

Validating Analytical Derivatives for Enhanced Accuracy in Academic Score Modeling

Anita Rahayu^{1*}, Noryanti Muhammad²

¹ Computer Science Department, School of Computer Science, Bina Nusantara University, Jakarta, Indonesia 11480

² Centre for Mathematical Sciences, Universiti Malaysia Pahang Al-Sultan Abdullah, Lebuhr Persiaran Tun Khalil Yaakob, 26300 Kuantan, Pahang

*Corresponding author: anitarahayu@binus.ac.id

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ABSTRACT – The correct mathematical formulation and the determination of model that suit the characteristics of the data play crucial role in ensuring accurate modeling. Considering the various problems that exist today where complex mathematical formulations require advanced solutions, this study was conducted with the aim of testing the validity of analytical derivatives using relative differences and analysing the relationship between student academic achievement using the Generalized Linear Model (GLM). The initial stage of the study focused on testing the first derivative of the log-likelihood function for each estimated parameter. If the analytical derivative is correct, the next step is to analyse the regression relationship where the parameter estimation uses Maximum Likelihood Estimation (MLE). This study used secondary data from 40 students at University "X" in 2026, with final grades as the response variable; midterm and final exam, assignment, and self-study scores as predictor variables. The results showed that the relative differences for all parameters were equal to or close to zero, which means that the resulting analytical derivative was correct. Furthermore, analysis using GLM resulted in the conclusion that the estimated values were close to the actual values, so it can be said that the model has good accuracy and reliability.

Keywords – Analytical Derivatives, Generalized Linear Model, Maximum Likelihood Estimation, Student Academic.

I. INTRODUCTION

Data science is a field of science that combines mathematics, statistics, programming, and artificial intelligence to process raw data and is one of the fastest growing disciplines today. The resulting information can be used for strategic policy formulation and decision-making. Several stages in data science include data collection, data cleaning and pre-processing, exploratory data analysis, modeling, model evaluation, and implementation [1]. In the first stage, data is collected from various primary and secondary sources relevant to the problem being solved. This stage requires in-depth insight into the problem being analyzed to ensure the collected data is truly relevant and of high quality. Data can be structured, semi-structured, or unstructured [2].

The second step is data cleaning and pre-processing. Collected data often contains missing values, duplicates, or formatting errors that must be corrected. This step is crucial to ensure the data used is valid and reliable [3]. In this step, the data will be processed using techniques such as normalization, standardization, or categorical variable coding. This process is quite lengthy but is crucial for obtaining accurate results from data analysis [4].

The next step is exploratory data analysis, which is an initial investigative approach to analysing and understanding the main characteristics of a data set, often utilizing visualization methods and descriptive statistics. This step aims to find patterns, detect outliers, verify assumptions, and test hypotheses before modeling. Visualization methods such as histograms, box plots, or scatter plots are used to illustrate relationships between variables. By conducting in-depth exploration, appropriate further analysis techniques can be determined and decisions about necessary data processing can be made [5].

After exploratory data analysis, the next step is modeling. At this stage, researchers select the machine learning algorithm that best suits the problem at hand. The data is divided into two sets: training data for model building and test data for model performance testing [6]. The developed model is evaluated using a number of performance metrics. If the model cannot achieve the desired results, iteration and model refinement can be performed [7]. At the modeling stage, the resulting model is often quite complex and cannot be solved using analytical methods because the solution obtained produces a solution in the form of a mathematical function that can then be evaluated, while numerical methods are expressed in the form of numerical values. Numerical methods only produce an approximation to the exact solution, so the results are known as approximate solutions [8]. Numerical methods are generally formulated as algorithms that enable fast and efficient calculations. Due to their approximate nature, numerical algorithms involve iteration, which is the repetition of calculation steps. Each approximation inherently contains errors, and the magnitude of these errors depends on the analytical derivatives used in the algorithm. Correct analytical derivatives will produce smaller errors. Therefore, a validation process is necessary to ensure the accuracy of the analytical derivatives used [9].

Currently, methods for validating first derivatives are limited. While several concepts and software tools exist to determine the first derivative of a function, no tools are available to verify the validity of these derivatives. In fact, the `compareDerivatives` function in R is used as a well-established computational tool to support the validation process. The

real contribution of this research lies not in developing a new software routine, but in proposing a structured methodological framework for integrating derivative validation into analytical workflows and demonstrating its application in a specific research context. Based on this explanation, the purpose of this research is to test the validity of analytical derivatives in a mathematical model and apply it to data modeling to obtain estimates for each regression parameter.

