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Hybrid Principal Component-Based Estimators for Multicollinearity in Simultaneous Equation Models

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ABSTRACT
This study addresses the problem of multicollinearity in simultaneous equation models (SEMs) by proposing hybrid estimators that integrate Principal Component Analysis (PCA) with conventional estimation techniques. Multicollinearity, characterized by high correlations among explanatory variables, adversely affects the efficiency and stability of estimators such as Two-Stage Least Squares (2SLS), Three-Stage Least Squares (3SLS), and Full Information Maximum Likelihood (FIML). To mitigate this problem, correlated regressors are transformed into orthogonal principal components prior to estimation, leading to the PCR-based SEM estimators. The performance of both classical and hybrid estimators is evaluated through Monte Carlo simulations under varying levels of multicollinearity, sample sizes and error structures. Mean Squared Error (MSE) is used as the evaluation criterion. The results indicate that the hybrid PCR-FIML estimator consistently outperforms competing estimators in most experimental settings. Overall, incorporating PCA into SEM estimation improves predictive accuracy, reduces estimation variance, and enhances robustness in the presence of multicollinearity.

Keywords: Multicollinearity, Principal Component Regression, Simultaneous Equation Models, Monte Carlo Simulation, Hybrid Estimators

INTRODUCTION

Multicollinearity also known as high correlation among input variables is a pervasive challenge in econometric modelling particularly within Simultaneous Equation Models (SEMs). A simultaneous equation model (SEM) consists of a system of interrelated structural equations in which endogenous and exogenous variables interact simultaneously through stochastic disturbance terms. It involves modelling several equations concurrently. (Schmidt, 2005; Alabi, 2016). SEMs comprise a system of interdependent structural equations where endogenous variables appear on both sides of equations, making identification and estimation more complex than in single–equation regression models. Under multicollinearity, classical estimators such as Method of Least Squares or Two–Stage Least Squares (2SLS) suffer from inflated variances and unstable coefficients, thereby undermining inferential reliability and predictive precision. Several studies have investigated the impact of multicollinearity on estimation procedures in simultaneous equation models such as Olubusoye (2001), Johnson *et al.* (2010), Alabi and Oyejola (2015), Alabi (2016), among others.

In linear regression, ridge regression and Principal Component Regression (PCR) are well-established techniques for multicollinearity mitigation. Principal Component Analysis (PCA) reduces dimensionality by orthogonal transformation of predictors, effectively mitigating collinearity via latent orthogonal components (Alabi, *et al.* 2025). However, their application in SEMs remains underdeveloped. Multicollinearity in the structural system is not automatically taken into account by traditional SEM estimators. Despite the extensive application of PCA in linear regression, limited attention has been given to the integration of PCA with simultaneous-equation estimation procedures. Consequently, the relative performance of PCA-based hybrid SEM estimators remains largely unexplored.

This study aims to:

1. Develop PCA-based hybrid estimators for simultaneous equation models.
2. Compare their performance with conventional SEM estimators.
3. Assess estimator performance under varying levels of multicollinearity and sample sizes using Monte Carlo simulations.
4. Identify the most efficient estimator based on Mean Squared Error (MSE).

Multicollinearity in Regression and SEM

Regression with multicollinearity is more sensitive to sampling variability and inflates the variance of coefficient estimators (Fayose and Ayinde, 2019; Aladesuyi *et al.* 2025). Multicollinearity does not affect parameter estimates on conventional ordinary least squares regression, but it can make them statistically insignificant because of excessive variation (Fayose *et al.* 2023a; Fayose *et al.* 2023b). For mitigation, methods like PCR are frequently used (Leamer, 1978 and Alabi *et al.* 2025). PCR uses PCA to orthogonalize predictors before regression, thereby eliminating linear dependence among regressors.

