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Performance Analysis of Robust Functional Continuum Regression to Handle Outliers

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Abstract

Robust functional continuum regression (RFCR) is an innovation as a development of functional continuum regression that can be applied to functional data and is resistant to outliers. The resistance of RFCR depends on the applied weighting function. This study aims to evaluate the RFCR performance to handle outliers. We propose the various weighting functions in this evaluation, i.e., Huber, Hampel, Ramsay, and Tukey (Bisquare), which do not eliminate or give zero weight to observed data identified as outliers. This contribution is essential to determining the appropriate RFCR method without eliminating the outlier data. The result shows that the RFCR performance with the Huber weighting function is better than the others, based on the goodness of fit, consisting of the root means square error of prediction (RMSEP), the correlation between the actual data and the model, and the mean absolute error (MAE).
Keywords: functional data analysis; Huber weighted function; Hampel weighted function; Ramsay weighted function; Tukey (Bisquare) weighted function.

Abstrak

Regresi kontinum fungsional kekar (RFCR) merupakan inovasi yang merupakan pengembangan dari regresi kontinum fungsional yang dapat diaplikasikan pada data fungsional dan tahan terhadap outlier. Resistansi RFCR bergantung pada fungsi pembobotan. Penelitian ini bertujuan untuk mengevaluasi kinerja RFCR. Kami mengusulkan beberapa fungsi pembobotan dalam evaluasi tersebut, yaitu Huber, Hampel, Ramsay, dan Tukey (Bisquare), dengan tidak menghilangkan atau memberikan bobot nol pada data observasi yang teridentifikasi sebagai outlier. Kontribusi ini penting untuk menentukan metode RFCR yang tepat tanpa menghilangkan data outlier. Hasil menunjukkan bahwa kinerja RFCR dengan fungsi pembobotan Huber lebih baik dibandingkan fungsi pembobotan lain berdasarkan goodness of fit, yang terdiri dari root mean square error of prediksi (RMSEP), korelasi antara data aktual dan model, dan mean kesalahan absolut (MAE).
Kata Kunci: *analisis data fungsional; fungsi berbobot Huber; fungsi tertimbang Hampel; fungsi tertimbang Ramsay; fungsi berbobot Tukey (Bisquare).*

2020MSC: 62J99, 62R10

1. INTRODUCTION

Functional data is often inappropriate to analyze with conventional methods due to its complex and dynamic nature [1]. Functional data generally includes function-shaped variables that evolve over time or in the context of a specific domain closely related to continuity, such as curves, spectra, or images. The functions are often defined in terms of time but can also be spatial locations, wavelengths, probabilities, and more [2]. Intrinsically, functional data is infinite-dimensional. The inherently high dimensionality of these data brings challenges to theory and computation, and these challenges vary

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according to how the functional data is sampled [3]. However, high-dimensional or infinite data structures are a rich source of information, and there are many exciting challenges to data research and analysis.

A more advanced approach is often required to generate meaningful insights when dealing with functional data. Some commonly used methods for functional data analysis include [4]. Functional Analysis involves the use of mathematical and statistical techniques specifically designed to handle functional data; examples are harmonic Analysis, wavelet analysis, functional principal component regression (FPCR), or functional partial least square regression (FPLSR) approaches [5][6]. (1) Splines and Basis Functions: this approach approximates the functional data with basis functions such as splines or wavelets; the functional data is broken down into simpler components for further analysis [7]. (2) Nonlinear Models and Machine Learning for highly complex data. Nonlinear models and machine learning techniques can extract patterns hidden in functional data, such as neural networks, support vector machines, or decision trees applied to functional data [8]. (3) Spatial Analysis and Geostatistics If the functional data is related to the spatial dimension, such as satellite or medical image data, spatial Analysis and geostatistics methods can be used to understand the spatial and temporal patterns in the data [9].

Analysis methods must be selected according to the structure and nature of the specific functional data. A combination of different analysis techniques and modeling approaches is often required to understand the functional data comprehensively. The robust functional continuum regression (RFCR) is a development of the continuum regression originated by Stone & Brooks [10]. RFCR can be applied to functional data and is robust, i.e., resistant to outliers.