II. LITERATURE REVIEW

Analytical methods provide precise and exact solutions in the form of mathematical formulas or functions using standard algebra, suitable for simple problems, while numerical methods provide approximations in numerical form through repeated arithmetic operations (add, subtract, multiply, divide) and are highly dependent on computers, suitable for complex problems that cannot be solved analytically, but always contain errors [10].

Table 1 The Differences between Analytical and Numerical Methods Based on Conceptual and Methodological Characteristics

Features	Analytical Methods	Numerical Methods
Solution	Precise, exact, in the form of a mathematical function/formula (can be evaluated as a number)	Estimate (approximation), in numerical form
Error	Zero (none)	Always present (non-zero), needs to be minimized
Computer Dependence	Not always necessary (can be pencil and paper), more towards mathematical thinking	It is very necessary, because it involves repeated arithmetic operations
Complexity of the Problem	Suitable for simple and limited problems	Able to solve complex and complicated problems that cannot be solved analytically
Process	Using existing mathematical formulas (theorems, algebra)	Using computational algorithms (basic arithmetic operations)
Example	Finding the roots of $x^2 - 4 = 0$ (solution $x = \pm 2$)	Finding the roots of complex equations, integrating difficult functions (e.g. using Simpson's method, Runge-Kutta)

The point is that analytical methods seek perfect answers with formulas, while numerical methods seek good enough answers with repeated calculations, especially when perfect formulas do not exist or are too difficult, often with the help of computers [11].

The magnitude of the error resulting from the difference between the approximate solution and the true solution is determined by the analytical derivative used in the algorithm [12]. If the analytical derivative is constructed correctly, its value will be close to the numerical derivative, resulting in a smaller error [13]. Conversely, the error will be greater if the analytical derivative is incorrect. To compare analytical and numerical derivatives, the compareDerivatives function in R software can be used. This function compares the two types of derivatives and displays diagnostic information. CompareDerivatives is designed to test pre-programmed derivative routines in maximization algorithms. If the analytical derivative is correct, then the resulting relative difference should be less than ϵ , where ϵ represents a very small number. The formula below explains the relative difference calculation used [14].

$$\text{Relative differences} = \frac{\text{analytic gradient} - \text{numeric gradient}}{\frac{1}{2}(\text{analytic gradient} + \text{numeric gradient})} \quad (1)$$

Numerical methods and analytical methods differ in the solutions they produce and the degree of precision with which they are obtained. Numerical methods only produce solutions that approximate the true solution in numerical form, while analytical methods produce solutions in the form of mathematical functions that can be evaluated to exact values [15].

Table 2 The Differences between Analytic Gradient and Numeric Gradient Based on Computational Performance and Implementation

Features	Analytic Gradient	Numeric Gradient
Precision	Exact (within machine precision)	Approximate
Speed	Fast (constant time per weight)	Slow (proportional to number of parameters)
Implementation	Difficult/Time-consuming to derive	Easy (finite difference): $\frac{f(x+h) - f(x)}{h}$
Error Type	Algebraic errors	Discretization/Rounding errors
Best For	Production, Neural Networks	Gradient Checking, Debugging

III. METHODOLOGY

This study utilizes secondary data, where the final value is used as the response variable, while midterm exam scores, final exam scores, assignment scores, and independent learning are used as predictor variables. Validation of the first derivative of the log-likelihood function at each parameter is done by comparing the relative difference between the analytical gradient and the numerical gradient. After the validation process, the study continues with data modeling, where parameter estimation is carried out using the Maximum Likelihood Estimation (MLE) method. MLE is an estimation method that aims to maximize the probability function to obtain the parameter estimator value, and the flexibility in determining the probability function makes this method easier to estimate parameters. The data analysis stage in this study begins with data collection, followed by determining the data distribution so that the form of the probability density function can be determined, then determining the likelihood and ln-likelihood functions, and perform the first derivative of the ln-likelihood function for each estimated parameter. Next, the analytical derivative is validated by comparing it with the numerical derivative through the calculation of the relative difference value, where the analytical derivative is declared valid if the relative difference value is smaller than ε , with ε being a small number which in this study is set at 10^{-5} . If the analytical derivative has been declared correct, the analysis can continue to the data modeling stage using the MLE method for parameter estimation [16]. The following is the data structure used in this study.

