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Using Ridge regression to deal with the multicollinearity problem and make a comparison between different techniques to solve the problem

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Abstract: Multicollinearity is a familiar problem in linear regression analysis; this phenomena arise when the relationships among explanatory variables exist. Ordinary least squares (OLS) is used to estimate parameters in regression analysis when it is assumed that there is no correlation between explanatory variables. When the assumption of multicollinearity is not valid, one should attempt to use different techniques to deal with the problem, because it affects the accuracy of the regression coefficient. Ridge regression (RR) is a special case of OLS that allows Biase to estimate parameters more precisely. Partial least squares regression (PLSR) and Principal component analysis (PCA) are both techniques that build new predictor variables known as components as linear combinations of the original predictor variables. These components are built in different ways. PLSR builds a component to explain the observed variability in predictor variables and involves a response variable; also, PCA builds a component like PLSR without a response variable, it just transforms the predictors into uncorrelated components, and principal component regression (PCR) applies to the uncorrelated components to regress the outcome response variable on those components. The performance of RR, PLSR, and PCR was compared to detect the effective technique to overcome the collinearity problem in a real data set.

Keywords: Multiple regression, Multicollinearity, Ridge regression, Partial least squares, Principal component.

استخدام انحدار الحرف لمعالجة مشكلة الارتباط الخطي المتعدد وإجراء مقارنة بين التقنيات المختلفة لحل هذه المشكلة

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المستخلص: تُعدّ مشكلة الارتباط الخطي المتعدد شائعة في تحليل الانحدار الخطي وتنشأ هذه الظاهرة عند وجود علاقات بين المتغيرات التفسيرية. تُستخدم طريقة المربعات الصغرى العادية (OLS) لتقدير المعاملات في تحليل الانحدار عندما يُفترض عدم وجود ارتباط بين المتغيرات التفسيرية. عندما لا يكون افتراض الارتباط الخطي المتعدد صحيحًا، ينبغي محاولة استخدام تقنيات مختلفة للتعامل مع المشكلة، لأنها تؤثر على دقة معامل الانحدار. يُعدّ انحدار الحرف (RR) حالة خاصة من OLS تسمح بالتحيز بتقدير المعاملات بدقة أكبر. يُعدّ كل من انحدار المربعات الصغرى الجزئية (PLSR) وتحليل المكونات الرئيسية (PCA) تقنيتين تُنشئان متغيرات تنبؤية جديدة تُعرف بالمكونات، وذلك من خلال تركيبات خطية من المتغيرات التنبؤية الأصلية. تُبنى هذه المكونات بطرق مختلفة؛ إذ يُنشئ (PLSR) مكونًا لشرح التباين الملحوظ في المتغيرات التنبؤية ويتضمن متغير استجابة. كذلك، تُنشئ تقنية تحليل المكونات الرئيسية (PCA) مكونًا مشابهًا لتقنية الانحدار الجزئي للمربعات الصغرى (PLSR) دون متغير استجابة، حيث تُحوّل المتغيرات التنبؤية إلى مكونات غير مترابطة. وتُطبّق تقنية انحدار المكونات الرئيسية (PCR) على هذه المكونات غير المترابطة لتحليل متغير الاستجابة (النتيجة) بناءً على هذه المكونات. وقد تقارن أداء كل من انحدار الحرف (RR) وانحدار الجزئي للمربعات الصغرى (PLSR) وتقنية انحدار المكونات الرئيسية (PCR) لتحديد التقنية الأكثر فعالية للتغلب على مشكلة الارتباط الخطي في مجموعة بيانات حقيقية.

الكلمات المفتاحية: الانحدار المتعدد، الارتباط الخطي المتعدد، انحدار الحرف، انحدار المربعات الصغرى الجزئية، انحدار المكونات الرئيسية.