According to Cankaya and Eker (2025), in SEMs, multicollinearity presents unique challenges due to the simultaneous determination of endogenous variables. Standard estimators (2SLS, 3SLS, FIML, ILS and LIML) assume stable instruments and well-conditioned design matrices; when multicollinearity is severe, these estimators may yield unstable solutions (Cankaya and Eker, 2025). Bayesian extensions and penalized GMM approaches have been proposed to handle violations of classical assumptions such as multicollinearity and heteroscedasticity, though the focus has often been on robustness rather than explicit multicollinearity correction (Okeke *et al.* 2025).

PCA in Linear Models

PCA transforms correlated regressors into orthogonal components, which can then be regressed on the output variable, mitigating collinearity by discarding components associated with small eigen values. Studies have compared this approach and found its strengths depending on data and application context.

Simultaneous Equation Estimation

In SEMs, classical estimators include the following:

Two–Stage Least Squares (2SLS): An instrumental variables estimator that first predicts endogenous regressors using instruments, then uses predicted values in structural equations.

Three–Stage Least Squares (3SLS): A system estimator that combines 2SLS with a generalized least squares approach to account for equation error covariance.

Full Information Maximum Likelihood (FIML): A likelihood-based estimator that uses all system information simultaneously.

Limited Information Maximum Likelihood (LIML): An estimator that maximizes a part of the likelihood relevant to a particular equation without full system specification.

Indirect Least Squares (ILS): Derives parameter estimates indirectly using reduced–form coefficients.

These estimators have performance limitations when multicollinearity is present in the model, hence the need to infuse ridge parameter in the model and apply the PCA to the model separately and examine their performance.

MATERIALS AND METHODS

We consider a linear simultaneous equation system of the form:

$$
\begin{aligned}
y_{i1} &= \beta_{12}y_{i2} + \beta_{13}y_{i3} + \beta_{14}y_{i4} + \gamma_{14}x_{i4} + u_{i1} && \text{(i)} \\
y_{i2} &= \beta_{23}y_{i3} + \gamma_{21}x_{i1} + \gamma_{23}x_{i3} + u_{i2} && \text{(ii)} \qquad (1) \\
y_{i3} &= \beta_{31}y_{i1} + \beta_{34}y_{i4} + \gamma_{31}x_{i1} + \gamma_{32}x_{i2} + u_{i3} && \text{(iii)} \\
y_{i4} &= \beta_{41}y_{i1} + \beta_{42}y_{i2} + \gamma_{42}x_{i2} + u_{i4} && \text{(iv)}
\end{aligned}
$$

Where y_{i1} is an output variable, i = 1,2,3,4, x_{i1}, x_{i2}, x_{i3} and x_{i4} are the input variables

$$
\begin{bmatrix} u_{i1} \\ u_{i2} \\ u_{i3} \\ u_{i4} \end{bmatrix} \sim N(0, \Sigma), where\ i = 1,2,3,\dots,n
$$

and

$\beta_{12}, \beta_{13}, \beta_{14}, \beta_{23}, \beta_{31}, \beta_{34}, \beta_{41}, \beta_{42}, \gamma_{14}, \gamma_{21}, \gamma_{23}, \gamma_{31}, \gamma_{32}$ and γ_{42} are the structural parameters of the model. Equations (i) and (iii) are exactly identified while equations (ii) and (iv) are overidentified by both order and rank conditions.

$$
\begin{aligned}
&y_{i1} - \beta_{12}y_{i2} - \beta_{13}y_{i3} - \beta_{14}y_{i4} + 0x_{i1} + 0x_{i2} + 0x_{i3} - \gamma_{14}x_{i4} = u_{i1} && \text{(i)} \\
&0y_{i1} + y_{i2} - \beta_{23}y_{i3} + 0y_{i4} - \gamma_{21}x_{i1} + 0x_{i2} - \gamma_{23}x_{i3} + 0x_{i4} = u_{i2} && \text{(ii)} \qquad (2) \\
&-\beta_{31}y_{i1} + 0y_{i2} + y_{i3} - \beta_{34}y_{i4} - \gamma_{31}x_{i1} - \gamma_{32}x_{i2} + 0x_{i3} + 0x_{i4} = u_{i3} && \text{(iii)} \\
&-\beta_{41}y_{i1} - \beta_{42}y_{i2} + 0y_{i3} + y_{i4} + 0x_{i1} - \gamma_{42}x_{i2} + 0x_{i3} + 0x_{i4} = u_{i4} && \text{(iv)}
\end{aligned}
$$