Table 3 The Data Structure

Observation	Y_1	X_1	X_2	$\dots$	X_s
1	$y_{1,1}$	$x_{1,1}$	$x_{1,2}$	$\dots$	$x_{1,s}$
2	$y_{2,1}$	$x_{2,1}$	$x_{2,2}$	$\dots$	$x_{2,s}$
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
n	$y_{n,1}$	$x_{n,1}$	$x_{n,2}$	$\dots$	$x_{n,s}$

IV. RESULTS AND DISCUSSIONS

Descriptive statistics for the final score as the response variable, as well as midterm exam scores, final exam scores, assignment scores, and independent learning scores as predictor variables are presented in Table 4.

Table 4 Descriptive Statistics

Variable	Total	Mean	Standard Deviation	Variance	Minimum	Q1	Median	Q3
Y	40	89.63	9.76	95.32	55	85.5	93.5	97
X_1	40	96.78	8.59	73.87	66	98	100	100
X_2	40	87.88	16.55	273.96	20	81.25	94	100
X_3	40	73.875	5.716	32.676	70	70	70	75
X_4	40	88.08	15.13	228.79	38	80.25	95.5	100

Based on the descriptive statistics in Table 4, all variables analyzed, namely Y, X_1 , X_2 , X_3 , and X_4 , each have a total of 40 observations. The average value of variable Y is 89.630, with a standard deviation of 9.760, which shows that the data is moderately distributed. Variable Y has a minimum value of 55 and a median of 93.500, indicating that most of the data falls within a relatively high range. Variable X_1 has the highest mean value of 96.780 and a standard deviation of 8.590, indicating limited variability in the data. The median and third quartile are equal to 100, indicating that most observations in variable X_1 are clustered around the maximum value. Variable X_2 has a mean value of 87.880 with the highest standard deviation of 16.55 and a variance of 273.96, indicating the greatest dispersion of the data compared to other variables. The wide range of values, indicated by the minimum value of 20 and the third quartile of 100, indicates quite extreme differences in the data. Variable X_3 has the lowest mean value of 73.875 with a standard deviation of 5.716. The similarity of the minimum value, the first quartile, and the median at 70 indicates a strong concentration of data at that value. Meanwhile, the mean value for variable X_4 is 88.080 and the standard deviation is 15.13, indicating significant variation in the data. The minimum value of 38, the median of 95.500, and the third quartile of 100 indicate that although most of the data has high values, there are still some observations with relatively low values. In general, these descriptive statistics provide an initial overview of the data patterns and distribution that can be used as a basis for further analysis.

After the descriptive analysis is performed, the next step is to test whether the distribution of the response variables conforms to a normal distribution. This test is intended to obtain an initial indication of the likelihood of a normally distributed residual distribution, aid in the selection of an appropriate regression model, and improve the reliability of statistical inference results. This distribution test was conducted using the Kolmogorov-Smirnov test. Figure 1 shows a P-value < 0.01 , indicating that the final score data does not follow a normal distribution. This is supported by the pattern of points that do not follow a normal line, with the points deviating quite clearly from the line, especially in the lower

and upper tails. There is clustering of data around the 95–100 value, as well as several outliers. If the data is normally distributed, the red points will follow the straight blue line.

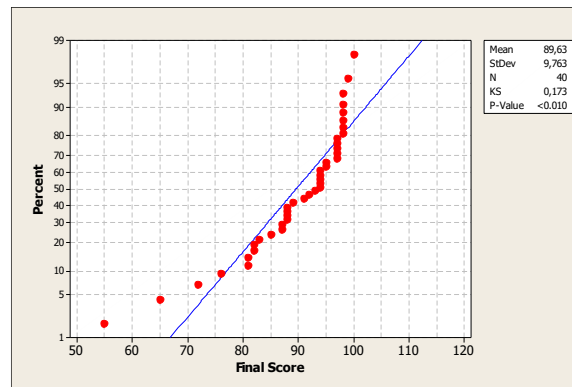


Figure 1 Probability Plot of Final Score

Because the response variable does not follow a normal distribution, the residuals were then tested for normal distribution. Figure 2 shows that the p-value is less than α (5%), indicating that the residuals do not follow a normal distribution. Therefore, classical linear regression is not suitable for this study. The appropriate method is regression that does not require the assumption of normality. This study uses the Generalized Linear Model (GLM). The concept of the GLM method is an extension of classical linear regression that allows modeling of response variables that do not have to be normally distributed and have a direct nonlinear relationship with the predictor variables.