An outlier is an observation significantly different from the general pattern in the data and can affect the analysis results [11]. Outliers are only sometimes a nuisance, but sometimes they can provide important information or valuable insights due to the natural variability of the data [12]. One alternative that can deal with outliers is assigning a lower weight value to observations considered outliers, thus reducing their influence on the analysis results. Weighting functions help to reduce possible bias by proportionally decreasing the impact of outliers rather than eliminating them [13]. The robustness of RFCR depends on the weighting function chosen. Commonly used weighting functions are Huber, Hampel, Ramsay, and Tukey (Bisquare) [14].

Based on these weighting functions, this study will examine the performance of RFCR against the presence of outliers with the four weighting functions as Huber, Hampel, Ramsay, and Tukey (Bisquare). The weights obtained based on the criteria in each method in Table 1 will be normalized by adding the weight value with a constant and dividing each weight with the minimum value of a set of weights, with normalization it will avoid the occurrence of reduction (zero weight) as it applies to the Hampel and Tukey (Bisquare) weight function.

2. METHODS

This section will discuss the performance of RFCR in modeling with simulated data and will be applied to empirical data to illustrate the theoretical results. We evaluated the performance of RFCR with both data based on the goodness of fit values, namely the correlation of the observed value (y_i) with the predicted value $(\hat{y}_i)$ for each of the n observations, root means square error of prediction (RMSEP) and mean absolute error (MAE) using R software:

$$\text{Correlation} = \frac{\sum(y_i-\bar{y}_i)(\hat{y}_i-\bar{\hat{y}}_i)}{(n-1)s_y s_{\hat{y}}},$$

where s_y and $s_{\hat{y}}$ are the standard deviations of the observed and estimated data, respectively.

$$\text{RMSEP} = \sqrt{\frac{\sum(y_i-\hat{y}_i)^2}{n}},$$

$$\text{MAE} = \frac{\sum|y_i-\hat{y}_i|}{n}.$$

Table 1 shows four weighted functions: Huber, Hampel, Ramsay, and Tukey (Bisquare). It also shows their respective weighting function formulas, which are used for analysis.

Table 1. Weighted Function

No	Metode	Weighted Function	Reference
1	Huber	$w(e_i) = \begin{cases} 1 & \text{for } \lvert e_i\rvert \le k \\ \frac{k}{\lvert e_i\rvert} & \text{for } \lvert e_i\rvert > k \end{cases}$ $k_1 = 1.345$	[15]
2	Hampel	$w(e_i) = \begin{cases} 1 & \text{for } \lvert e_i\rvert \le k_1 \\ \frac{k_1}{\lvert e_i\rvert} & \text{for } k_1 < \lvert e_i\rvert < k_2 \\ k_1 \frac{\frac{k_1 - \lvert e_i\rvert}{k_3 - k_2}}{\lvert e_i\rvert} & \text{for } k_2 < \lvert e_i\rvert < k_3 \\ 0 & \text{for } \lvert e_i\rvert > k_3 \end{cases}$ $k_1 = 1.7;\ k_2 = 3.4;\ k_3 = 8.5$	[14]
3	Ramsay	$w(e_i) = exp(-k\lvert e_i\rvert)$ for $\lvert e_i\rvert < \infty$ $k = 0,3$	[16]
4	Tukey (Bisquare)	$w_T(e) = \begin{cases} \left[1 - \left(\frac{e}{k}\right)^2\right]^2 & \text{for } \lvert e\rvert \le k \\ 0 & \text{for } \lvert e\rvert > k \end{cases}$ $k = 4.685$	[15]

Where the constant $k_1,\ k_2,\ k_3$ in Hampel, k in other are called tuning constants satisfying $0 < k_1 < k_2 < k_3 < \infty$ and $0 < k < \infty$, the residuals are given by $e_i = y_i - \hat{y}_i$. The functional continuum regression algorithm developed by Zhou [18] is as follows:

Algorithm 1. The functional continuum regression algorithm [18]

for (p, α) in finite set **do** # p and $\alpha \in [0,1)$ are the tuning parameters
  for i from 1 to n **do**
    if $p = 1$ **then**
      $\hat{X}_i^{(p,\alpha)} \leftarrow X_i - \bar{X}$ # X_i ith observation data (independent variable), $\bar{X}$ mean of X, $\hat{X}_i$ estimated data X_i
      $\hat{Y}_i^{(p,\alpha)} \leftarrow Y_i - \bar{Y}$ # Y_i ith observation data (dependent variable) $\bar{Y}$ mean of Y, $\hat{Y}_i$ estimated data Y_i
      $\hat{\beta}_{p-1,\alpha} \leftarrow 0$ # $\hat{\beta}$ model coefficient estimator
    else
      $\hat{X}_i^{(p,\alpha)} \leftarrow \hat{X}_i^{(p-1,\alpha)} - c_2.c_3.\hat{V}_X(\hat{\omega}_{p-1,\alpha})$ # $\hat{V}_X$ the covariance estimator X, $\hat{\omega}$ basis