This can be written in matrix form as:

$$
\beta y_i + \Gamma x_i = u_i \qquad (3)
$$

Where

$$
\beta = \begin{bmatrix} 1 & -\beta_{12} & -\beta_{13} & -\beta_{14} \\ 0 & 1 & -\beta_{23} & 0 \\ -\beta_{31} & 0 & 1 & -\beta_{34} \\ -\beta_{41} & -\beta_{42} & 0 & 1 \end{bmatrix} \qquad
\Gamma = \begin{bmatrix} 0 & 0 & 0 & -\gamma_{14} \\ -\gamma_{21} & 0 & -\gamma_{23} & 0 \\ -\gamma_{31} & -\gamma_{32} & 0 & 0 \\ 0 & -\gamma_{42} & 0 & 0 \end{bmatrix} \qquad
y_i = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{bmatrix}
$$

$$
x_1 = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} \text{ and } u_i = \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{bmatrix}
$$

Now, from equation (3),

$$
\beta^{-1}\beta y_i = \beta^{-1}\Gamma x_i = \beta^{-1}u_i \qquad (4)
$$

Data Generation of Input Variables

The input variables were generated using the procedure proposed by Ayinde (2007) and later adopted by Alabi (2019) to produce normally distributed regressors with predetermined correlation structures. The equations are given as:

$$
x_1 = \mu_1 + \sigma_1 z_1
$$

$$
x_2 = \mu_2 + \rho_{12}\sigma_2 z_1 + \left(\sqrt{m_{22}}\right) z_2
$$

$$x_3 = \mu_3 + \rho_{13}\sigma_3 z_1 + \frac{m_{23}}{\sqrt{m_{22}}} z_2 + \left(\sqrt{n_{33}}\right) z_3$$

$$x_4 = \mu_3 + \rho_{14}\sigma_4 z_1 + \frac{m_{24}}{\sqrt{m_{22}}} z_2 + \frac{n_{34}}{\sqrt{n_{33}}} z_3 + \sqrt{0_{44}}\, z_4$$

where $m_{22} = \sigma_2^2(1-\rho_{12}^2)$ $m_{23} = \sigma_2\sigma_3\left(\rho_{23} - \rho_{12}\rho_{13}\right)$ $m_{24} = \sigma_2\sigma_4\left(\rho_{24} - \rho_{12}\rho_{14}\right)$,

$m_{33} = \sigma_3^2\left(1-\rho_{13}^2\right)$, $m_{44} = \sigma_4^2\left(1-\rho_{14}^2\right)$, $0_{44} = n_{44} - \frac{n_{34}^2}{n_{33}}$, $n_{44} = m_{44} - \frac{m_{24}^2}{m_{22}}$,

$n_{34} = m_{34} - \frac{m_{23}m_{24}}{m_{22}}$, $n_{33} = m_{33} - \frac{m_{23}^2}{m_{22}}$

And $Z_i \sim N(0,1)$, i = 1, 2, 3, 4 and $\left|\rho_{ij}\right| < 1$ is the value of correlation between the two variables i and j (Ayinde, 2007; Alabi, 2019).

The input variables were generated to be normally distributed with mean zero and unity variance. i.e. $x \sim N(0,1)$, i = 1,2,3,4 and $\left|\rho_{ij}\right| < 1$ is the value of correlation between the two variables i and j. In addition, the study used $\rho_{12} = \rho_{13} = \rho_{14} = \rho_{23} = \rho_{24} = \rho_{34} = \rho =$ 0.3, 0.6, 0.9 and 0.99 as scenarios where collinearity existed between the model's regressors