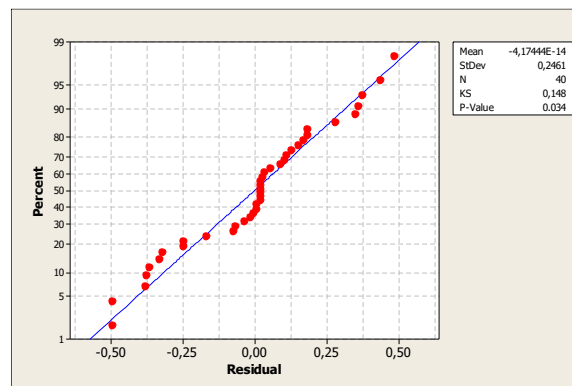


Figure 2 Probability Plot of Residual

The likelihood function for the probability density function y_{il} is:

$$L(\gamma, \lambda, \beta) = \prod_{l=1}^n f(y_{il}) = \prod_{l=1}^n \left(\frac{(y_{il} - \lambda)^{\alpha-1} e^{-\frac{y_{il}-\lambda}{\gamma}}}{\gamma^{\alpha} \Gamma(\alpha)} \right). \quad (2)$$

The ln-likelihood function from equation (2) is:

$$\begin{aligned} \ln L(\gamma, \lambda, \beta) &= \prod_{l=1}^n \ln \left(\frac{(y_{il} - \lambda)^{\alpha-1} e^{-\frac{y_{il}-\lambda}{\gamma}}}{\gamma^{\alpha} \Gamma(\alpha)} \right) \\ &= \sum_{l=1}^n \frac{e^{x_{il}^T \beta} - \lambda - \gamma}{\gamma} \ln(y_{il} - \lambda) - \sum_{l=1}^n \frac{y_{il} - \lambda}{\gamma} - \sum_{l=1}^n \frac{e^{x_{il}^T \beta} - \lambda}{\gamma} \ln \gamma - \sum_{l=1}^n \ln \Gamma \left(\frac{e^{x_{il}^T \beta} - \lambda}{\gamma} \right). \end{aligned} \quad (3)$$

The ln-likelihood function will be maximum if the result of the first derivative of the function with respect to each estimated parameter and equal to zero is in closed form.

The ln-likelihood function is derived with respect to the γ parameter first, as explained below.

$$\frac{d \ln L(\gamma, \lambda, \beta)}{d\gamma} = \sum_{i=1}^n \left(\frac{\lambda - e^{x_i^T \beta}}{\gamma^2} \ln(y_{i1} - \lambda) \right) - \sum_{i=1}^n \left(\frac{\lambda - y_{i1}}{\gamma^2} \right) - \sum_{i=1}^n \left(\frac{e^{x_i^T \beta} - \lambda}{\gamma^2} (1 - \ln \gamma) \right) - \sum_{i=1}^n \left(-\frac{1}{\gamma^2} \left(\Psi \left(\frac{e^{x_i^T \beta} - \lambda}{\gamma} \right) \right) (e^{x_i^T \beta} - \lambda) \right). \quad (4)$$

The ln-likelihood function is derived with respect to the λ parameter first, as explained below.

$$\frac{d \ln L(\gamma, \lambda, \beta)}{d\lambda} = \sum_{i=1}^n \left(-\frac{\ln(y_{i1} - \lambda)}{\gamma} - \frac{e^{x_i^T \beta} - \lambda - \gamma}{\gamma(y_{i1} - \lambda)} \right) + \frac{n}{\gamma} + \frac{n \ln \gamma}{\gamma} - \sum_{i=1}^n \left(-\frac{1}{\gamma} \Psi \left(\frac{e^{x_i^T \beta} - \lambda}{\gamma} \right) \right). \quad (5)$$

The ln-likelihood function is derived with respect to the β parameter first, as explained below.

