

Estimation of Nonorthogonal Problem Using Time Series Dataset

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Abstract

Based on the presentation of the principles of nonorthogonal problem, we discuss the difference in some of the approaches. A simple procedure to include the R-squared and Root Mean Square Error (RMSE) is proposed and tested. The results showed that the Partial Least Square Regression provides better predictions due to a small RMSE value.

Key words: Nonorthogonal, Mean Square, Partial Least Square, R Square

1.0 Introduction

Partial Least Square Regression (PLSR) was first proposed by Herman Wold around 1975 as a method of regressing complicated, collinear, many and even incomplete data sets in terms of chains of matrices [1]. It is becoming a powerful tool to explore the vague relationship between the independent variables and dependent variables. PLSR attempts to extract latent (non-observable) variables so that they collect most of the variation of the real θ (observable) variables in such a way that they may also be used to model the ψ response (dependent) variable [2].

According to [3], multicollinearity refers to a situation in which two or more predictor variables in a multiple regression model are highly correlated. If multicollinearity is perfect, the regression coefficients are indeterminate and their standard errors are infinite but if it is less than perfect; then regression coefficients although determinate but possess large standard errors which means that the coefficients cannot be estimated with great accuracy [4]. We can define multicollinearity through the concept of orthogonality, when the predictors are orthogonal or uncorrelated, all eigenvalues of the design matrix are equal to one and the design matrix is of full rank. If at least one eigenvalue is different from one, especially when equal to zero or near zero, then nonorthogonality exists, meaning that multicollinearity is present [5]. The variables of multivariate partial least square was derived in [1].

The general recommendations for the use of Partial least squares regression, which include: data that is highly collinear, has large predictor variables compared to the number of observations and is not normal was listed in [6]. A comparison of covariance-based and variance-based structural equation models based on their respective variances was highlighted in [7]. Small survey sample size and skewed dataset with partial least square path modelling was handled in [8]. The use of partial least squares equation modelling in marketing data was assessed in [9]. Partial least squares regression with other prediction methods: Ordinary Least Squares (OLS), Ridge Regression (RR) and PCR to handle problem of multicollinearity on Gross Domestic Product (GDP) data of Pakistan was compared in [10]. The use of Partial least squares (PLS) structural equation modelling for building and testing behavioural causal theories was illustrated in [11]. The use and the misuse of structural equation modelling in management research was written in [12]. The inconsistency of Partial least squares path coefficient estimates in the case of reflective measurement can have adverse consequences for hypothesis testing as was shown in [13]. Thus consistent PLS provides correction for estimates when PLS is applied to reflective constructs. An alternative approach based on multitrait-multimethod matrix to assess discriminant validity since other approaches like Larcker criterion and examination of cross-loadings do not reliably detect the lack of discriminant validity in common research situations was proposed in [14].

The PLS methodology has also achieved an increasingly popular role in empirical research in international marketing, which may represent an appreciation of distinctive methodological features of PLS.

This paper focuses on using the R squared and Root mean square error for estimation of nonorthogonal problems and the performance is evaluated in comparison with the method involved. The paper proposes a simple method to incorporate times

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series dataset in Nonorthogonal problem.

Section 2 describes the definition and algorithms of Ordinary least square. Ridge, regression and partial least square regression. Section 3 introduces the applicability of the method involved in the Nonorthogonality with illustrative example.

Discussions on the differences between the regression methods is hereby presented.

2.0 The Ordinary Least Square Model (OLS)

The OLS general model is defined as

$$\psi = \theta B + E \text{ (matrix notation)} \quad (1)$$

where ψ is $n \times 1$ vector of observations on the dependent variable.

θ is $n \times p$ matrix of predictors.

B is $p \times 1$ vector of regression parameters.

E is $n \times 1$ vector of errors.

When the matrix θ has a full rank of p , the OLS estimator B_{OLS} can be obtained by minimizing the sum of squared residuals, hence

$$B_{OLS} = (\theta' \theta)^{-1} \theta' \psi \quad (2)$$

where B_{OLS} is $p \times 1$ vector of OLS estimated parameters.

