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OVERCOMING UNIDENTIFIABILITY IN LINEAR FUNCTIONAL RELATIONSHIP MODEL USING BALANCED REPLICATED DATA

(*Mengatasi Isu Ketidakbolehpastian dalam Model Hubungan Fungsi Linear Menggunakan Data Replikasi Seimbang*)

AZURAINI MOHD ARIF*, YONG ZULINA ZUBAIRI
& MOHD SYAZWAN MOHAMAD ANUAR

ABSTRACT

This paper proposes a balanced replicated linear functional relationship model (LFRM) to overcome the unidentifiability issue present in the unreplicated LFRM, where both the predictor and response variables are measured with errors. In the unreplicated LFRM, parameter estimation relies on the restrictive assumption of a known ratio of error variances, denoted as λ. This study demonstrates that by transforming unreplicated data into balanced groups, all parameters namely the intercept, slope, incidental parameters, and two error variances, can be independently estimated using the Maximum Likelihood Estimation (MLE) method. A simulation study was conducted to evaluate the performance of the proposed model. To illustrate the practical application of the balanced replicated LFRM, a fat mass measurement dataset is used. The results demonstrate robustness, as the error variances are estimated without prior assumptions. This novel approach eliminates the need for λ based assumptions, offering an unbiased and consistent solution for LFRM parameter estimation.

Keywords: errors-in-variable model; model performance; parameter estimation; robustness

ABSTRAK

Kertas kerja ini mencadangkan model hubungan fungsian linear bereplika seimbang untuk mengatasi isu ketidakbolehpastian yang wujud dalam model hubungan fungsian linear tanpa replika di mana kedua-dua pembolehubah diukur dengan ralat. Dalam model hubungan fungsian linear tanpa replikasi, penganggaran parameter bergantung kepada andaian terhadap nisbah ralat varians diketahui iaitu λ. Kajian ini menunjukkan dengan mengelompokkan data tanpa replikasi, semua parameter iaitu, pintasan, kecerunan, parameter sampingan dan dua ralat varians, boleh dianggarkan secara bebas menggunakan kaedah kebolehjadian maksimum. Satu kajian simulasi telah dijalankan untuk menilai prestasi model yang dicadangkan. Bagi menggambarkan aplikasi praktikal model fungsian linear bereplika seimbang, satu set data pengukuran jisim lemak telah digunakan. Hasil kajian menunjukkan keteguhan model ini kerana ralat varians boleh dianggarkan tanpa memerlukan andaian awal. Pendekatan baharu ini menghapuskan keperluan terhadap andaian mengenai λ sekaligus menawarkan penyelesaian yang saksama dan konsisten untuk penganggaran parameter model hubungan fungsian linear.

Kata kunci: model ralat pengukuran; prestasi model; anggaran parameter; keteguhan

1. Introduction

The linear functional relationship model (LFRM), a branch of the errors-in-variables model, is essential for analysing the relationship between two variables, *X* and *Y*, when both variables are subject to measurement errors. The LFRM is widely used in many fields, including economics, industrial quality control, biomedical research, environmental monitoring and many more (Buonaccorsi 2010; Stevens *et al.* 2017; Duwarahan & Nawarathna 2022; Lee 2022; Sharif *et* *al.* 2022). Since its early development by Adcock in 1878, the errors-in-variables model has gained significant attention (Arif *et al.* 2021; Jamaliyatul *et al.* 2024). Adcock (1878) investigated the estimation properties of standard linear regression models when both the independent variable, x, and the dependent variable, y, were subject to measurement errors. He applied the least squares method to estimate the slope parameter under the assumption both variables had equal error variances (Adcock 1878). However, this early work was limited to cases with identical error variances.