function estimator

$\hat{Y}_i^{(p,\alpha)} \leftarrow \hat{Y}_i^{(p-1,\alpha)} - \hat{\eta}_{p-1,\alpha}(X_i)$ # $\hat{\eta}$ conditional expected value estimator

end if

end for

$\hat{\lambda}_j^{(p,\alpha)}, \hat{\phi}_j^{(p,\alpha)} \leftarrow$ the jth eigenvalue and eigenfunction of $\hat{V}_{\hat{X}^{(p,\alpha)}}$

$a_j \leftarrow \widehat{cov}\left\{\hat{Y}^{(p,\alpha)}, \int_{\mathbb{T}} \hat{X}^{(p,\alpha)}\hat{\phi}_j^{(p,\alpha)}\right\}$

$b_j \leftarrow \widehat{var}\left\{\int_{\mathbb{T}} \hat{X}^{(p,\alpha)}\hat{\phi}_j^{(p,\alpha)}\right\}$

$$Q_{p,\alpha}(\delta) \leftarrow \left\{\sum_{j=1}^{\infty} \frac{a_j^2}{\hat{\lambda}_j^{(p,\alpha)} + \frac{\hat{\lambda}_1^{(p,\alpha)}}{\delta}}\right\}^2 \left\{\sum_{j=1}^{\infty} \frac{a_j^2}{\left(\hat{\lambda}_j^{(p,\alpha)} + \frac{\hat{\lambda}_1^{(p,\alpha)}}{\delta}\right)^2}\right\}^{\frac{\alpha}{(1-\alpha)}} \left\{\sum_{j=1}^{\infty} \frac{a_j^2 b_j}{\left(\hat{\lambda}_j^{(p,\alpha)} + \frac{\hat{\lambda}_1^{(p,\alpha)}}{\delta}\right)^2}\right\}^{\frac{\alpha}{(1-\alpha)}-1}$$

$\hat{\delta}^{(p,\alpha)} \leftarrow \operatorname{argmin}_{\delta \in (-1,0)\cup(0,\infty)} - \ln Q_{p,\alpha}(\delta)$

$$\widehat{\omega}_{p,\alpha} \leftarrow \left\{\sum_{j=1}^{\infty} \frac{a_j^2}{\left(\hat{\lambda}_j^{(p,\alpha)} + \frac{\hat{\lambda}_1^{(p,\alpha)}}{\delta^{(p,\alpha)}}\right)^2}\right\}^{\frac{1}{2}} \sum_{j=1}^{\infty} \frac{a_j}{\hat{\lambda}_j^{(p,\alpha)} + \frac{\hat{\lambda}_1^{(p,\alpha)}}{\delta^{(p,\alpha)}}} \hat{\phi}_j^{(p,\alpha)}$$

$c_1 \leftarrow \widehat{\mathrm{cov}}\left(Y, \int_{\mathbb{T}} X\widehat{\omega}_{p,\alpha}\right)$

$c_2 \leftarrow \widehat{\mathrm{var}}^{-\frac{1}{2}}\left(\int_{\mathbb{T}} X\widehat{\omega}_{p,\alpha}\right)$

$c_3 \leftarrow \int_{\mathbb{T}} \hat{X}_i^{(1,\alpha)}\widehat{\omega}_{p,\alpha}$

$\hat{\beta}_{p,\alpha} \leftarrow \hat{\beta}_{p-1,\alpha} + c_1 c_2 \widehat{\omega}_{p,\alpha}$

for i from 1 to n **do**

$\hat{\eta}_{p,\alpha}(X_i) \leftarrow \bar{Y} + \int_{\mathbb{T}} \hat{X}_i^{(1,\alpha)}\hat{\beta}_{p,\alpha}$

end for

$\mathrm{GCV}(\mathrm{p},\alpha) \leftarrow (\mathrm{n}-\mathrm{p}-1)^{-2}\sum_{i=1}^{n}\left\{Y_i - \hat{\eta}_{p,\alpha}(X_i)\right\}^2$ # generalized cross-validation (GCV)

end for

$\mathrm{optimal}(\mathrm{p},\alpha) \leftarrow \underset{(\mathrm{p},\alpha)}{\mathrm{argmin}}\mathrm{GCV}(\mathrm{p},\alpha)$