Using unbiased linear estimation with minimum variance or maximum likelihood estimation when the random vector E is normal gives (2) as an estimate of B and this gives minimum sum of squares of the residuals.

2.1 Partial Least Square Regression (PLSR) for Nonorthogonal Problems

In general, according to [15] the variables of a multivariate PLS is derived as follows:

$$\theta = TP^t + \delta \quad (3)$$

$$\psi = UQ^t + \omega \quad (4)$$

where θ is $n \times m$ matrix of predictors

ψ is $n \times p$ matrix of responses

T and U are $n \times 1$ matrices which are respectively the projection of θ and ψ

P and Q are respectively $m \times 1$ and $p \times 1$ orthogonal loading matrices and

δ and ω are their respective error terms.

Formally, the pattern of relationships between the columns of θ and ψ is stored in $m \times n$ cross-product matrix, denoted by

ξ (that is, usually a correlation matrix in that we compute it θ_0 and ψ_0 instead of θ and ψ). ξ is computed as:

$$\xi = \theta_0^T \psi_0 \quad (5)$$

The main analytical tool for PLS is the singular value decomposition (SVD) of a matrix. The matrix of correlations (or covariance) between θ_0 and ψ_0 (mean-centered and normalized variables) is computed as

$$\xi = W \Delta C^T \quad (6)$$

where

W is $n \times n$ eigenvectors of RR^T

C is $m \times m$ eigenvectors of $R^T R$ and

Δ is an $n \times m$ diagonal matrix made up of the square roots of the non-zero eigenvalues of both RR^T and $R^T R$.

The first pair of singular vector (that is the first columns of W and C) are denoted by w_1 and c_1 and the first singular value (that is the first diagonal entry) is denoted by Δ_1 .

The first latent variable of θ is given by

$$t_1 = \theta_0^T w_1 \quad (7)$$

$$p_1 = \theta_0^T t_1 \quad (8)$$

$$\hat{\theta}_1 = t_1 p_1^T \quad (9)$$

The first pseudo latent variable for ψ is given by

$$U_1 = \psi_0 c_1$$

Reconstituting ψ from its pseudo latent variable as

$$\hat{\psi}_1 = u_1 c_1^T \quad (10)$$

$$\psi = t_1 b_1 c_1^T \quad (11)$$

$$\text{With } b_1 = t_1^t u_1 \text{ (first regression coefficient)} \quad (12)$$

Matrices $\hat{\theta}_1$ and $\hat{\psi}_1$ are then subtracted from the original θ_o and ψ_o respectively

$$\text{That is } \theta_1 = \theta_0 - \hat{\theta}_1 \text{ and } \psi_1 = \psi_0 - \hat{\psi}_1$$

The iterative process continues until θ is completely decomposed into L components (that is, θ is now a null matrix and L is the rank of X). When this happens, we have succeeded in obtaining all the latent variables for the model.

The predicted ψ scores are now given by

$$\psi = TBC^T = \theta B_{PLS} \quad (13)$$

where

$$B_{PLS} = (P^{T+})BC^T \quad (14)$$

(P^{T+}) is the Moore – penrose pseudoinverse of P^T

$$\text{That is, } (P^{T+}) = (AA^T)^{-1}A \quad (15)$$

2.2 Ridge Regression (RR)

The standard regression model can be written as

$$\psi = \theta\beta + \varepsilon \quad (16)$$

where ψ is the $n \times 1$ vector of “n” observations,

θ is the $n \times p$ matrix

β is a $p \times 1$ vector of regression coefficients

ε is the $n \times 1$ vector of random errors with zero mean and variance $\sigma^2 I$