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Introduction

The OLS method is a classical technique that is used in regression analysis for estimating parameters under the related assumptions with a view to selecting the best regression line that minimizes the sum of the squares of errors. In case the assumptions are not valid, OLS does not provide a precise result. Multicollinearity is one of the assumptions that should be paid attention to, to deal with it properly, and it appears when some explanatory variables are correlated or collinear. RR, PLSR, and PCA are selected to face this problem and make a comparison between them. This paper applied techniques to real data.

Previously, researchers conducted many investigations about multicollinearity, RR was used and compared with other techniques, and most of them used simulated data. A Monte Carlo simulation technique was used to detect the effectiveness of methods between RR, PLSR, and PCR to overcome multicollinearity (Adnan et al., 2006). Evaluate the effectiveness of RR and compare it to OLS in handling different levels of multicollinearity (Herawati et al., 2018). Many different methods of Ridge regression are used to solve the multicollinearity problem, including Direct ridge regression (DRR), Ordinary ridge regression (ORR), and Generalized ridge regression (GRR) (Rashwan, 2011). Using data simulation to compare the effectiveness between Ordinary ridge regression (ORR) and Ordinary least squares (OLS) by (Muhamad, S(2014). A Case study used the Partial Least Squares method to solve the problem of multicollinearity (Wondola et al., 2020). The partial least squares modeling method is used to solve the multicollinearity problem (Mao, 2018).

This paper aims to focus on the multicollinearity problem in regression models and display methods of handling the collinearity problem. Furthermore, this investigation seeks to compare RR, PLSR, and PCR techniques using minimum squared error MSE and others.

1st: Methodology

1- Multicollinearity:

One of the most important assumptions in linear regression analysis is that collinearity among explanatory variables does not exist. The multicollinearity problem states that the association between two or more explanatory variables leads to a strong linear relationship in which the effect of the dependent variable cannot be separated from that of the explanatory variables. Orthogonality is another concept that describes this phenomenon. When explanatory variables are orthogonal, it means there is no relationship between explanatory variables, and all the eigenvalues are equal to one. If one of these is less than one or equal to zero, it is not orthogonal, leading to the problem of multicollinearity.

Multicollinearity is divided into two types:

First, the perfect multicollinearity: in this type, the specific matrix of information $(X^{-}X)$ has a determinant equal to zero ($|X^{-}X| = 0$). Therefore, it is impossible to estimate the coefficient of the regression model because the inverse matrix cannot be found.
Second, Semi-multicollinearity: It is our concern when the specific matrix of information $(X^{-}X)$ has a determinant that is very small or close to zero ($|X^{-}X| \simeq 0$). Possible to estimate the coefficient of the regression model, but it affects the accuracy of the regression coefficient because of the high variance of the coefficient. (Roman et al., 2017)

2- Ridge regression:

Ridge regression is one of the techniques suggested by Hoerl and Kennard to deal with the multicollinearity problem. OLS has a deficiency in overcoming this problem because it assumes that there is no collinearity among explanatory variables. The core of RR is that it adds just enough bias to improve the estimator's accuracy. In contrast, OLS produces an unbiased estimator. (Hoerl & Kennard, n.d.)
The OLS estimates the best linear unbiased estimator:

$$\widehat{B} = (\acute{X}X)^{-1}\acute{X}Y \qquad \text{...... (1)}$$

The OLS estimator has several properties, which can be summarized as follows:

$$E(\widehat{B}) = B \qquad \text{...... (2)}$$

$$V(\widehat{B}) = \sigma^2\,(\acute{X}X)^{-1} \qquad \text{...... (3)}$$

$$MSE(\widehat{B}) = \sigma^2\, trace(\acute{X}X)^{-1} \qquad \text{...... (4)}$$

The RR estimates a biased estimator:

$$\widehat{B_R} = (\acute{X}X+kI)^{-1}\acute{X}Y \qquad \text{...... (5)}$$

Where:
I: Identity matrix
k: Ridge parameter
The RR estimator has several properties, which can be summarized as follows:

$$\begin{aligned} E(\widehat{B_R}) &= (\acute{X}X+kI)^{-1}E(\acute{X}Y) \\ &= (\acute{X}X+kI)^{-1}\,(\acute{X}X)E(B) \\ &= A_k\,B \qquad \text{...... (6)} \end{aligned}$$

