\beta}(k)$$

$$\tilde{u}_m(k) = GZ'H^{-1}(y - X\tilde{\beta}_m(k))$$

where $\hat{\beta}(k)$ is the ridge estimator given by Eq. (3).

Prediction of linear combinations of β and u can be infered as $\mu = L'\beta + M'u$ for specific matrices $L \in \mathbb{R}^{p\times\dot{s}}$ and $M \in \mathbb{R}^{q\times\dot{s}}$ (see [27]; [28]; [29] for $\dot{s} = 1$). Following [30], MMSE of any predictor $\tilde{\mu} = L'\tilde{\beta} + M'\tilde{u}$ is given as

$$MMSE(\tilde{\mu}) = E\left((\tilde{\mu} - \mu)(\tilde{\mu} - \mu)'\right) = Var(\tilde{\mu}) + Var(\mu) + Bias(\tilde{\mu})Bias(\tilde{\mu})' - Cov(\tilde{\mu}, \mu) - Cov(\mu, \tilde{\mu}) \tag{5}$$

where $Bias(\tilde{\mu}) = E(\tilde{\mu} - \mu)$.

[26] is obtained the predictor of μ under the BLUPs and the jackknifed ridge predictors, respectively, as

$$\hat{\mu} = L'\hat{\beta} + M'\hat{u} = \mathbb{Q}\hat{\beta} + M'GZ'H^{-1}y$$

$$\tilde{\mu}_k = L'\tilde{\beta}(k) + M'\tilde{u}(k) = \mathbb{Q}\tilde{\beta}(k) + M'GZ'H^{-1}y$$

and [26] also found by using Eq. (5)

$$MMSE(\hat{\mu}) = \mathbb{Q}MMSE(\hat{\beta})\mathbb{Q}' + \sigma^2 M'(G - GZ'H^{-1}ZG)M$$

$$MMSE(\tilde{\mu}_k) = \mathbb{Q}MMSE(\tilde{\beta}(k))\mathbb{Q}' + \sigma^2 M'(G - GZ'H^{-1}ZG)M$$

where

$$MMSE(\hat{\beta}) = \sigma^2 Q\Lambda^{-1}Q'$$

$$MMSE\left(\tilde{\beta}(k)\right) = \sigma^2 Q(\Lambda + kI_p)^{-2}(\Lambda + 2kI_p)\,\Lambda(\Lambda + 2kI_p)(\Lambda + kI_p)^{-2}Q' + k^4(\Lambda + kI_p)^{-2}Q'\beta\beta'Q(\Lambda + kI_p)^{-2}$$

where there arises a $p \times p$ orthogonal matrix Q such that $Q'Q = QQ' = I_p$ and $Q'X'H^{-1}XQ = \Lambda = diag(\lambda_1, \cdots, \lambda_p)$ where λ_i, $i = 1, \cdots, p$, are the eigenvalues of $X'H^{-1}X$.

By following [26], we derive $\tilde{\mu}_{m,k}$ as $\tilde{\mu}_{m,k} = L'\tilde{\beta}_m(k) + M'\tilde{u}_m(k) = \mathbb{Q}\tilde{\beta}_m(k) + M'GZ'H^{-1}y$ and so, we introduce $MMSE(\tilde{\mu}_{m,k})$ by using Eq. (5)

$$MMSE(\tilde{\mu}_{m,k}) = \mathbb{Q}MMSE(\tilde{\beta}_m(k))\mathbb{Q}' + \sigma^2 M'(G - GZ'H^{-1}ZG)M$$

where

$$\begin{aligned} MMSE\left(\tilde{\beta}_m(k)\right) = {} & \sigma^2 Q(I_p - k^2(\Lambda + kI_p)^{-2})(I_p - k(\Lambda + kI_p)^{-1}) \\ & \times \Lambda^{-1}(I_p - k(\Lambda + kI_p)^{-1})(I_p - k^2(\Lambda + kI_p)^{-2})Q' + k^2(I_p + k(\Lambda + kI_p)^{-1} \\ & - k^2(\Lambda + kI_p)^{-2})(\Lambda + kI_p)^{-1}Q'\beta\beta'Q(\Lambda + kI_p)^{-1}(I_p + k(\Lambda + kI_p)^{-1} - k^2(\Lambda + kI_p)^{-2}) \end{aligned}$$

and then, with the help of [26], it can be seen that the superiority of $MMSE(\tilde{\mu}_{m,k})$ over $MMSE(\hat{\mu})$ and $MMSE(\tilde{\mu}_k)$ is equipollent to the superiority of $MMSE\left(\tilde{\beta}_m(k)\right)$ over $MMSE(\hat{\beta})$ and $MMSE\left(\tilde{\beta}(k)\right)$.