$$\frac{d \ln L(\gamma, \lambda, \beta)}{d\beta} = \sum_{i=1}^n \left(\ln(y_{i1} - \lambda) \right) \frac{x_i^T e^{x_i^T \beta}}{\gamma} - \sum_{i=1}^n \left(\left(\Psi \left(\frac{e^{x_i^T \beta} - \lambda}{\gamma} \right) \right) \frac{x_i^T e^{x_i^T \beta}}{\gamma} \right). \quad (6)$$

The functions obtained in equations (4) to (6) are quite complex, so a method is needed to test the truth of analytical derivatives in a mathematical model. This test is carried out using the relative differences values shown in equation (1). If the analytical derivative is correct, then the relative differences value is expected to be smaller than ε , with ε is a very small number. In this study, we used $\varepsilon = 10^{-5}$. Table 5 shows the relative differences values for each parameter.

Table 5 Relative Differences for Each Parameter

Number	Parameter	Analytic Gradient	Numeric Gradient	Relative Differences
1	γ	-19.84341	-19.84341	0.00000
2	λ	0.226158	0.226158	0.00000
3	β_0	19.72864	19.72864	0.00000
4	β_1	1900.842	1900.842	0.00000
5	β_2	1650.879	1650.879	0.00000
6	β_3	1468.834	1468.834	0.00000
7	β_4	1664.492	1664.492	0.00000

Table 5 shows that the analytic gradient value is equal to or close to the numeric gradient value for each parameter, so the relative differences are equal to or close to zero. Based on these results, it is concluded that the analytical derivative, in other words, the first derivative of the ln-likelihood function for each estimated parameter is valid and can be used in further analysis. Figure 3 shows that the analytic gradient and numeric gradient coincide, this is what causes the relative differences to be equal to or close to zero.

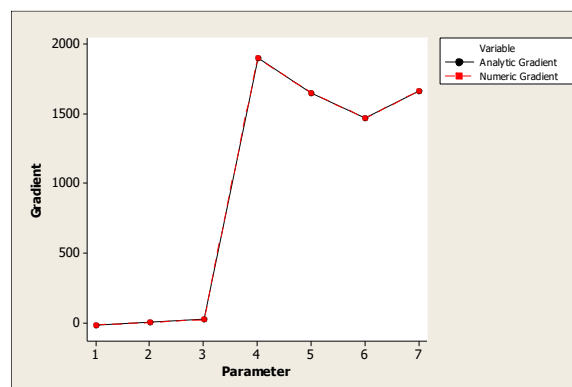


Figure 3 Comparison of Analytic and Numeric Gradient

Figure 4 shows a graph of the relative differences for each parameter. There are two curves on the graph: the relative differences, indicated by the black line, and ε , indicated by the red line. The graph shows that the relative differences are very close to zero for all parameters, while the ε value remains relatively constant at around 10^{-5} . The interpretation of this graph is that the relative differences generated for each parameter are very small, even approaching zero. This indicates that changes or variations in the parameters do not significantly affect the observed results, or in other words, the model used is stable and consistent with these parameter variations. The red line (ε) can be understood as error tolerance, and because the relative differences are well below this limit, the results obtained can be considered accurate

and acceptable. Overall, this graph shows that the model used has a very small error rate and low sensitivity to parameter changes, so the analysis results can be said to be robust.

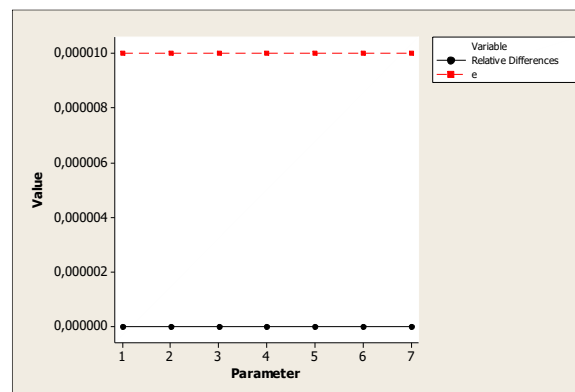


Figure 4 Relative Differences Values

Because the analytical derivative value is correct, the analysis can be continued for regression modeling with GLM. Figure 5 shows the relationship between actual values and estimated values, with the horizontal axis representing the actual value and the vertical axis representing the estimated value. The red dots indicate data pairs between actual and estimated values, while the blue line represents the linear regression line. The distribution of points that are very close to the regression line indicates a strong positive linear relationship between the two variables. Thus, this estimation method can provide results that are close to the true value, with a low margin of error and without any noticeable bias.