Where:

$$A_k = (\,I + k(\acute{X}X)^{-1})^{-1} \qquad \text{...... (7)}$$

$$\begin{aligned} V(\widehat{B_R}) &= (\acute{X}X+kI)^{-1}\acute{X}X(\acute{X}X+kI)^{-1}\sigma^2 \\ &= \sigma^2\,A_k(\acute{X}X)^{-1}\,\acute{A}_k \qquad \text{...... (8)} \end{aligned}$$

$$\begin{aligned} MSE\,\widehat{B_R} &= E\,[(\,\widehat{B_R} - B\acute{)}(\,\widehat{B_R} - B)] \\ &= \sigma^2 trace\,[A_k(\acute{X}X)^{-1}\,\acute{A_k}] + \acute{\widehat{B}}\,(1 - A_k\acute{)}(1 - A_k)\widehat{B} \qquad \text{...... (9)} \end{aligned}$$

3- Partial least squares regression

Partial least squares regression was defined as another technique for overcoming the problem of multicollinearity. It is known as soft modeling in contrast to the OLS, which requires hard assumptions, such as no collinearity among explanatory variables. Soft modeling refers to the softening of these assumptions. (R.Frank Falk & Nancy B. Miller, 1992). A PLSR is appropriate when the matrix of predictors has more variables than observations and when there is multicollinearity among explanatory variables. A PLSR makes a linear model by decomposing matrices from explanatory and dependent variables into bilinear terms. (Gentle et al., n.d.). The general underlying of PLSR:

$$\boldsymbol{X = T\acute{P} + E} \qquad \text{...... (10)}$$

$$\boldsymbol{Y = U\acute{Q} + F} \qquad \text{...... (11)}$$

Where:
X: is an nxm matrix of predictors
Y: is an nxp matrix of responses
T: is an nx1 matrix projection of X (X score, component)
U: is an nx1 matrix projection of Y (Y score)
P: is an mx1 orthogonal loading matrix
Q: is an px1 orthogonal loading matrix
E and F : error term
The decompositions of X and Y are built to maximize the covariance between T and U.

4- Principal component

Principal component analysis is a very useful method for reducing dimensionality. It was proposed by Pearson (1901) and Hotelling (1933). After a long time, Principal Component Regression was introduced by Massey (1965) as a technique to overcome multicollinearity by combining principal component analysis with multiple linear regression. PCR was used as a principal component of the regressor instead of regressing the response variable on the regressors directly. When multicollinearity occurs, least square estimators are biased, so the principal component regression technique is used to handle collinearity among explanatory variables (Arum et al., 2025). The general underlying line of PCR. (Alibuhtto & Peiris, 2015)

$$\boldsymbol{Y = X\beta +} \text{ €} \qquad \text{...... (12)}$$

Where $\boldsymbol{Y}$ is an n x 1 matrix of the dependent variable, $\boldsymbol{X}$ is an n x p matrix of the independent variables, $\boldsymbol{\beta}$ is a p x 1 vector of unknown constants, and € is an n x 1 vector of random errors.
Restated the regression model in terms of the principal component as:

$$\boldsymbol{Y = ZB_{pcr} +} \text{ €} \qquad \text{...... (13)}$$

$$\boldsymbol{\acute{C}(\acute{X}X)C} = \wedge \text{ and } \boldsymbol{\acute{C}C = C\acute{C} = 1} \qquad \text{...... (14)}$$

Where:
$\wedge$ is a diagonal matrix with ordered characteristic roots of $\boldsymbol{\acute{X}X}$ on the diagonal. It's denoted by $\boldsymbol{\lambda_1 \geq \lambda_2 \geq \ldots.., \lambda_p}$. Could be the new set of explanatory variables calculated as:

$$\boldsymbol{(Z_1, Z_2, \ldots Z_p) = Z = XC = (X_1, X_2, \ldots\ X_p)} \qquad \text{...... (15)}$$

$$\boldsymbol{B_{pcr} = C\beta} \qquad \text{...... (16)}$$

$$\boldsymbol{\acute{Z}Z = \acute{C}\acute{X}XC = \acute{C}C \wedge \acute{C}C} \qquad \text{...... (17)}$$