Methods of Generating Output Variables

Following (Ayinde, 2007; Alabi, 2019), The output variables were created using equation (4) by using the parameters' actual values as:

$$\beta = \begin{bmatrix} 1 & -\beta_{12} & -\beta_{13} & -\beta_{14} \\ 0 & 1 & -\beta_{23} & 0 \\ -\beta_{31} & 0 & 1 & -\beta_{34} \\ -\beta_{41} & -\beta_{42} & 0 & 1 \end{bmatrix} = \begin{bmatrix} 1 & -3.2 & -0.2 & -1.2 \\ 0 & 1 & -3.8 & 0 \\ -1.6 & 0 & 1 & -1.0 \\ -2.8 & -2.2 & 0 & 1 \end{bmatrix}$$

$$\Gamma = \begin{bmatrix} 0 & 0 & 0 & -\gamma_{14} \\ -\gamma_{21} & 0 & -\gamma_{23} & 0 \\ -\gamma_{31} & -\gamma_{32} & 0 & 0 \\ 0 & -\gamma_{42} & 0 & 0 \end{bmatrix} = \begin{bmatrix} 0 & 0 & 0 & -0.8 \\ -3.0 & 0 & -1.3 & 0 \\ -1.5 & -0.6 & 0 & 0 \\ 0 & -2.6 & 0 & 0 \end{bmatrix}$$

Generation of Correlated Error Term

The mean of the disturbance are zero and unit variance. i.e. 1 as adopted by (Ayinde, 2007; Alabi, 2019). The correlation values are $\lambda_{12} = \lambda_{13} = \lambda_{14} = \lambda_{23} = \lambda_{24} = \lambda_{34} = \lambda$ and $\left|\lambda_{ij}\right| < 1$ is the value of correlation between the two error terms i and j. $\lambda_{12} = \lambda_{13} = \lambda_{14} = \lambda_{23} = \lambda_{24} = \lambda_{34} = \lambda = 0$ was used in this investigation as the scenario in which there is no correlation at all between the model's error terms.

Classical SEM Estimators

Two–Stage Least Squares (2SLS)

2SLS uses instrumental variables to obtain consistent estimates in the presence of endogeneity. First, endogenous regressors are projected onto instruments; second, predicted values are used in the structural equation. This estimator is consistent but not efficient under general disturbance covariance.

Three–Stage Least Squares (3SLS)

3SLS combines 2SLS with a generalized least squares adjustment exploiting the cross–equation error covariance matrix:

Full Information Maximum Likelihood (FIML)

FIML estimates parameters by maximizing a joint likelihood function under multivariate normal assumptions, using all equations simultaneously.

Indirect Least Squares (ILS) and LIML

ILS uses reduced–form parameters to derive structural coefficients. LIML is a maximum likelihood estimator for individual equations, requiring limited systemic information.

PCA SEM Estimators

Principal Component Analysis (PCA) was applied to the correlated explanatory variables to obtain orthogonal principal components. Components satisfying the selected retention criterion were subsequently used as regressors in the estimation procedures. This transformation removes linear dependence among regressors and reduces the adverse effects of multicollinearity.

The orthogonalized regressors mitigate multicollinearity by construction. This yields PCR-2SLS, PCR-3SLS, PCR-FIML, PCR-ILS and PCR-LIML etc (Judge, *et al.* 1985; De Jong and Kiers, 1992; Cankaya and Eker, 2025).

Criterion for Selecting Principal Components

The principal components were selected based on the Kaiser criterion, whereby components with eigenvalues greater than one were retained while components with eigenvalues less than or equal to one were excluded. This criterion was adopted because an eigenvalue represents the amount of variance explained by each principal component; therefore, retaining components with eigenvalues greater than one ensures that each retained component explains more variance than an individual standardized original variable. The criterion also provides a simple and objective rule for reducing the dimensionality of highly correlated regressors while preserving the major information contained in the original variables. The retained components were then used as regressors in the proposed PCA-based simultaneous equation estimators (PCR-2SLS, PCR-3SLS, PCR-FIML, PCR-ILS and PCR-LIML). This approach reduces multicollinearity because the retained principal components are mutually orthogonal. Consequently, the procedure improves the numerical stability of the estimation without retaining components that contribute relatively little information to the model.