2.1. The MMSE comparisons

Theorem 2.1. $\tilde{\beta}_m(k)$ overhelms $\hat{\beta}$ in the sense of the MMSE sense iff

$$\beta'(Ł^{-1}(\sigma^2 H + k^2(\Lambda + kI_p)^{-1}\beta\beta'(\Lambda + kI_p)^{-1})Ł^{-1})^{-1}\beta \leq 1$$

is satisfied with $Ł = k(I_p + k(\Lambda + kI_p)^{-1} - k^2(\Lambda + kI_p)^{-2})(\Lambda + kI_p)^{-1}$ and $H = Var(\hat{\beta}) - Var(\tilde{\beta}_m(k))$.

Theorem 2.2. $\tilde{\beta}_m(k)$ overhelms $\tilde{\beta}(k)$ in the sense of the MMSE sense iff

$$\beta'(Ł^{-1}(\sigma^2 Ŧ + k^4(\Lambda + kI_p)^{-2}\beta\beta'(\Lambda + kI_p)^{-2})Ł^{-1})^{-1}\beta \leq 1$$

is satisfied with $Ŧ = Var\left(\tilde{\beta}(k)\right) - Var(\tilde{\beta}_m(k))$.

To see the proof of Theorems 2.1 and 2.2, [17] can be investigated under linear mixed models.

3. Estimators of Biasing Parameters

Three methods of the selection of k that are used in ridge regression to the modified jackknifed ridge predictors are generalized in this part.

Firstly, [9] recommended estimator of k. Then, [25] extended to the linear mixed models estimator of k as $\hat{k}_h = \frac{p\hat{\sigma}^2}{\hat{\alpha}'\hat{\alpha}}$ where $\hat{\sigma}^2 = (y - X\hat{\beta})'H^{-1}(y - X\hat{\beta})/(n - p)$ and we use $\hat{k}_h$ as the first estimator of k.

Secondly, by following [16], the second estimator of k is taken as $\hat{k}^h = \frac{p\hat{\sigma}^2}{\sum\{\hat{\alpha}_i^2/[1+\sqrt{1+\lambda_i(\frac{\hat{\alpha}_i^2}{\hat{\sigma}^2})}]\}}$ where λ_i's are the eigenvalues of $X'H^{-1}X$.

Concisely, with the help of [31], the third estimator of k is used as $\hat{k}_{LW} = \frac{p\hat{\sigma}^2}{\sum \lambda_i \hat{\alpha}_i^2}$.

4. A Real Data Analysis

Gases that trap radiation and make the planet softer in the atmosphere are called greenhouse gases. (see the offical United States Environmental Protection Agency (EPA) website [32]).

The transportation segment is the greatest component of greenhouse gas emissions and transportation gas emissions are produced from burning fossil fuel for cars, light/heavy trucks-buses, motorcycles and railways (see EPA website [32]).

We describe the response (y) as 297 fuel combustion in transport (in million tonnes) that is randomly taken from 27 zones throughout 2006-2016 inclusive years. Then, the explanatory variables are taken as fuel combustions in cars (x_1), light duty trucks (x_2), heavy duty trucks-buses (x_3), motorcycles (x_4) and railways (x_5) that are declared as fixed effects and because the 27 zones are randomly taken from the zones, the zones factor effect on the response is declared as random effect. Hence, the random intercept and slope model (RISM) is expressed as

$$y_{ij} = \beta_1 x_{ij1} + \beta_2 x_{ij2} + \beta_3 x_{ij3} + \beta_4 x_{ij4} + \beta_5 x_{ij5} + u_1 + u_2 t_{ij} + \varepsilon_{ij}, i = 1, \cdots, 27 \;\; j = 1, \cdots, 11$$

where y_{ij} indicates the ith observation of the jth zone of the response, x_{ijs} indicates the ith observation of the jth zone of the explanatory variable x_s, $s = 1, \cdots, 5$ and t_{ij} demonstrates time corresponding to y_{ij} (see [26]).

With the help of Matlab R2014a, unstructured (UN), diagonal (UN(1)), compound symmetry (CS) and variance components (VC) models are handled. Then, by utilizing the Akaike's Information Criterion (AIC) and Bayesian Information Criterion (BIC), the selection among models is performed and the estimation of the covariance matrices are computed by maximum likelihood (ML) or restricted maximum likelihood (REML) methods.