Ordinary least squares estimators obtained by minimizing the sum of squared residuals as

$$(\theta^T \theta)^{-1} \theta^T \psi = \hat{\beta}_{OLS} \quad (17)$$

$$\text{Var}(\hat{\beta}) = \hat{\sigma}^2 (\theta^T \theta)^{-1} \quad (18)$$

$$\text{M.S.E } (\hat{\beta}) = \hat{\sigma}^2 \text{trace}(\theta^T \theta)^{-1} = \hat{\sigma}^2 \sum_{i=1}^p \lambda_i \quad (19)$$

where $\hat{\sigma}^2$ is the mean squares error. This estimator $\hat{\beta}$ is unbiased and has a minimum variance. However, if $\theta^T \theta$ is ill-conditioned (singular), the OLS estimate tends to become too erratic and some of the coefficients have wrong sign [16]. In order to prevent these difficulties of O.L.S, ridge regression as an alternative procedure to the OLS method in regression analysis was suggested in [17]. The ridge technique is based on adding a biasing constants IK's to the diagonal of Benson matrix before computing $\hat{\beta}'$ s by using method of [17]. Therefore, the ridge solution is given by:

$$\beta_{\text{ridge}} = (\theta^T \theta + KI)^{-1} \theta^T \psi, \quad K \geq 0 \quad (20)$$

Iterative Method for estimating K

Iterative point method to find out the best value of ridge constant was given in [17]. Start with the value of k which has already been calculated by fixed point method then determine as:

$$k_1 = \frac{p\hat{\sigma}^2(0)}{\sum_{j=1}^p [\hat{\beta}_j(k_0)]^2} \quad (21)$$

Then compute k_2 as

$$k_2 = \frac{p\hat{\sigma}^2(0)}{\sum_{j=1}^p [\hat{\beta}_j(k_1)]^2} \quad (22)$$

where p is the number of regressor variables

$\hat{\beta}_j$ is the j th regression parameter estimate.

$\hat{\sigma}^2(0)$ is the standardized residual mean square.

k_0 is the arbitrarily chosen K value.

When the difference of estimates is moderately small, then stop the iterative procedure.

3.0 Results and Discussions

3.1 Illustrative Example

Nigeria Insurance company expenditure dataset were used (N' Million). Let the independent variables be claims, Fire, Accident, Motor, Employers Liability, Marine and Miscellaneous while the dependent variable is the Total expenditure.

Table 1: Correlation Matrix of the Insurance Company dataset

Variables	Claims	Fire	Accident	Motor	Employers	Marine	Misce	Total Expenditure
Claims	1.000	0.801	0.973	0.984	0.931	0.954	0.818	0.968
Fire	0.801	1.000	0.664	0.802	0.560	0.623	0.330	0.863
Accident	0.973	0.664	1.000	0.957	0.965	0.970	0.888	0.918
Motor	0.984	0.802	0.957	1.000	0.901	0.917	0.764	0.984
Employers	0.931	0.560	0.965	0.901	1.000	0.991	0.949	0.832
Marine	0.954	0.623	0.970	0.917	0.991	1.000	0.930	0.863
Misce-	0.818	0.330	0.888	0.764	0.949	0.930	1.000	0.680
Total Expenditure	0.968	0.863	0.918	0.984	0.832	0.863	0.680	1.000

Table 2: Multicollinearity Statistics

Multicollinearity statistics:							
Statistic	Claims	Fire	Accident	Motor	Employers	Marine	Misce
Tolerance	0.000	0.002	0.004	0.002	0.004	0.005	0.002
VIF	4406.366	468.931	233.686	486.067	255.674	185.715	580.127

The correlation matrix showed that there is a perfect correlation between each variable and itself. The correlation values for between each variable and others are significantly closer to unity indicating a positive relationship and high collinearity amongst variables. Looking at both the tolerance and VIF rows in the multicollinearity diagnostic table, all the independent variables are significantly highly collinear since the VIF and tolerance values are greater than 10 and closer to zero respectively. The determinant of the correlation matrix above was calculated to be 0.0000000000696125 indicating the extreme dependency among variables.

Ordinary Least Squares Result

Table 3: Analysis of variance

Analysis of variance					
Source	DF	Sum of squares	Mean squares	F	Pr> F
Model	7	9166191209.744	1309455887.106	153.789	< 0.0001
Error	8	68117032.630	8514629.079		
Corrected	15	9234308242.374			
Total					

The Analysis of Variance for the O.L.S.R above yield a significant regression model since the probability value is less than 0.05 level of significance. The mean squares are very high due to the presence of multicollinearity.