Computational Complexity and Convergence Characteristics of the Hybrid Estimators

The proposed hybrid estimators involve two computational stages: principal component transformation and simultaneous equation estimation. In the first stage, the covariance structure of the input variables is decomposed into orthogonal principal components. For (n) observations and (p) input variables, the computational cost of constructing the covariance matrix is of order ($O(np^2)$), while the eigenvalue–eigenvector decomposition is approximately ($O(p^3)$). Given the relatively small number of input variables considered in the simulation design, the additional computational burden associated with the PCA transformation is expected to be limited.

In the second stage, the retained principal components are incorporated into the respective simultaneous equation estimators. Thus, PCR-2SLS, PCR-3SLS, PCR-FIML, PCR-ILS and PCR-LIML retain the fundamental computational structure of their corresponding classical estimators, with the PCA transformation serving as a preprocessing step. Although this introduces an additional computational operation, the orthogonalization of the regressors is expected to improve the numerical conditioning of the estimation problem, particularly under severe multicollinearity.

With respect to convergence, the PCA transformation is expected to enhance the numerical stability of the hybrid estimators because the retained principal components are mutually orthogonal. Consequently, near-linear dependence among the original input variables is substantially reduced before estimation. This effect is expected to be particularly important for PCR-FIML, whose full-information likelihood estimation uses information from all equations simultaneously. By improving the conditioning of the regressor structure, PCA may facilitate more stable numerical optimization and reduce the likelihood of unstable parameter estimates under high levels of multicollinearity.

It should, however, be noted that the present Monte Carlo experiment was designed primarily to compare estimator performance using mean squared error and did not explicitly record computational time, iteration counts, convergence failures, or optimization tolerances. Therefore, the convergence characteristics discussed here represent the expected numerical implications of the PCA transformation rather than direct empirical measures of convergence speed.

Criteria for Assessment

Using Monte Carlo simulations, we evaluate the characteristics of estimators at various stages of multicollinearity, sample sizes, and instrument strength. Estimator performance was evaluated using Mean Squared Error (MSE), defined as

$MSE(\hat{\beta}) = E[(\hat{\beta} - \beta)^2]$

where $\hat{\beta}$denotes the estimator and βrepresents the true parameter value. The MSE is defined as: $MSE\left(\hat{\theta}_{ij}\right)=\dfrac{1}{R}\sum_{i=1}^{R}\left(\hat{\theta}_{ij}-\theta_{ij}\right)^2$, i = 1, 2, ……, R, where R = 1000.

In the study, $\hat{\theta}$ is used to represent the estimator of any of the parameters in the model (1) under consideration. Using the R programming language, the mean square error values for each parameter across the estimation methods and equation were arrived at for all sample sizes at all correlation value levels for gaussian distributed regressors.

Summary of the Procedure for Identifying the Best Estimators under MSE Criterion

i. At each level of multicollinearity, error variance and lambda, the MSE produced by each estimator were ranked.

ii. The number of occasions on which each estimator recorded the least MSE was evaluated under varying levels of multicollinearity, error variance and lambda values.

iii. An estimator is considered best if it has highest number of counts.

RESULTS AND DISCUSSION

This section compares the performance of the estimators with and without collinearity, respectively. The simulation results are presented pictorially for PCR-SEM.

Results from all Estimation Methods with and without PCA Combination

The results of the investigations under all estimation methods from the simulation study at various sample sizes, multicollinearity levels, error variances and lambda errors is pictorially presented in Figure 1 and Figure 2 respectively.