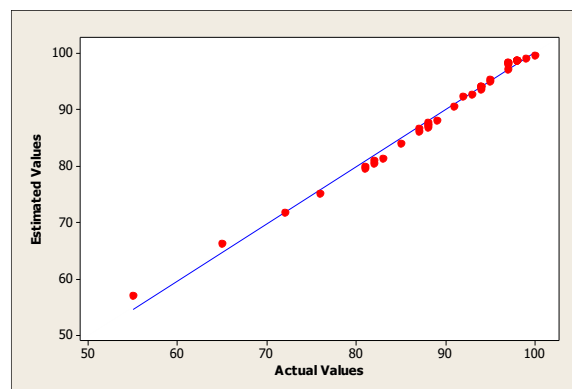


Figure 5 Regression Line Equation

Figure 6 shows a comparison between actual and estimated values according to the order of observations. The horizontal axis shows the observation number, and the vertical axis shows the value magnitude. The black lines and dots represent the actual values, while the red lines and dots represent the estimated values. Both curves have very similar patterns and move in the same direction, indicating that the estimates adequately reflect the dynamics of changes in actual values, despite some sharp fluctuations in certain values. Small differences between the two lines indicate estimation errors, but they are still within relatively small limits. Overall, this graph indicates that the estimation model or method used has a good level of accuracy and consistency in predicting actual values across various observation conditions.

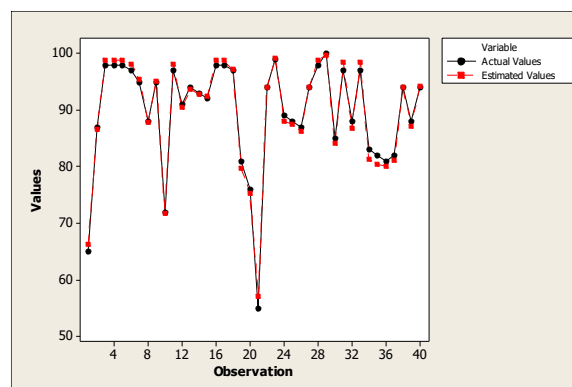


Figure 6 Comparison of Actual and Estimated Values

V. CONCLUSIONS AND SUGGESTIONS

Analytical derivative accuracy testing is necessary before modeling data because analytical derivatives are the main calculation basis in many modeling methods, especially those involving optimization, nonlinear regression, and gradient-based modeling. In this study, the test uses relative differences, where the analysis results show that the relative differences for all parameters are equal to or close to zero, which means that the analytical derivative is correct. Then the next analysis is regression using GLM because the response variable does not follow a normal distribution and has a direct nonlinear relationship with the predictor variable. The resulting estimated value is close to the actual value, this indicates that the model or estimation method used has a good level of accuracy and the model is able to represent the relationship between variables accurately, so that the estimated values closely approximate the actual values. In addition, this condition also indicates that the estimation error is low and the model does not experience significant bias, either in the form of overestimation or underestimation. Thus, the model can be said to be reliable and valid for use in predicting or representing actual data in the analysed observation range.

Future research is recommended to validate the proposed framework using substantially larger and more diverse datasets in order to improve parameter stability, strengthen empirical reliability, and enhance the generalizability of the model across broader contexts. Second, further research can consider comparisons with other methods or models to determine the strengths and limitations of the current method. Finally, parameter sensitivity testing and validation using independent data are highly recommended to ensure the model remains stable and accurate when applied to data outside the research sample.

DATA AVAILABILITY

The data used in this research are secondary data derived from https://binusianorg-my.sharepoint.com/personal/anitarahayu_binus_ac_id/_layouts/15/guestaccess.aspx?share=IQBpZaB8mdwVSaWKnm_NQgP1AW_MDchrwJbP0Y2ZOHqE04U&e=A6HXIL.

AUTHORSHIP STATEMENT

Anita Rahayu contributed to the project through conceptualizing the research idea, developing the software, and drafting as well as revising the manuscript. She also participated in study validation, conceptual framework development, methodology design, and supervision of the overall project execution. Noryanti Muhammad contributed by supporting the research design, assisting in data analysis and validation, and reviewing and refining the manuscript to improve the quality and clarity of the study.

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