

COMPARISON OF SIMPLEX AND NELDER-MEAD OPTIMIZATION METHODS IN QUANTILE REGRESSION FOR BOGOR CITY RAINFALL ANALYSIS

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ABSTRACT

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Predicting extreme rainfall is crucial for supporting planning in the agricultural sector, infrastructure development, and disaster mitigation in the city of Bogor. However, the asymmetric distribution of daily rainfall and the presence of outliers make linear regression methods less suitable. Quantile regression offers an alternative that captures the influence of explanatory variables across different parts of the data distribution, particularly in the extreme regions. This study compares the Simplex and Nelder-Mead methods for estimating quantile regression parameters on extreme rainfall data in Bogor. Daily rainfall data were obtained from the West Java BMKG Climate Station for the period from May 2024 to April 2025, comprising 365 observations, with four explanatory variables: average temperature, average humidity, sunshine duration, and average wind speed. Modeling was conducted at the 0.75, 0.85, and 0.95 quantiles to represent extreme rainfall. The results show that the Simplex method outperformed Nelder-Mead, as indicated by lower Pinball Loss and Mean Absolute Error (MAE) values at most quantiles. Humidity and average wind speed had a significantly positive effect on extreme rainfall intensity, while average temperature had a negative effect. Sunshine duration showed less consistent effects. Overall, the Simplex method is recommended for quantile regression optimization in extreme rainfall data due to its greater stability and accuracy in generating model parameters. However, this study is limited by the number of explanatory variables and the relatively short observation period. Incorporating additional variables such as air pressure, ENSO index, or topographical data, along with extending the observation period, could improve model accuracy and generalizability in future research.



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1. INTRODUCTION

Rainfall is an important climate component that affects the agriculture, trade, and livestock sectors through its pattern and distribution. However, these rainfall patterns can be disrupted by extreme climate phenomena such as El Nino and La Nina, which are phenomena that affect the climate in Indonesia [1], causing drought or excessively wet conditions in the surrounding area [2]. Extreme rainfall can cause negative impacts such as floods, landslides, and crop failures, which ultimately reduce the work of businesses in the affected areas [3]. One of the areas in Indonesia that often experiences extreme rainfall is Bogor City, which is known as the "rain city" because it has an average rainfall above 50 mm [4].

According to research [5], the presence of extreme rainfall will make the rainfall distribution deviate far from the normal pattern. In this condition, the use of simple linear regression becomes inappropriate because the estimation is strongly affected by the outlier value. Quantile regression is a suitable alternative method because it can evaluate the effect of explanatory variables on the entire distribution, including outliers from the data [6]. However, the loss function of quantile regression is non-differentiable and complex, making parameter estimation require an efficient optimization method [7]. One of the optimization methods used for quantile regression estimation is Simplex and Nelder-Mead. The Simplex method is a classic linear program-based optimization technique by iteratively moves between feasible corner points to improve the objective function value [8]. Meanwhile, Nelder-Mead uses a derivative-free algorithm with a geometric simplex approach that is adaptive for complex functions [9].

Previous research shows that the Nelder-Mead method excels in optimizing complex and non-differentiable loss functions, such as in quantile regression for rainfall data that is asymmetric and contains outliers. It can adapt to non-smooth functions, resulting in more stable and accurate parameter estimates. Meanwhile, the Simplex method remains relevant as an effective optimization technique for linear functions and provides a meaningful comparison in the context of quantile regression [9]. Therefore, the research entitled "Comparison of Simplex and Nelder-Mead Optimization Methods in Quantile Regression for Bogor City Rainfall Analysis" was chosen to directly evaluate the advantages and disadvantages of both methods in quantile regression parameter estimation. In addition, the purpose of this study is to compare the performance of Simplex and Nelder-Mead optimization methods in estimating quantile regression parameters and determining influential variables of rainfall in Bogor City.

2. METHODS

Data and Data Sources

The data used in this study are daily data obtained from daily data published by the Meteorology, Climatology, and Geophysics Agency (BMKG) in Bogor City. The data was collected from the West Java Climatology Station with a time span of May 1, 2024 to April 30, 2025, covering 365 observations. The selection of variables in this study refers to a previous study, [10] and [11], with one response variable and four predictor variables which can be seen in table 1.