The LFRM is commonly classified into unreplicated and replicated models (Dorff & Gurland 1961). Traditionally, the parameters in LFRM are intercept (β_0), the slope (β_1), two error variances (σ^2 and τ^2) and the incidental parameter (X_i). In the unreplicated LFRM, the estimation of the error variances remains a challenge due to the unidentifiability problem (Hussin 2004; Christiansen 2014; Ghapor *et al.* 2017). Unidentifiability occurs when the number of parameters increases in relation to the number of observations, i. Lindley (1947) demonstrated that the likelihood equations become inconsistent, requiring prior information on the parameters to handle this issue. Lindley (1947) also estimated the parameters of the unreplicated LFRM using Maximum Likelihood Estimation (MLE) with the assumption that the ratio of error variances, $\lambda = \tau^2/\sigma^2,$ is known. However, in the unreplicated model, consistent estimation of all parameters is not possible because the number of parameters increases with the number of observations and can only be estimated if the ratio of error variances is fixed or assumed, limiting its practical applicability. Consequently, many subsequent studies have relied on the assumption that the ratio of error variances is known or equal error variances, $\lambda = 1$ (Hussin *et al.* 2010; Ghapor *et al.* 2014; Abuzaid *et al.* 2021; Mokhtar *et al.* 2022; Jamaliyatul *et al.* 2023).

Unfortunately, in many practical scenarios, this ratio of error variances is often unknown, making model estimation unreliable. Klepper and Leamer (1984) highlighted the challenges of unidentifiability when λ is unknown, emphasising the need for alternative solutions, namely obtaining replication of observations. Kendall and Stuart (1979) discussed overcoming unidentifiability problems in unreplicated models using the properties of replicated errors. Barnett (1970) explored MLE in replicated LFRM by considering different error structures applicable in biological and medical research. Several researchers have proposed forming pseudo-replicates from unreplicated data to allow for parameter estimation, especially in circular data scenarios (Hussin *et al.* 2005; Mokhtar *et al.* 2017; Moslim *et al.* 2021). Badarisam and Anuar (2023) also highlighted the importance of unequal error variances in parameter estimation. In the replicated model, the key advantage is that the number of parameters remains fixed as the number of observations increases, allowing for consistent estimation (Hokama *et al.* 2021).

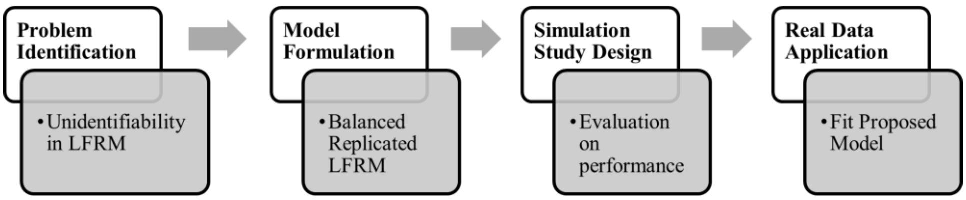

Figure 1: Research design flowchart

To address the limitations of unreplicated LFRM, a balanced replicated LFRM is proposed. The balanced replicated LFRM overcomes unidentifiability by grouping unreplicated data into balanced replicates in each group. In this model, equal-sized observations in each group allow for independent estimation of all parameters without requiring any assumption about the ratio of error variances, λ. In this case, the ratio of error variances could be greater than, less than or equal to one, making the balanced replicated LFRM a robust and flexible alternative to the unreplicated model. Figure 1 presents an overview of the entire process conducted in this study.

2. The Balanced Replicated Linear Functional Relationship Model

Given a particular pair, there may be replicated observations of X_i and Y_i occurring in p groups with m elements in each group. For this model, the linear relationship between X_i and Y_i is given by

$$Y_i = \beta_0 + \beta_1 X_i \tag{1}$$

where $x_{ij} = X_i + \delta_{ij}$ and $y_{ik} = Y_i + \varepsilon_{ik}$ for $i = 1,2,\cdots,p$, $j = 1,2,\cdots,m$ and $k = 1,2,\cdots,m$. β_0 and β_1 are the intercept and the slope parameters respectively. In this case, the error terms δ_{ij} and ε_{ik} are independently distributed and are assumed to follow normal distribution with mean zero and variance σ^2 and τ^2 respectively, i.e. $\delta_{ij} \sim N(0,\sigma^2)$ and $\varepsilon_{ik} \sim N(0,\tau^2)$. In balanced replicated LFRM, it is assumed the observations in each group are the same size ($j = k = 1,2,\cdots,m$). In other words, the observations within each group are balanced and each group has the same number of observations.