Table 4:Model parameters

Source	Value	Std error	t	Pr> t	Lower bound (95%)	Upper bound (95%)
Intercept	1346.411	2425.234	0.555	0.594	-4246.189	6939.012
Claims	2.868	2.355	1.218	0.258	-2.562	8.298
Fire	-3.789	3.977	-0.953	0.369	-12.961	5.383
Accident	-2.211	2.951	-0.749	0.475	-9.016	4.595
Motor	0.779	2.751	0.283	0.784	-5.565	7.122
Employers	-17.477	57.365	-0.305	0.768	-149.762	114.807
Marine	-1.367	3.986	-0.343	0.741	-10.559	7.826
Misce-	-3.196	3.415	-0.936	0.377	-11.070	4.678

Partial Least Square Regression Result

Table 5:Model quality

Model quality			
Index	Comp 1	Comp 2	Comp 3
Q ² cum	0.859	0.941	0.976
R ² Y cum	0.894	0.967	0.988
R ² X cum	0.871	0.985	0.994

Consider as PLSR model quality. We should be interested in the quality of prediction we want to achieve. Perhaps we ought to use the latent variable that explains much information about the Y variable. Comp 1, Comp 2, Comp 3 and Comp 4 has the following Q^2_i values as 0.859, 0.584, 0.590 and 0.03 respectively. This automatically makes Comp1 the chief latent variable and Comp 4 the least latent variable. Consequently, we are supposed to drop Comp 4 because it only explained 3% of information in Y variable and dropping it will not cause much harm as seen in the cumulative Q^2_i value table. We still had a cumulative value of 0.976 with or without Comp 4.

Table 6: Model parameters

Variable	Total Expenditure
Intercept	-20.656
Claims	0.339
Fire	0.527
Accident	2.115
Motor	2.756
Employers	-16.801
Marine	-1.517
Misce-	-0.540

Ridge Regression

Table 7: Variance Inflation Factor Section

Variance Inflation Factor Section							
k	Claims	Fire	Accident	Motor	Employers	Marine	Miscellaneous
0.000	4406.366	468.9307	233.6862	486.0673	255.674	185.7148	580.1272
0.001	89.6244	18.5617	42.2834	35.1855	73.742	89.7348	34.5996
0.002	29.4692	10.783	35.4836	26.3248	54.8802	65.6983	24.5075
0.003	16.0242	8.3782	31.4218	22.7937	43.5515	50.7256	20.7886
0.004	10.7703	7.1223	28.2625	20.4624	35.8502	40.6236	18.4471
0.005	8.0919	6.3167	25.6452	18.6638	30.2876	33.448	16.6858
0.005	8.0919	6.3167	25.6452	18.6638	30.2876	33.448	16.6858
0.006	6.4929	5.7421	23.4198	17.1853	26.0965	28.1478	15.2579
0.007	5.4336	5.3045	21.4994	15.9302	22.8349	24.1087	14.0554

0.008	4.6787	4.9562	19.8249	14.8435	20.2303	20.9509	13.0196
0.009	4.1113	4.6696	18.3528	13.89	18.1061	18.4287	12.1138
0.01	3.6675	4.4279	17.0499	13.045	16.3429	16.3775	11.3132
0.02	1.7164	3.0933	9.3801	7.9295	7.7244	7.0838	6.5282
0.03	1.0602	2.458	6.0461	5.521	4.6825	4.178	4.362
0.04	0.7357	2.06	4.268	4.1349	3.1929	2.8335	3.1747
0.05	0.5476	1.7823	3.1963	3.2436	2.338	2.0807	2.447
0.06	0.4279	1.5765	2.4952	2.6283	1.7975	1.6087	1.9656
0.07	0.3466	1.4179	2.009	2.1818	1.4322	1.2899	1.629
0.08	0.2888	1.2917	1.6566	1.8458	1.173	1.0627	1.3834
0.09	0.2461	1.1891	1.3924	1.5855	0.982	0.8943	1.198
0.1	0.2135	1.1038	1.1887	1.3793	0.8369	0.7655	1.0541
0.2	0.0913	0.6754	0.4008	0.5175	0.2957	0.2722	0.4752
0.3	0.0614	0.5023	0.2095	0.284	0.168	0.1515	0.3124
0.4	0.0485	0.4012	0.1339	0.1862	0.1163	0.1026	0.2352
0.5	0.0413	0.3326	0.0961	0.1353	0.0892	0.0774	0.189
0.6	0.0367	0.2822	0.0744	0.1051	0.0727	0.0625	0.1578
0.7	0.0333	0.2435	0.0606	0.0855	0.0617	0.0527	0.135
0.8	0.0307	0.2128	0.0512	0.0719	0.0538	0.0458	0.1176
0.9	0.0286	0.1879	0.0446	0.062	0.0478	0.0407	0.1039
1	0.0269	0.1674	0.0395	0.0545	0.0432	0.0368	0.0927