We propose the algorithm for RFCR is as follows:

1. Regress y and y' using the FCR method,
2. Calculate the residuals (e_i) for each observation based on the model obtained in step 1,
3. Calculate $\hat{\sigma}$, where $\hat{\sigma} = 1{,}4826(median|e_i - median(e_i)|$,
4. Calculate the weight value for each observation (w_i) based on the value of the residuals obtained in Step 2; the weight formulation uses Table 1.
5. Normalize the weight value $w^*(e_i) = \frac{w(e_i)+0{,}1}{min\,(w(e_i)+0{,}1)}$,
6. Generate data y and y' as much as each weight obtained in Step 5,

7. Regress the generated data in Step 6 using the FCR method,
8. Repeat Steps 2 to 7 until the value converges. The convergent value is obtained when $|e_n - e_{n-1}| \leq 0{,}00001$ and the maximum iteration is 10. This iteration number is selected based on the previous simulation, and the convergent value is obtained at the 10th iteration.

3. RESULTS

3.1. Simulation Data

In the simulated data, we assume that there are 365 independent variables, which are functions of $sin\ (i\pi/45) + \text{distribusi uniform}\ (91, -0.1, 0.1), i = [0,90]$. One response variable $y_i = \sum_{j=1}^{365} x_{i,j}, j = 1, 2, .., n$, each variable has 50 replicates, and the generation data prepared are $n = 50, n = 100$, and $n = 200$, and the provision of outliers that vary (3%, 6%, and 10%). Table 2 show the goodness of fit from the simulation data. Based this table, RFCR performs well when the amount of data increases and decreases when the percentage of outliers increases; all weighting functions consistently experience this.

Table 2. Goodness of fit

Goodness of Fit	Weighted Function	$n = 50$			$n = 100$			$n = 200$		
		3%	6%	10%	3%	6%	10%	3%	6%	10%
RMSEP	Huber	2,5791	3,4568	4,2168	1,7912	2,4650	3,1401	1,3224	1,8006	2,2881
	Hampel	2,6185	3,5394	4,4205	1,7877	2,4667	3,1577	1,3155	1,7943	2,2842
	Ramsay	2,5991	3,4978	4,3251	1,7893	2,4658	3,1496	1,3185	1,7973	2,2861
	Tukey (Bisquare)	2,6160	3,5320	4,3993	1,7897	2,4694	3,1603	1,3172	1,7967	2,2869
Correlation	Huber	0,2034	0,1883	0,2034	0,4859	0,3727	0,3056	0,5926	0,4709	0,3954
	Hampel	0,1535	0,1313	0,1538	0,4838	0,3692	0,2992	0,5926	0,4705	0,3944
	Ramsay	0,1822	0,1685	0,1859	0,4849	0,3711	0,3025	0,5927	0,4708	0,3950
	Tukey (Bisquare)	0,1607	0,1427	0,1675	0,4838	0,3693	0,2994	0,5925	0,4705	0,3944
MAE	Huber	1,3698	1,9227	2,6394	0,6366	0,9371	1,3429	0,4841	0,6348	0,8363
	Hampel	1,3666	1,9097	2,6035	0,6463	0,9406	1,3340	0,4969	0,6452	0,8431
	Ramsay	1,3612	1,9055	2,5998	0,6406	0,9381	1,3367	0,4897	0,6392	0,8392
	Tukey (Bisquare)	1,3622	1,9053	2,5989	0,6424	0,9369	1,3310	0,4929	0,6413	0,8395

RFCR with the Huber weighting function obtained the smallest RMSEP value compared to the other methods when n=50 but became the largest when n increased (n=100 and n=200). On the other hand, the MAE value of RFCR with the Huber weighting function is the largest when n is small (n=50) and becomes the smallest when n=100 and n=200. Meanwhile, the correlation value obtained by RFCR with the Huber weighting function is consistently greater than the other methods for all n.