Unlike unreplicated LFRM, the ratio of error variances, λ, must be known to estimate the parameters (Ghapor *et al.* 2015). By organizing data into balanced replicated groups, the number of parameters remains fixed as the number of observations increases, ensuring reliable estimation (Barnett 1970; Hussin *et al.* 2005; Arif *et al.* 2020).

3. Maximum Likelihood Estimation of the Model

The Maximum Likelihood Estimation (MLE) method is employed to estimate the parameters of the balanced replicated LFRM to obtain an unbiased and a consistent estimator (Barnett 1970; Hussin 2005). This method has previously been applied in similar contexts, such as in replicated data modeled using the von Mises distribution and in linear structural relationship model (Mokhtar *et al.* 2017; Alshargawi *et al.* 2019; Moslim *et al.* 2021; Saari *et al.* 2023a). By assuming the observations in each group are the same size ($j = k = 1,2,\cdots,m$), the log-likelihood function for balanced replicated LFRM is shown below:

$$\begin{aligned} \log L\left(\beta_0,\beta_1,\sigma^2,\tau^2,X_1,\ldots,X_p;x_{ij},y_{ik}\right) &= -n\log 2\pi - \frac{n}{2}(\log\sigma^2 + \log\tau^2) - \\ &- \frac{1}{2}\left\{\sum_{i=1}^{p}\sum_{j=1}^{m}\frac{\left(x_{ij}-X_i\right)^2}{\sigma^2} + \sum_{i=1}^{p}\sum_{k=1}^{m}\frac{(y_{ik}-\beta_0-\beta_1X_i)^2}{\tau^2}\right\} \end{aligned} \tag{2}$$

There are $(p+4)$ parameters to be estimated as given in Eq. (2) namely the intercept (β_0), the slope (β_1), the incidental parameter (X_i) and two error variances (σ^2 and τ^2). In this case, by grouping data into balanced replicates, the number of parameters remains fixed as the number of observations increases. Thus, to estimate these parameters, the first partial derivative of the log likelihood function with respect to $\beta_0, \beta_1, X_i, \sigma^2$ and τ^2 are obtained and equating to zero. Details on derivations for the MLE and variance-covariance matrix of the balanced replicated model can be found in (Arif *et al.* 2021).

$$\hat{\beta}_0 = \frac{\sum_{i=1}^{p} m(\bar{y}_{i.} - \hat{\beta}_1 \hat{X}_i)}{\sum_{i=1}^{p} m} \quad (3)$$

$$\hat{\beta}_1 = \frac{\sum_{i=1}^{p} m\hat{X}_i(\bar{y}_{i.} - \hat{\beta}_0)}{\sum_{i=1}^{p} m\hat{X}_i^2} \quad (4)$$

$$\hat{\sigma}^2 = \frac{\sum_{i=1}^{p}\sum_{j=1}^{m}(x_{ij} - \hat{X}_i)^2}{\sum_{i=1}^{p} m} \quad (5)$$

$$\hat{\tau}^2 = \frac{\sum_{i=1}^{p}\sum_{k=1}^{m}(y_{ik} - \hat{\beta}_0 - \hat{\beta}_1\hat{X}_i)^2}{\sum_{i=1}^{p} m} \quad (6)$$

$$\hat{X}_i = \frac{1}{\hat{\Delta}}\left\{\frac{m\bar{x}_{i.}}{\hat{\sigma}^2} + \frac{m\hat{\beta}_1}{\hat{\tau}^2}\left(\bar{y}_{i.} - \hat{\beta}_0\right)\right\} \quad (7)$$

where $\bar{x}_{i.} = \frac{\sum x_{ij}}{m}$, $\bar{y}_{i.} = \frac{\sum y_{ik}}{m}$, and $\hat{\Delta}_i = \frac{m}{\hat{\sigma}^2} + \frac{m\hat{\beta}_1^2}{\hat{\tau}^2}$.