The least squares estimator of $\boldsymbol{B_{pcr}}$ is

$$\boldsymbol{\widehat{B}_{pcr}} = (\boldsymbol{\acute{Z}Z}\,)^{-1}\boldsymbol{\acute{Z}Y} = \wedge^{-1}\boldsymbol{\acute{Z}Y} \qquad \text{...... (18)}$$

The variance-covariance matrix of $\boldsymbol{\widehat{B}_{pcr}}$ is

$$V(\boldsymbol{\widehat{B}_{pcr}}) = \boldsymbol{\sigma^2}(\boldsymbol{\acute{Z}Z}\,)^{-1} = \boldsymbol{\sigma^2}\wedge^{-1} \qquad \text{...... (19)}$$

In principal component estimators, consider that the regressors are arranged in order of decreasing eigenvalues $\lambda_1 \geq \lambda_2 \geq \ldots.., \lambda_p > 0$, and the principal components corresponding to near-zero eigenvalues are removed from the analysis, and least squares is applied to the remaining components.

2nd: Result and Discussion

1- Multicollinearity Test

The data was obtained from the meteorological directorate of Sulaimani for the period (2006 – 2021). Statgraphics 19 X64 has been used for analyzing. The data included one dependent variable and sixteen independent variables, and the number of observations for each variable is 192:

a. Temperature-Max (X1)
b. Temperature-Min (X2)
c. wind speed (X3)
d. Vapour Max (X4)
e. Vapour Min (X5)
f. Sunshine (X6)
g. Cloud cover (X7)
h. Sea pressure (X8)
i. Soil Temperature-SUR (X9)
j. Soil Temperature-5CM (X10)
k. Soil Temperature-10CM (X11)
l. Soil Temperature-20CM (X12)
m. Soil Temperature-30CM (X13)
n. Soil Temperature-50CM (X14)
o. Soil Temperature-100CM (X15)
p. Precipitation (X16)
q. Relative humidity (Y)

For checking multicollinearity using the correlation matrix and VIF. These results are shown in Table 1. There was severe multicollinearity among explanatory variables.

Table (1): Correlation matrix and VIF for explanatory variables

Variable	x1	x2	x3	x4	x5	x6	x7	x8	x9	x10	x11	x12	x13	x14	x15	x16	VIF
x1	1	.990**	.281**	.853**	.760**	.881**	-.854**	-.719**	.988**	.992**	.992**	.988**	.969**	.980**	.931**	-.663**	116.7
x2		1	.276**	.854**	.773**	.854**	-.819**	-.728**	.986**	.990**	.990**	.985**	.967**	.976**	.926**	-.624**	75.6
x3			1	.284**	.231**	.309**	-.175*	-.196**	.287**	.285**	.285**	.286**	.247**	.251**	.199**	-0.141	1.2
x4				1	.945**	.691**	-.577**	-.562**	.859**	.866**	.866**	.871**	.839**	.848**	.791**	-.406**	18.6
x5					1	.561**	-.440**	-.500**	.769**	.780**	.781**	.791**	.772**	.774**	.734**	-.287**	14.5
x6						1	-.863**	-.623**	.875**	.872**	.873**	.868**	.833**	.855**	.807**	-.696**	7.2
x7							1	.595**	-.829**	-.832**	-.833**	-.830**	-.825**	-.851**	-.850**	.759**	11.6
x8								1	-.718**	-.717**	-.715**	-.707**	-.688**	-.693**	-.650**	.432**	2.3
x9									1	.997**	.996**	.991**	.971**	.975**	.920**	-.634**	264.5
x10										1	.999**	.996**	.975**	.983**	.932**	-.633**	1794.9
x11											1	.997**	.977**	.987**	.938**	-.636**	1437.9
x12												1	.976**	.989**	.945**	-.628**	202.8
x13													1	.978**	.945**	-.616**	28.7
x14														1	.976**	-.635**	258.8
x15															1	-.629**	51.4
x16																1	2.8