The consequences are attached by Table 1 and by examining Table 1, we favour UN(1) model in BIC and ML approaches (see for the details [26]; [33]). Then, we estimate UN(1) variance-covariance matrices as

$$\hat{G}_{ML} = \begin{bmatrix} 2.1913 & 0 \\ 0 & 0.0755 \end{bmatrix}$$

and $\widehat{W}_{ML} = 0.25451 I_{297}$. Hence, by using $H = ZGZ' + W$, $\widehat{H}_{ML}$ is found.

The eigenvalues of the matrix $X'\widehat{H}_{ML}^{-1}X$ are figured out as $\lambda_1 = 1.4326 \times 10^{+7}$, $\lambda_2 = 1.5085 \times 10^{+4}$, $\lambda_3 = 4.7251 \times 10^{+3}$, $\lambda_4 = 247.7243$ and $\lambda_5 = 41.5100$. Hence, the condition number is computed as $\frac{\lambda_{max}}{\lambda_{min}} = 345120$ that is larger 1000, it shows severe multicollinearity.

$\hat{k}_h = 0.9324$, $\hat{k}^h = 15.1795$ and $\hat{k}_{LW} = 7.2215 \times 10^{-7}$ are derived by following Section 3.

With the help of Table 2, we see respectively, the parameter estimators, predictors, the scalar mean square error (SMSE) values of fixed effects.

Table 2 indicates that the situation of the estimators based on in accordance with the biasing parameter used. For $\hat{k}_h$, jackknifed ridge estimator, the blue and modified jackknifed ridge estimator; for $\hat{k}^h$, blue, jackknifed ridge estimator and modified jackknifed estimator; for $\hat{k}_{LW}$, modified jackknifed ridge estimator, jackknifed ridge estimator and blue have the minimum SMSE values.

Table 1. Goodness-of-fit results (model fit statistics)[1]

Cov. Struc.	Est. Met. for Cov. Par.	AIC	BIC
UN	ML	337.30	374.24
	REML	362.03	398.76
UN(1)	ML	339.42	372.67
	REML	362.87	395.93
VC	ML	391.56	421.11
	REML	416.72	446.11
CS	ML	393.42	426.67
	REML	418.60	451.66

Table 2. Parameter estimates of fixed and random effects, SMSE values for $\hat{k}_h$, $\hat{k}^h$ and $\hat{k}_{LW}$ (Greenhouse Gases Data).

	β_1	β_2	β_3	β_4	β_5	$SMSE$		u_1	u_2
$\hat{\beta}$	1.024744842890595	1.050073767439245	0.933047790125021	3.343610285450398	3.678983322307381	0.146934583387170	$\hat{u}$	0.548830170504787	−0.078066966087015
$\tilde{\beta}(\hat{k}_h)$	1.024814210301806	1.050109885233066	0.932994950376863	3.342217512844979	3.677067790930870	0.146819359552921	$\tilde{u}(\hat{k}_h)$	0.548938532485973	−0.078083061569482
$\tilde{\beta}_m(\hat{k}_h)$	1.028024042902154	1.051705902727657	0.930517265690817	3.277526670770907	3.590874629722005	0.148373867083482	$\tilde{u}_m(\hat{k}_h)$	0.553830386847995	−0.078802183878643
$\tilde{\beta}(\hat{k}^h)$	1.035052390564944	1.055453092842452	0.925198513622418	3.136169165113276	3.394792624603533	0.253559688429873	$\tilde{u}(\hat{k}^h)$	0.564902511503670	−0.080452852670506
$\tilde{\beta}_m(\hat{k}^h)$	1.071654348563221	1.073282177704197	0.896785435545271	2.397437240066398	2.423730433054158	1.538053111200660	$\tilde{u}_m(\hat{k}^h)$	0.620095564683005	−0.088529407552526
$\tilde{\beta}(\hat{k}_{LW})$	1.024744842890595	1.050073767439245	0.933047790125021	3.343610285450397	3.678983322307380	0.146934583387170	$\tilde{u}(\hat{k}_{LW})$	0.548830170504789	−0.078066966087015
$\tilde{\beta}_m(\hat{k}_{LW})$	1.024744845432904	1.050073768704577	0.933047788162454	3.343610234217020	3.678983253993676	0.146934578929192	$\tilde{u}_m(\hat{k}_{LW})$	0.548830174396600	−0.078066966657172

[1] The abbreviations "Cov. Struc." and "Est. Met. for Cov. Par." refer to "Covariance Structures" and "Estimation Methods for Covariance Parameters".