Overall, the goodness of fit value of RFCR obtained for all weighting functions is similar, as shown in Figure 1. The graphs tend to overlap, so in this study, we apply the performance of RFCR with various weighting functions when dealing with outliers. The novelty of this study is that it does not eliminate or give zero weight to observed data identified as outliers.

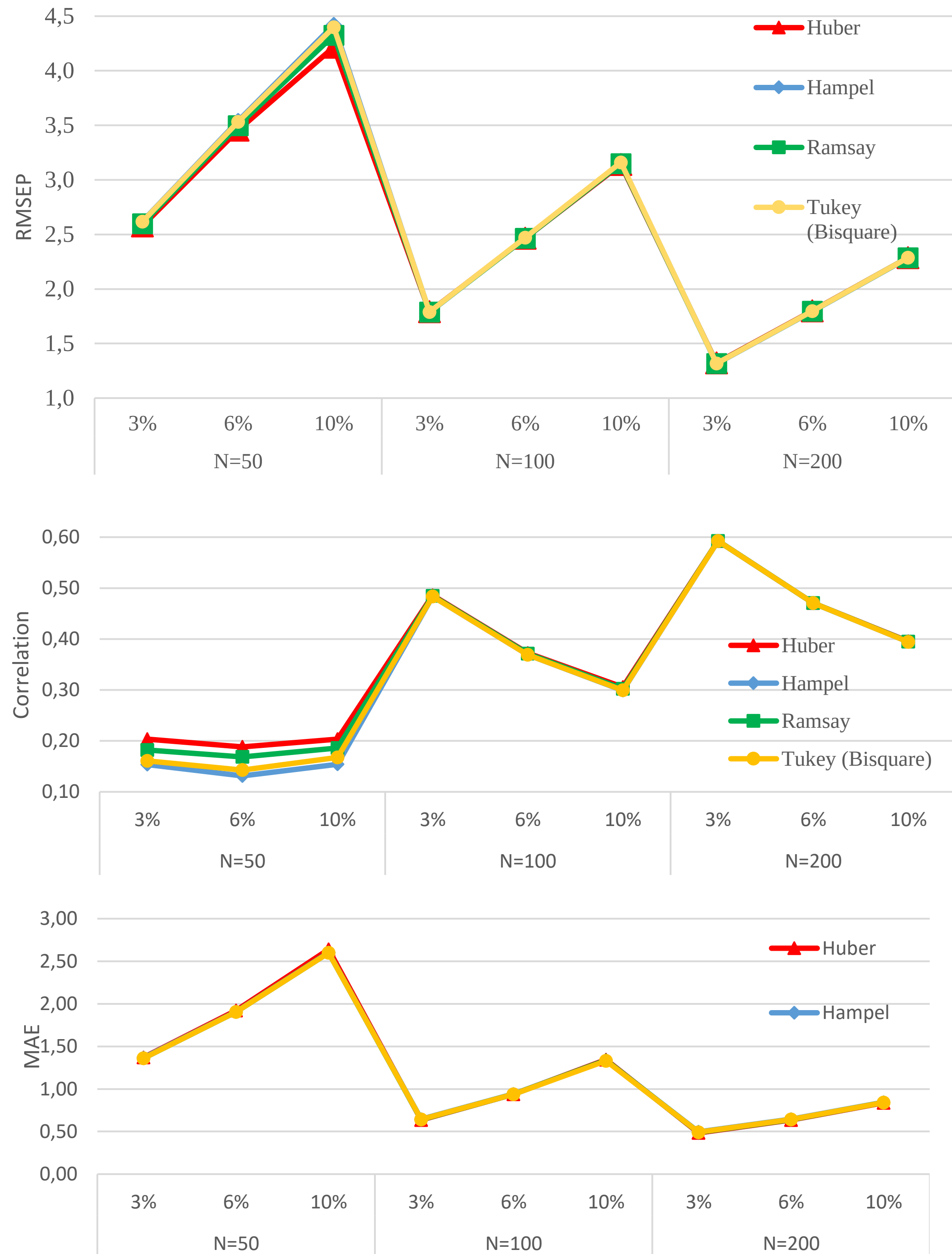

Figure 1. Goodness of fit of simulation data: RMSEP (top), correlation between actual data and model (middle), and MAE (bottom)

3.2. Empirical Data

The data used in this study are blood glucose data measured using invasive techniques by the PRODIA Laboratory of IPB Indonesia (y) and invasive techniques using the Spectroscopy-Based Non-Invasive Blood Glucose Detection Tool Prototype developed by the Physics and Statistics Team of IPB in 2019 (y'). The data sample obtained was 74 people who were the general public living in the IPB Bogor Indonesia neighborhood, aged 21-87 years.