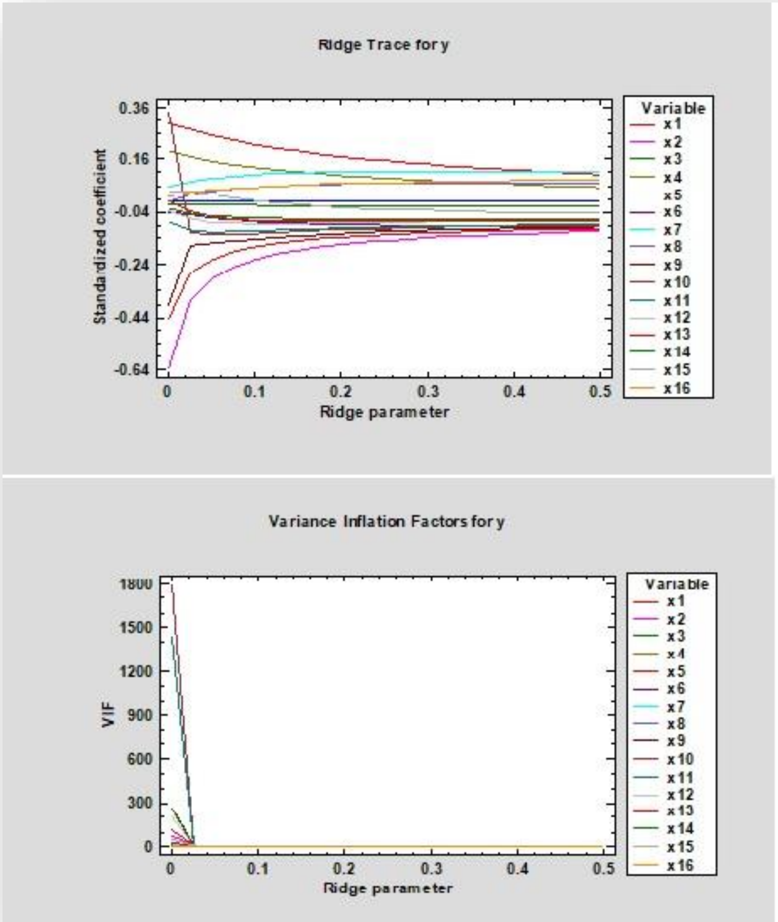
**. Correlation is significant at the 0.01 level (2-taile)

2- Ridge Regression

After standardizing the explanatory variables, applying RR, according to Hoerl and Kennard (1970), we could select the shrinkage (biasing) parameter k by using a ridge trace, which shows the ridge coefficients as a function of k . the shrinkage parameter $k = 0.175$ chosen as the smallest value of k that introduced the small bias, also by using the cross-validation technique, and the model has stabilized, which is shown in graph (1).

Table (2): Model Results

Parameter	Estimate	VIF
CONSTANT	1.639	
x1	-0.025	0.314
x2	-0.031	0.476
x3	-0.003	0.770
x4	0.019	0.857
x5	0.032	0.850
x6	-0.015	1.234
x7	0.020	1.078
x8	0.011	1.063
x9	-0.023	0.324
x10	-0.020	0.161
x11	-0.019	0.140
x12	-0.015	0.216
x13	-0.013	0.742
x14	-0.012	0.247
x15	-0.003	0.947
x16	0.012	1.061