Figures 1 and 2 are produced for other k values. The plots of the $SMSE(\tilde{\beta}(k))$, $SMSE(\tilde{\beta}_m(k))$ and $SMSE(\hat{\beta})$ versus k intervals (0,20) and (0,1) are presented by Figures 1 and 2, respectively. Under SMSE, Figures 1 and 2 indicate that $\tilde{\beta}_m(k)$ has smaller SMSE values than $\tilde{\beta}(k)$ and $\hat{\beta}$ for k values in the interval (0,0.734). We see that the difference between $SMSE(\tilde{\beta}(k))$ and $SMSE(\hat{\beta})$ values increases as k values increase. On the other hand, we say that $\tilde{\beta}(k)$ overhelms $\tilde{\beta}_m(k)$ and $\hat{\beta}$ when k values are larger than 0.734.

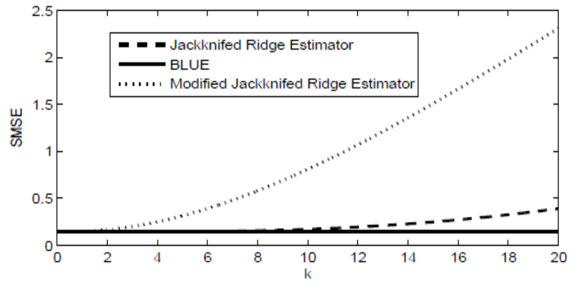

Figure 1. Plots of $SMSE(\tilde{\beta}(k))$, $SMSE(\tilde{\beta}_m(k))$ and $SMSE(\hat{\beta})$ values versus k (Greenhouse Gases Data).

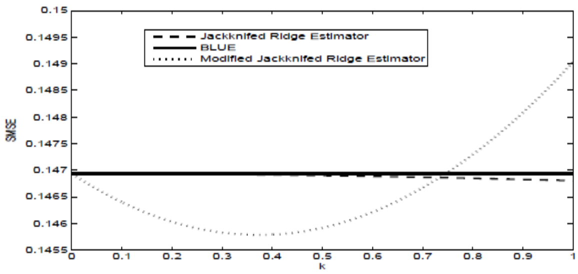

Figure 2. Plots of $SMSE(\tilde{\beta}(k))$, $SMSE(\tilde{\beta}_m(k))$ and $SMSE(\hat{\beta})$ values versus k (Greenhouse Gases Data).

Theorem 2.1 condition is figured out as $14.4426 \nless 1$ for $\hat{k}_h$, hence $\hat{\beta}$ has smaller MMSE values $\tilde{\beta}_m(\hat{k}_h)$. Theorem 2.1 condition is figured out as $182.3097 \nless 1$ for $\hat{k}^h$, so $\hat{\beta}$ has smaller MMSE values than $\tilde{\beta}_m(\hat{k}^h)$. For $\hat{k}_{LW}$, Theorem 2.1 condition is calculated as 1.1424×10^{-5}, since it is smaller than 1, $\tilde{\beta}_m(\hat{k}_{LW})$ has smaller MMSE values than $\hat{\beta}$.

Theorem 2.2 condition is calculated as 5.2938 for $\hat{k}_h$; $1.0530 \times 10^{+3}$ for $\hat{k}^h$, hence $\tilde{\beta}(\hat{k}_h)$ and $\tilde{\beta}(\hat{k}^h)$ have smaller MMSE values than $\tilde{\beta}_m(\hat{k}_h)$ and $\tilde{\beta}_m(\hat{k}^h)$. For $\hat{k}_{LW}$, Theorem 2.2 condition is found as 3.2170×10^{-12} which is smaller than 1, so $\tilde{\beta}_m(\hat{k}_{LW})$ has a good performance than than $\tilde{\beta}(\hat{k}_{LW})$ under MMSE criterion.

For suitable k values, it is seen that $\tilde{\beta}_m(k)$ has a good performance (that is, $\tilde{\beta}_m(k)$ has small MMSE and SMSE values) than $\hat{\beta}$ and $\tilde{\beta}(k)$.

4. Conclusions

In this article, the modified jackknifed ridge way is recommended in the linear mixed models. Then, the MMSE comparisons and several different methods for k are given. Finally, greenhouse gases data analysis is done to demonstrate theoretical findings.

When the appropriate biasing parameter is used, this study is confirmed that the modified jackknifed ridge way guarantees smaller MSE than the jackknifed ridge way under multicollinearity.

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