Given that Eq. (2) through Eq. (6) rely on the value of Eq. (7), $\hat{X}_i$, thus, a closed-form solution cannot be obtained. Nonetheless, estimates can be calculated through iteration until all parameters reach convergence by selecting suitable initial values i.e., from unreplicated LFRM. The asymptotic variances of the estimators can be obtained by inverting the estimated Fisher information matrix for a balanced replicated LFRM (Arif *et al.* 2021). Thus, the variances are given as follows: where $n = \sum_{i=1}^{p} m = m \times p$

$$V\hat{a}r(\hat{\beta}_0) = \frac{(m\hat{\tau}^2 + m\hat{\beta}_1^2\hat{\sigma}^2)\sum_{i=1}^{p}\hat{X}_i^2}{m^2\left\{p\sum_{i=1}^{p}\hat{X}_i^2 - \left(\sum_{i=1}^{p}\hat{X}_i\right)^2\right\}} \quad (8)$$

$$V\hat{a}r\,(\hat{\beta}_1) = \frac{(m\hat{\tau}^2 + m\hat{\beta}_1^2\hat{\sigma}^2)p}{m^2\left\{p\sum_{i=1}^{p}\hat{X}_i^2 - \left(\sum_{i=1}^{p}\hat{X}_i\right)^2\right\}} \quad (9)$$

$$V\hat{a}r\,(\hat{\sigma}^2) = 2\hat{\sigma}^4/n \quad (10)$$

$$V\hat{a}r\,(\hat{\tau}^2) = 2\hat{\tau}^4/n \quad (11)$$

where $n = \sum_{i=1}^{p} m = m \times p$.

4. Simulation Study

A simulation study was conducted using R software to evaluate the performance of the estimated parameters of the balanced replicated LFRM. Without loss of generality, we fixed the true value of the intercept, $\beta_0 = 1$ and the slope, $\beta_1 = 1$ while varying the value of error variances, $\sigma^2 = 0.8, 1$ and $\tau^2 = 0.8, 1$ to investigate the robustness of the parameter. Three cases of the ratio of error variances, $\lambda = \tau^2/\sigma^2$ are considered. Case 1: $\lambda > 1$, where $\sigma^2 = 0.8$ and $\tau^2 = 1$, Case 2: $\lambda < 1$, where $\sigma^2 = 1$ and $\tau^2 = 0.8$, and Case 3: $\lambda = 1$ where both σ^2 and τ^2 are equal to one. Case 3 will act as the baseline for comparison. The values of λ chosen are intended to cover more realistic and different situations where the value of λ is usually unknown (Saari *et al.* 2023b). The number of simulations, s is set to be 10000. The sample sizes are chosen to be $n = 40, 80$ and 120 with p-subgroups 5, 8 and 8 respectively. Details on data grouping for balanced replicated LFRM can be found in (Arif *et al.* 2021). To measure the accuracy and biasness of the model parameters, the estimated bias and the mean square error were computed as follows:

$$\text{Estimated Bias} = \left|\hat{b} - b\right|$$

and

$$\text{Mean Square Error} = \frac{1}{s}\sum_{i=1}^{s}\left(\hat{b} - b\right)^2$$

with b be a generic term for the parameters and s is the number of simulations. The following tables summarize the simulation results for each case:

Table 1: Case 1: Estimated bias and mean square error when $\lambda > 1$

Parameter	Estimated Bias			Mean Square Error		
	$n = 40$	$n = 80$	$n = 120$	$n = 40$	$n = 80$	$n = 120$
$\hat{\beta}_0$	0.04	0.05	0.05	0.23	0.12	0.08
$\hat{\beta}_1$	0.01	0.01	0.01	0.01	0.00	0.00
$\hat{\sigma}^2$	0.11	0.06	0.04	0.06	0.03	0.02
$\hat{\tau}^2$	0.30	0.25	0.23	0.12	0.08	0.07

Table 2: Case 2: Estimated bias and mean square error when $\lambda < 1$

Parameter	Estimated Bias			Mean Square Error		
	$n = 40$	$n = 80$	$n = 120$	$n = 40$	$n = 80$	$n = 120$
$\hat{\beta}_0$	0.06	0.07	0.07	0.24	0.12	0.08
$\hat{\beta}_1$	0.01	0.01	0.01	0.01	0.00	0.00
$\hat{\sigma}^2$	0.30	0.25	0.23	0.12	0.08	0.06
$\hat{\tau}^2$	0.11	0.06	0.04	0.06	0.01	0.01