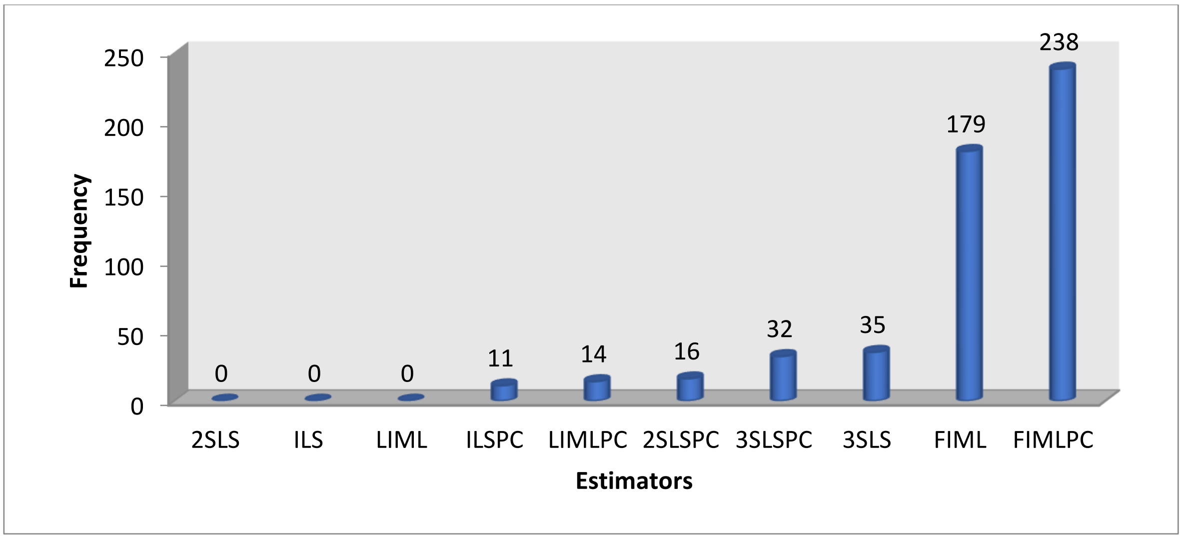

Figure 1. Frequency with which each Estimator Achieved the Minimum MSE across all Simulation Scenarios

Figure 1 shows that the PCR-FIML estimator attained the highest frequency of minimum MSE values across the experimental settings. This result suggests that combining PCA with FIML substantially improves estimation efficiency in the presence of multicollinearity. The conventional FIML estimator ranked second, followed by 3SLS and PCR-3SLS.

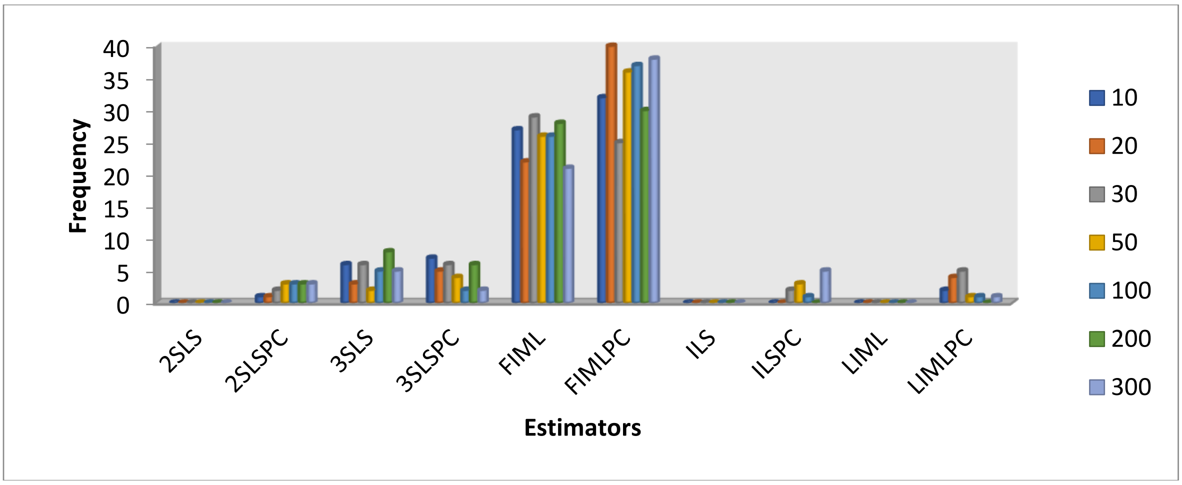

Figure 2. Distribution of minimum-MSE frequencies across sample sizes for all estimators.