Graph (1): Ridge Trace and Variance Inflation Factors and VIF

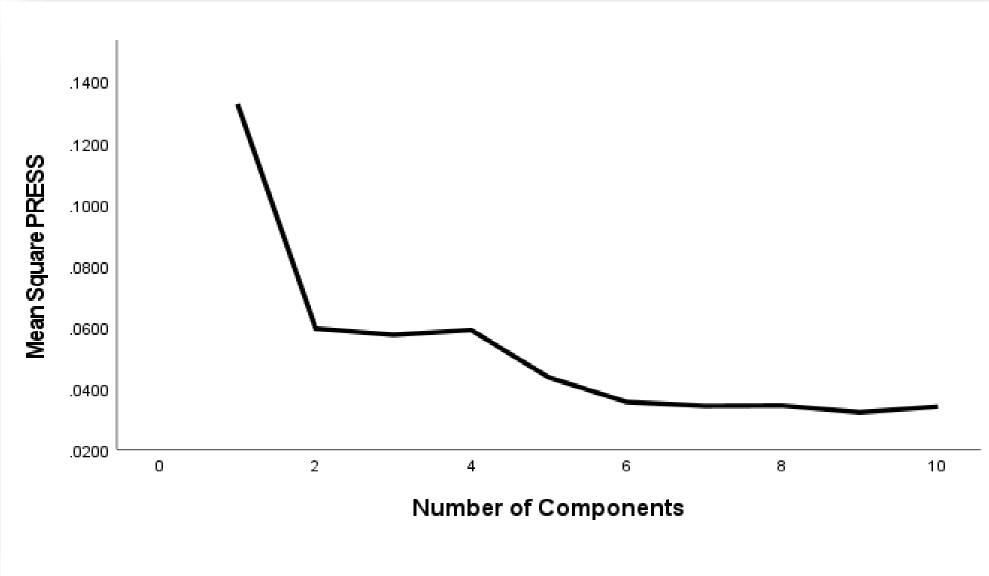
The RR coefficients and variance inflation factor can be summarized in Table 2. It seemed the RR could overcome the collinearity among explanatory variables.

3- Partial Least Squares Regression

Also, for partial least squares, standardize both the explanatory and dependent variables. A PLSR component is a weighted linear combination of explanatory variables constructed to maximize covariance with the dependent variable to build an orthogonal component that overcomes multicollinearity. The number of components extracted is ten, consequently a PLSR model with nine components was observed to have the maximum average prediction R-square and minimum PRESS.

Table (3): displays variation and average prediction R-squared for different components

Component	% Variation in X	Cumulative % of X	% Variation in Y	Cumulative % of Y	Average Prediction R-Squared
1	79.2807	79.2807	87.5351	87.5351	86.6762
2	6.71823	85.9989	7.21007	94.7452	94.0337
3	2.91943	88.9183	1.36929	96.1145	94.2372
4	3.70995	92.6283	0.612781	96.7273	94.0824
5	3.0903	95.7186	0.214151	96.9414	95.6346
6	1.92885	97.6474	0.0896395	97.0311	96.4377
7	0.307211	97.9546	0.305598	97.3367	96.569
8	1.05061	99.0052	0.0392849	97.376	96.5572
9	0.220224	99.2255	0.0771537	97.4531	96.7743
10	0.321453	99.5469	0.0319255	97.485	96.5877



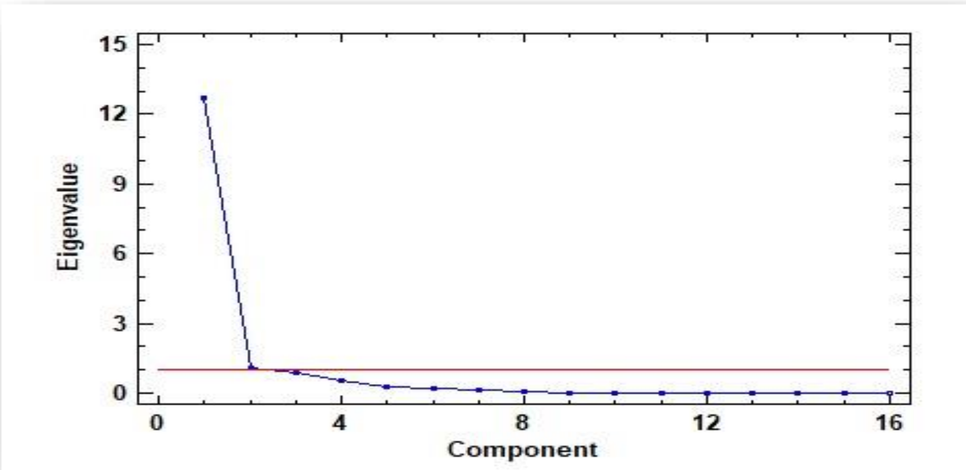
Graph (2): display Mean Square PRESS for different components