Table 3: Case 3: Estimated bias and mean square error when $\lambda = 1$

Parameter	Estimated Bias			Mean Square Error		
	$n = 40$	$n = 80$	$n = 120$	$n = 40$	$n = 80$	$n = 120$
$\hat{\beta}_0$	0.01	0.01	0.01	0.29	0.13	0.08
$\hat{\beta}_1$	0.00	0.00	0.00	0.01	0.00	0.00
$\hat{\sigma}^2$	0.08	0.06	0.04	0.06	0.03	0.02
$\hat{\tau}^2$	0.08	0.06	0.04	0.06	0.03	0.02

The estimated bias in Table 1 for $\lambda > 1$ (Case 1) shows that the values are close to zero for all sample sizes and parameters, indicating unbiased estimation. Meanwhile, the mean square error in Table 1 decreases with increasing sample sizes, indicating that the parameter estimates are consistent. Similar trends can be found in Table 2 for $\lambda < 1$ (Case 2) where the estimated bias is also close to zero. In other words, unbiasedness indicates that the estimated parameters approximate the true values. The mean square error in Table 2 also decreases with increasing sample sizes from 40 to 120 for all parameters. This shows the estimated parameters are consistent. Similar results can also be found in Table 3 under equal error variances, $\lambda = 1$

(Case 3), where all parameters demonstrate good accuracy with estimated bias value close to zero.

Next, the robustness across different ratios of error variances, $\lambda = \tau^2/\sigma^2$, was investigated. For Case 1, the value of error variance, $\hat{\sigma}^2$ is greater than $\hat{\tau}^2$ and for Case 2, the value of error variance $\hat{\sigma}^2$ is less than $\hat{\tau}^2$. Meanwhile, in Case 3, the error variances $\hat{\sigma}^2$ and $\hat{\tau}^2$ are equal. In both Case 1 and Case 2, the model shows that the estimated parameters can be obtained independently without making any assumptions on the ratio of error variances. The results in Case 3 (Table 3) offer the optimal solution, as the estimated bias and mean square error for all parameters are smaller than those in Case 1 (Table 1) and Case 2 (Table 2). Nevertheless, the results from Case 1 and Case 2 show that the model performs well regardless of whether the ratio of error variances is greater than or less than one, demonstrating the model's flexibility and applicability to various practical scenarios. Overall, the parameter estimates are both unbiased and consistent, indicating that the proposed model is adequate.

5. Application of The Model

The applicability of the balanced replicated LFRM is illustrated by using a fat mass measurement dataset. The dataset consists of 96 observations from children, with body fat measured using two techniques, namely the skinfold thickness (ST), x_i, and bioelectrical resistance (BR), y_i, (Goran *et al.* 1996). The techniques involved are subject to errors due to factors such as instrument precision, environmental conditions and operator variability (Giménez & Patat 2005; Wimmer & Witkovský 2007). Since only one observation pair, x and y exists for each subject, the original dataset is considered unreplicated. In this case, it is not possible to estimate all parameters unless an assumption is made regarding the ratio of error variances. Thus, to estimate the parameters namely the intercept, the slope and the error variances without making any assumption on the ratio of error variances, the dataset is transformed into replicated data. It is assumed that the replication can be made available based on each observation measured, enabling parameter estimation using the maximum likelihood method. For this data, two models were considered, either using 6 groups or 8 groups. Akaike's Information Criterion (AIC) is used to select the best model with the lowest AIC among competing models (Mokhtar *et al.* 2020). AIC is straightforward to compute, requiring the log-likelihood and the number of parameters. AIC is calculated as follows:

$$AIC = -2(log\ L) + 2 * (p + 4)$$

To obtain replication, the first model is divided into 6 groups, each containing 16 observations and for the second model, the dataset is divided into 8 groups, each containing 12 observations. This grouping ensures that data is balanced and equal-sized, which is necessary for applying the balanced replicated LFRM. In both models, the observations X_i and Y_i are referring to skinfold thickness (ST) and bioelectrical resistance (BR) techniques respectively which are observed with errors. The data is fitted with balanced replicated LFRM and can be shown as follows:

$$BR_i = \hat{\beta}_0 + \hat{\beta}_1\ ST_i \text{ for } i = 1,2,\cdots,p \text{ and } j = 1,2,\cdots,m.$$

To estimate the parameters, the MLE method is used. Table 4 shows the estimated parameters with variances as explained in Section 3.