Figure 2 shows that the proposed PCA-FIML estimator performed consistently across all sample sizes and outperformed the other estimators and their PCA-based counterparts. The conventional FIML estimator also performed relatively well across the sample sizes. In contrast, the conventional 2SLS, ILS and LIML estimators did not attain the minimum MSE at any of the sample sizes considered.

Table 1: Frequency with Which Each Estimator Attained the Minimum MSE across levels of Multicollinearity, Error Variance and lambda errors based on Sample Size

	Sample Size (n)								
Estimators	10	20	30	50	100	200	300	TOTAL	RANK
2SLS	0	0	0	0	0	0	0	0	10th
PCR-2SLS	1	1	2	3	3	3	3	16	5th
3SLS	6	3	6	2	5	8	5	35	3rd
PCR-3SLS	7	5	6	4	2	6	2	32	4th
FIML	27	22	**29**	26	26	28	21	179	2nd
PCR-FIML	**32**	**40**	25	**36**	**37**	**30**	**38**	238	1st
ILS	0	0	0	0	0	0	0	0	10th
PCR-ILS	0	0	2	3	1	0	5	11	7th
LIML	0	0	0	0	0	0	0	0	10th
PCR-LIML	2	4	5	1	1	0	1	14	6th

NOTE: Estimator with highest frequency at each sample size is bolded

From Table 1, it can be observed that the best / most efficient estimator is the proposed combined estimator (PCR-FIML) i.e. Full Information Maximum Likelihood with Principal Component Analysis estimator followed by its existing estimator (FIML) i.e. Full Information Maximum Likelihood estimator and (3SLS) i.e. existing Three Stage Least Square estimator and proposed combined estimator (PCR-3SLS) i.e. proposed Three Stage Least Square with Principal Component Analysis estimator respectively.

Table 1 indicates that PCR-FIML consistently dominates competing estimators across most sample sizes. The superiority of PCR-FIML becomes increasingly pronounced as sample size increases, demonstrating both stability and robustness under severe multicollinearity.

CONCLUSION

This study investigated the impact of multicollinearity on the performance of estimators in simultaneous equation models (SEMs) and evaluated the effectiveness of integrating Principal Component Analysis (PCA) with conventional estimation techniques. Through extensive Monte Carlo simulations conducted under varying sample sizes and correlation structures, the study assessed estimator performance using Mean Squared Error (MSE) as the primary evaluation criterion.

The findings demonstrate that multicollinearity significantly undermines the efficiency, stability and reliability of traditional SEM estimators, including Two-Stage Least Squares (2SLS), Three-Stage Least Squares (3SLS), Full Information Maximum Likelihood (FIML), Limited Information Maximum Likelihood (LIML) and Indirect Least Squares (ILS). To address this limitation, PCA was incorporated into the estimation framework to transform highly correlated explanatory variables into orthogonal components, thereby reducing redundancy and improving parameter estimation.

The simulation results consistently reveal that PCA-based hybrid estimators outperform their classical counterparts across most experimental conditions. In particular, the PCR–FIML estimator exhibited the lowest MSE and the highest frequency of optimal performance, indicating superior efficiency and robustness in the presence of severe multicollinearity. Similarly, PCR–3SLS and other hybrid approaches showed notable improvements over conventional methods.

Overall, the study establishes PCR-based hybrid estimation as a practical and effective strategy for mitigating multicollinearity in SEMs. Future research may extend this framework to non-Gaussian settings, heteroscedastic error structures and real-world economic datasets to further validate its applicability and generalizability.

AUTHOR CONTRIBUTIONS

i. Conceptualization: A. Aladesuyi

ii. Methodology: A. Aladesuyi, O.O. Alabi

iii. Software: A. Aladesuyi

iv. Supervision: O.O. Alabi, A.H. Bello

v. Writing – Original Draft: A. Aladesuyi

vi. Writing – Review & Editing: All authors

DATA AVAILABILITY STATEMENT

The data generated during the simulation study are available from the corresponding author upon reasonable request.

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DECLARATION OF COMPETING INTEREST

The authors declare no competing interests.

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