Table 7 shows the VIF values for the several independent variables at different k trial values. Observe that the multicollinearity reduces with increased k value since the VIF's kept reducing.

Table 8:Ridge vs. Least Squares Comparison Section for k = 0.005000

Independent Variable	Regular Ridge Coeff's	Regular L.S. Coeff's	Standardized Ridge Coeff's	Standardized L.S. Coeff's	Ridge Standard Error	L.S. Standard Error
Intercept	1493.466	1346.411				
Claims	0.494533	2.867821	0.4233	2.4548	0.134311	2.354801
Fire	0.446711	-3.78929	0.0739	-0.6264	0.614432	3.977479
Accident	0.872502	-2.21072	0.1372	-0.3477	1.301242	2.9512
Motor	2.939932	0.778697	0.7155	0.1895	0.717422	2.750741
Employers	-37.0777	-17.4773	-0.3138	-0.1479	26.27917	57.36528
Marine	-0.59686	-1.36654	-0.062	-0.1419	2.251593	3.986157
Miscellaneous	-0.0153	-3.19616	-0.0033	-0.6846	0.770782	3.414654

At k value of 0.005, the Least square standard errors for parameter estimates were reduced as compared above since RR reduced the effect of multicollinearity.

Table 9: Ridge Regression Coefficient Section for $k = 0.005000$

Independent Variable	Regression Coefficient	Standard Error	Standardized Regression Coefficient	VIF
Intercept	1493.466			
Claims	0.494533	0.134311	0.4233	8.0919
Fire	0.4467107	0.614432	0.0739	6.3167
Accident	0.8725019	1.301242	0.1372	25.6452
Motor	2.939932	0.7174224	0.7155	18.6638
Employers	-37.07767	26.27917	-0.3138	30.2876
Marine	-0.596858	2.251593	-0.062	33.448
Miscellaneous	-0.01530452	0.7707824	-0.0033	16.6858

Notice that the VIF values are now smaller, which means that the multicollinearity has reduced due to Ridge regression parameter estimates.

Table 10: Analysis of Variance Section for $k = 0.005000$

Source	DF	Sum of Squares	Mean Square	F-Ratio	Prob Level
Intercept	1	9.64E+09	9.64E+09		
Model	7	9.11E+09	1.30E+09	86.314	0.000001
Error	8	1.21E+08	1.51E+07		
Total (Adjusted)	15	9.23E+09	6.16E+08		

Table 11: Comparison of the different estimation methods.