Table 4: Parameter estimation for fat mass measurements data

Parameter	Estimate (Variance) with $p = 6$	Estimate (Variance) with $p = 8$
$\hat{\beta}_0$	0.59 (8.94)	0.91 (4.93)
$\hat{\beta}_1$	0.99 (0.35)	0.93 (0.19)
$\hat{\sigma}^2$	8.97 (1.66)	8.58 (1.54)
$\hat{\tau}^2$	10.82 (2.43)	10.53 (2.31)
AIC	1004.58	1001.19

From Table 4, the result shows that both models yield similar parameter estimates, but the variances of the estimated parameters are smaller in the second model ($p = 8$) compared to the first model ($p = 6$). Additionally, the second model also has a lower AIC value compared to the first model, indicating better model fit and precision. Hence, the second model is preferred for this dataset and can be fitted as follows:

$$BR_i = 0.91 + 0.93\, ST_i \quad \text{for } i = 1,2,\cdots,8 \text{ and } j = 1,2,\cdots,12.$$

The estimated slope indicates a strong positive relationship between skinfold thickness (ST) and bioelectrical resistance (BR). The estimated ratio of error variances, $\lambda = \tau^2/\sigma^2$, is approximately 1.2, suggesting more variability in bioelectrical resistance (BR) measurements. Furthermore, the estimated variance for the error variance parameter by skinfold thickness (ST) is smaller than the estimated variance for the error variance parameter by bioelectrical resistance (BR), suggesting that the skinfold thickness (ST) yields more accurate measurements. These findings can help the researchers develop better calibration methods for bioelectrical resistance (BR) devices and improve the accuracy of body fat measurements in children. Thus, by estimating error variances separately, the proposed model offers insights into the reliability of different measurement methods, enabling better calibration and accuracy.

6. Discussion and Conclusion

This paper proposes the balanced replicated LFRM as a robust solution to the unidentifiability problem inherent in unreplicated LFRM. The proposed model, which divides unreplicated data into balanced and equal-sized observations, allows that all parameters; the intercept, slope, incidental parameters, and two error variances to be estimated independently using Maximum Likelihood Estimation (MLE). Furthermore, the proposed model provides unbiased and consistent parameter estimates that eliminate the need for precise assumptions on the ratio of error variances (λ).

Despite its strength, the balanced replicated LFRM has several limitations. The model assumes balanced and equal-sized observations, which is often unlikely in practice. Furthermore, the iterative estimation technique for MLE can be computationally expensive, particularly with large datasets. The model's performance in datasets with extreme values or outliers has not been thoroughly examined, which could impact its robustness in certain applications. Addressing these limitations with methodological improvements and alternative estimation techniques could improve the model's practicality. Future research should focus on extending the model to handle unbalanced datasets, exploring computationally efficient estimation methods and assessing its performance in a wide range of applications.

In conclusion, the balanced replicated LFRM successfully overcomes the limitations on unreplicated models. By transforming unreplicated data into replicated data, the balanced replicated LFRM can be used to estimate all parameters, eliminating the necessity for the assumption on the ratio of error variances, unlike in the unreplicated LFRM. By overcoming these challenges, the balanced replicated LFRM provides reliable parameter estimation and improves measurement accuracy in various fields.

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Department of Mathematics
Centre for Defence Foundation Studies
National Defence University of Malaysia
57000 Kuala Lumpur, MALAYSIA
E-mail: azuraini@upnm.edu.my, m.syazwan@upnm.edu.my*

Institute of Advanced Studies
Universiti Malaya
50603 Kuala Lumpur, MALAYSIA
E-mail: yzulina@um.edu.my

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*Corresponding author