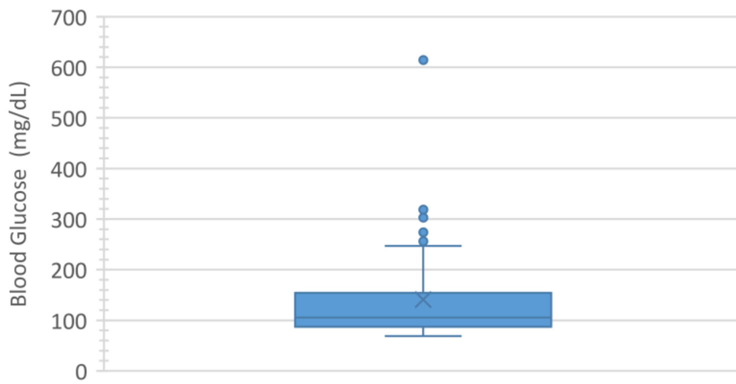

Figure 2. Visualization of blood glucose level data

Data on blood glucose levels in this study showed the lowest value was 69 mg/dL, and the highest was 614 mg/dL, with an average of 140.7 mg/dL. The American Diabetes Association (ADA) divides blood glucose levels into three categories, namely normal (< 100 mg/dL), prediabetes (100 mg/dL - 125 mg/dL) and diabetes (> 125 mg/dL) (American Diabetes Association 2014), so based on these categories, data obtained as many as 35 respondents were included in the normal category, 11 respondents were included in the prediabetes category. There were 28 respondents included in the diabetes category. Data visualization is shown in Figure 1; respondents' blood glucose levels tend to be close to 100 mg/dL rather than above 100 mg/dL. There are eight respondents' blood sugar levels that are outliers, including 256 mg/dL, 258 mg/dL, 274 mg/dL, 282 mg/dL, 303 mg/dL, 319 mg/dL, 328 mg/dL, and 614 mg/dL.

Intensity Residual Data Visualization of intensity residual value data: A sample of 5 out of 74 respondents in the first replication is taken so that the pattern of each respondent's data can be seen, as shown in Figure 3. It is evident in Figure 3 that the patterns formed are almost similar between respondents; it can be seen that the data patterns overlap. The amount of data generated varies between respondents and between replicates, so it is necessary to cut (reduce) the data to obtain the same amount between respondents. It replicates so that data analysis can be carried out. The cutting technique uses the trapezoidal rule's numerical method to determine the curve's area value. The cutting results show that the number of variables for each respondent for one replication is 20, so 100 variables are received for five replications. Figure 4 shows the data visualization of the cutting results on the first respondent; the cutting results have a consistent pattern in each replication; the data that forms the peak is the 1st to 5th replication data; this result looks different from Figure 3 before cutting.

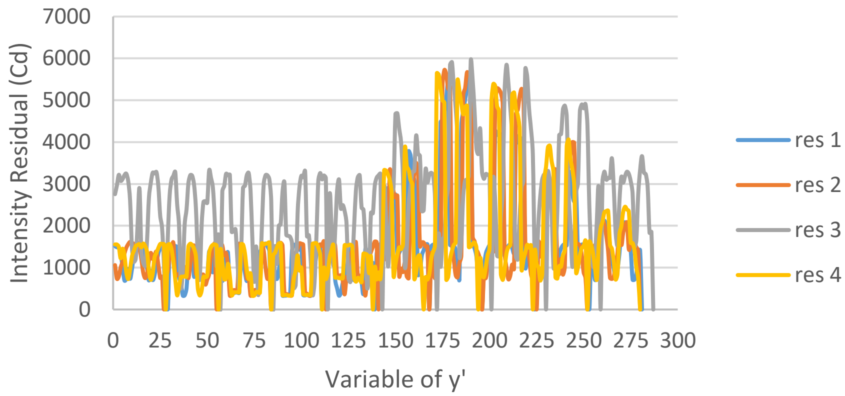

Figure 3. Visualization of Glucose Data from respondents 1, 2, 3, and 4 in the second repetition