4- Principal Component Analysis

Principal component analysis was applied to standardized explanatory variables to obtain a small number of linear combinations of the sixteen variables that account for most of the variability in the data set to handle severe multicollinearity. The component number was determined by using an eigenvalue that is greater than one and scree plot monitoring. Two orthogonal components have been extracted because these two components had eigenvalues greater than one, and together they were explaining 86% of the variability in the data. Principal component regression applies to the uncorrelated components to regress the outcome response variable on those components, to compare with other techniques that were mentioned previously.

Table (3): displays variability and component number

Component Number	Eigenvalue	Percent of Variance	Cumulative Percentage
1	12.6923	79.327	79.327
2	1.10024	6.877	86.204
3	0.914111	5.713	91.917
4	0.522155	3.263	95.18
5	0.289299	1.808	96.988
6	0.187016	1.169	98.157
7	0.122284	0.764	98.922
8	0.0715854	0.447	99.369
9	0.0356306	0.223	99.592
10	0.0291086	0.182	99.774
11	0.0171158	0.107	99.881
12	0.00729718	0.046	99.926
13	0.00620818	0.039	99.965
14	0.00344423	0.022	99.987
15	0.00182181	0.011	99.998
16	0.000333734	0.002	100



Graph (3): Scree Plot

Discussion

Variance inflation factors for several explanatory variables exceeded ten, its indicated that there was severe multicollinearity among explanatory variables, and it affects the accuracy of the regression coefficient. After applying Ridge regression to the data, the VIF drops sharply. It indicated that the problem has been very well resolved by ridge regression. PLSR model with nine components builds a linear combination of explanatory variables constructed to maximize covariance with the dependent variable, and to make an orthogonal component which eliminating multicollinearity among explanatory variables. PCA was applied to standardized explanatory variables, and two orthogonal components were extracted, which they were explaining 86% of the variability in the data. PCR was applied to the uncorrelated component to regress the outcome response variable on those components. To compare the performance of RR, PLS, and PCA, MSE, RMSE, PRESS, and R^2 of the three methods are calculated. The results for RR, PLS, and PCA can be seen in Table 4.

Table (4): MSE, RMSE, PRESS, and R^2 for different techniques

	Method		
Criteria	**PCA**	**PLSR**	**RR**
MSE	0.00217924	0.0265312	0.00088606
RMSE	0.046682331	0.162884	0.029766
PRESS	0.418414085	5.093989912	0.17011
R^2	93.2872	97.4531	94.3552

As seen in Table 4, the MSE, RMSE, and PRESS values of the RR are smaller than those of other techniques, indicating a premium predictive performance and robustness to multicollinearity. PLSR produced the highest $R^{2,}$ indicating superior explained variance in the response variable compared to the others. The MSE, RMSE, and PRESS values of the PCA are smaller than those of PLSR, but produced the lowest value of R^2. In addition, RR was found to be a better method for overcoming multicollinearity when prediction matters because it achieved lower prediction error.

Conclusion

According to the results of this study, the superior method was Ridge regression, under severe multicollinearity among explanatory variables, to achieve the lowest prediction metrics MSE, RMSE, and PRESS. Partial least squares regression is showing the largest proportion of variance explained in the response variable while simultaneously overcoming multicollinearity. While Principal component regression did not reach the highest variance explanation.

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