RR				OLSR		PLSR	
Year	Actual	Predicted	Residual	Predicted	Residual	Predicted	Residual
1996	5,916.14	2,662.29					
			3,253.85	3,276.22	2,639.92	2,020.39	3,895.75
1997	6,499.40	3,483.50	3,015.90	3,658.44	2,840.96	2,801.59	3,697.81
1998	7,174.28	3,874.73	3,299.56	3,844.41	3,329.87	3,024.78	4,149.50
1999	5,923.18	7,502.31	-1,579.13	8,367.28	- 2,444.10	7,560.00	- 1,636.82
2000	5,629.52	6,330.17	-700.65	6,009.15	- 379.63	5,857.19	- 227.67
2001	6,110.52	7,286.43	-1,175.91	8,354.04	- 2,243.52	7,241.56	- 1,131.04
2002	6,856.15	9,433.87	-2,577.73	9,370.65	- 2,514.51	7,478.80	- 622.65
2003	9,415.20	12,359.90	-2,944.70	12,035.07	- 2,619.87	12,643.05	- 3,227.85
2004	12,084.04	13,535.59	-1,451.55	12,176.93	- 92.89	15,074.19	- 2,990.15
2005	12,402.40	16,106.77	-3,704.37	13,689.05	- 1,286.65	17,336.87	- 4,934.47
2006	76,276.11	76,001.85	274.25	75,950.58	325.53	75,438.15	837.96
2007	25,133.24	22,825.94	2,307.30	24,002.70	1,130.54	24,054.89	1,078.35
2008	37,412.55	36,345.20	1,067.35	35,164.29	2,248.26	37,686.21	- 273.66
2009	61,969.15	61,528.85	440.30	61,511.82	457.33	60,609.04	1,360.11
2010	53,815.35	55,812.01	-1,996.66	56,556.87	- 2,741.52	5,942.62	- 2,127.27
2011	60,204.76	57,732.58	2,472.18	58,854.50	1,350.26	58,052.66	2,152.10

Table 12: Prediction error comparison of the different methods.

Year	RR	OLS	Difference	RR	PLSR	Difference
1996	3253.846	2639.918	-	3253.846	3895.753	-
1997	3015.896	2840.962	-	3015.896	3697.814	-
1998	3299.555	3329.875	+	3299.555	4149.498	-
1999	-1579.13	-2444.100	-	-1579.13	-1636.815	+
2000	-700.651	-379.630	+	-700.651	-227.669	-
2001	-1175.91	-2243.516	-	-1175.91	-1131.035	-
2002	-2577.73	-2514.508	+	-2577.73	-622.652	-
2003	-2944.7	-2619.866	+	-2944.7	-3227.852	+
2004	-1451.55	-92.887	+	-1451.55	-2990.152	+
2005	-3704.37	-1286.655	+	-3704.37	-4934.471	+
2006	274.2549	325.534	+	274.2549	837.964	-
2007	2307.304	1130.544	-	2307.304	1078.349	+
2008	1067.349	2248.257	+	1067.349	-273.661	+
2009	440.2982	457.328	+	440.2982	1360.109	-
2010	-1996.66	-2741.522	-	-1996.66	-2127.274	+
2011	2472.178	1350.265	-	2472.178	2152.097	+

Here, we try to compare the precision of the methods through their prediction residuals. A positive sign means that RR performed better than OLSR while a positive sign in the other end means that PLSR performed better than RR. The signs are as a result of the difference between errors due to prediction results by the methods being compared. Notice that RR performed better than OLSR but PLSR performed equally the same way as RR on the basis of the plus and minus signs. This leaves us with no doubt that PLSR performed better than OLSR.

Table 13: General Comparison

	OLSR	RR	PLSR
R-Squared	0.993	0.9869	0.988
M.S.E	8,514,629.079	15,083,863.6	6,695,165.045
R.M.S.E	2917.984	3883.795	2587.502

When model fitting is the aim and not prediction, we observe that O.L.S.R gave higher R-squared value than PLSR and RR. This means that OLSR fits the data well even in the presence of multicollinearity but failed to predict better than PLSR since its RMSE value is higher compared to PLSR. Note, not all high values of R-square indicates good model fit because R-squared values increases monotonously with the variables, whether important or irrelevant for the prediction of the dependent variable.

4.0 Conclusion

The PLSR model provided more précised prediction as compared with the OLSR and RR methods to handle the problem of multicollinearity on Nigeria Insurance company's expenditure data when predictors are highly correlated.

5.0 Recommendation

It is highly recommended that a correlation matrix and collinearity diagnostics be computed on any data before embarking on regression analysis, this will enable one know the exact model that fits the data well. If the X variables are found to be collinear then the researcher should consider the following remedial measures to tackle the multicollinearity problem: Dropping some variables, transformation of variables, additional or new data and very importantly try using other shrinkage regression methods like Principal component regression (PCR), Ridge Regression (RR), Total least squares (TLS) and Partial Least Square regression (PLSR).

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