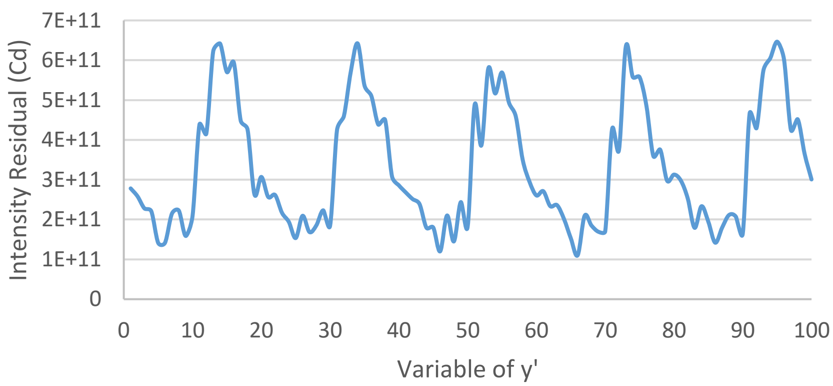

Figure 4. Visualization of area data

The results of data analysis using the RFCR approach with the Huber weighting function obtained the goodness of fit value in Table 3. The RMSEP value obtained was 83.84, the correlation was 36.48%, and the MAE value was 48.97. We evaluate the goodness of the model through the data pattern formed. The estimated data obtained by the RFCR method has the same pattern as the actual data, as shown by the level of correlation obtained. Figure 5 shows the estimate of blood glucose using RFCR compare to the actual data.

Table 3. Goodness of fit RFCR: empirical data

RMSEP	Correlation	MAE
83,84	0,3648	48,97

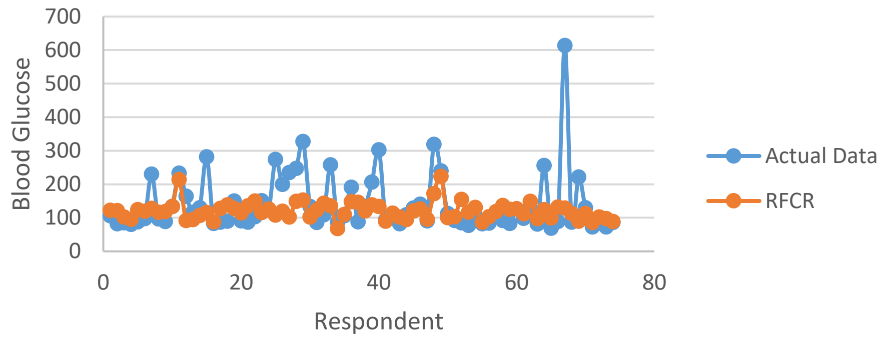

Figure 5. The estimate of blood glucose using RFCR compare to the actual data

4. DISCUSSION

RFCR is an improved method of FCR initiated by Zhou [18] that is resistant to outliers. The resistance of RFCR to outliers depends on the applied weighting function. The study of the four weighting functions Huber, Hampel, Ramsay, and Tukey (Bisquare) applied to FCR so that FCR becomes resistant to outliers and is referred to as RFCR.

The results of the Huber weighting function show better RFCR performance than others based on the goodness of fit values obtained, namely RMSEP, the correlation between actual data and models, and MAE. This study's results align with research by Nawaz et al. [19]. Still, the novelty of this study is that it does not eliminate (reduce) observed data identified as outliers because, in general, the measurement data is relatively complex to obtain because it requires high cost and a long time, so it is unfortunate if the data is reduced, besides that outliers are sometimes not a disturbance but a data phenomenon with high variability. Thus, outliers provide important and in-depth information.

As in the Hampel and Tukey (Bisquare) weighting functions, data reduction or zero weighting may show better performance, as in research by Pratiwi et al. [20]. Still, it will undoubtedly lose complete data. This research has the potential to be developed with other weighting functions, such as Andrew, Welsch, or others, as well as studies on other goodness of fit values, such as bias or mean square of error (MSE).

5. CONCLUSIONS

The simulation results show that the larger the amount of data, the RFCR performance with Huber, Hampel, Ramsay, and Tukey (bisquare) weighting functions increases. Still, on the contrary, it decreases when the percentage of outliers increases. The performance of RFCR with the Huber weighting function shows better results than the other three weighting functions. However, the difference is very small due to the normalization of the weight values obtained based on the criteria of each weighting function.

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