Table 1. Research Variable

Variable	Description	Unit
Y	Rainfall	Milimeter (mm)
X ₁	Average temperature	Celcius (°C)
X ₂	Relative humidity	Percent (%)
X ₃	Sunshine Duration	Hours
X ₄	Average Wind Force	m/s

Quantile Regression

Quantile regression analysis is a regression method to determine the effect of predictor variables on response variables, especially on outlier or extreme values. Quantile regression is at first glance like multiple linear regression, but with a different approach, namely minimizing the sum of weighted absolute differences (*Pinball Loss*) [12]. This method provides a more complete picture of the relationship between variables, especially in data with outliers. The objective function of quantile regression contains weights τ for positive errors and $1 - \tau$ for negative errors [13]. Parameter estimation β is obtained by minimizing the weighted combination of the absolute remainders as formulated in formula 1.

$$Y = X^T \beta_\tau + \varepsilon \tag{1}$$

where β_i is the regression parameter at the τ^{th} quantile.

Simplex Method Optimization

Simplex method is an algorithm to solve the optimization process of linear functions with linear constraints. This method utilizes the geometric structure of the solution, namely the *feasible* solution points forming a polyhedron. The simplex algorithm moves from one extreme point to another along the sides of the polyhedron until it reaches the optimum point [14]. *The simplex method* works systematically by selecting variables that enter and exit the base, then recalculating the solution and objective function value at each step. Although in theory it can take a long time, in practice this method is very efficient, especially because the matrix is often sparse (many zeros) and its shape can be adjusted for easy calculation.

The initial stage of the Simplex-Method algorithm is to determine the objective function of quantile regression *loss*. The objective function is presented in formula 2.

$$loss = \tau u_i + (1 - \tau)v_i \tag{2}$$

The objective function is limited by the constraints in formula 3.

$$X(\beta^+ - \beta^-) + u - v = y \text{ with } u, v \geq 0 \tag{3}$$

The objective function in Equation (2) and the constraints in Equation (3) can be re-represented into a standard linear program form as follows.

$$z^T = [\beta^+ \quad \beta^- \quad u \quad v] \in \mathbb{R}^{2p+2n} \tag{4}$$

$$c^T = [0 \quad 0 \quad \tau \quad (1 - \tau)] \tag{5}$$

$$A = [x^+ \quad -x^- \quad I_n \quad -I_n] \in \mathbb{R}^{n \times (2p+2n)} \tag{6}$$

$$b = y \in \mathbb{R}^n \tag{7}$$

Where z is the decision variable, c is the objective function coefficient, A is the constraint coefficient matrix, and b is the right-hand side of the constraint. Thus, quantile regression can be formulated in the form of a linear program in formula 7.

$$Loss = c^T z \text{ with } Az = b, \quad z \geq 0 \tag{8}$$

The Simplex Method optimization stage is then continued with the following algorithm:

- 1) Determine initial values for slack variables and decision variables. Generally, in the first iteration, all decision variables will be considered equal to 0.

$$\beta^+, \beta^- = 0, \quad u - v = y \quad (9)$$

β^+, β^- is a non-base column (N) and u, v belongs to the base column (B)

- 2) Calculate the shadow price (dual)

$$\pi^T = c_B^T A_b^{-1} \quad (10)$$

The matrix A_b is the column matrix of A representing the basis variables and c_B is the part vector c in the same row as the basis column (B).

- 3) Calculate reduced cost

$$r_N = c_N^T - \pi^T N \quad (11)$$

where N is the column matrix of A representing the non-base variables. If all $r_N \geq 0$, then the optimal solution has been determined. If not, then proceed to step 4.

- 4) Select the base entry variable. Index s with the smallest or most negatively $r_s < 0$.
- 5) Calculate the direction of change

$$d_B = B^{-1} A_s \quad (12)$$

Where A_s is the s -th column of matrix A.

- 6) Perform a minimum ratio to select the base exit variable.

$$\theta = \min_r \left\{ \frac{(x_B)_r}{(d_B)_r} \mid (d_B)_i > 0 \right\} \quad (13)$$

with the index i that satisfies the minimum is the variable that comes out of the base (exit variable).

- 7) Replace the B_r field with A_s
- 8) Calculate the new solution

$$z_B^{new} = z_B - \theta \quad d_B, \text{ and } z_s = \theta \quad (14)$$

where z_B denotes the current base column decision variable vector.

- 9) Update the objective function value
- 10) Repeat the process from step 2 until there are no more $r_N < 0$

Nelder Mead Optimization

The *Nelder–Mead* method is a numerical optimization method to find the minimum or maximum value of a function in multidimensional space. The advantage of this method is that it does not require a differentiable function, so it is suitable for functions with derivatives that are difficult to calculate. The *Nelder–Mead* method will form and modify a simple geometry called *simplex* to explore the solution space and iteratively move towards the local minimum point [15].

The initial stages of the Nelder-Mead algorithm for quantile regression with N variables require $N + 1$ starting points that form a simplex: $\beta^{(1)}, \beta^{(2)}, \dots, \beta^{(N+1)}$. Where $\beta^{(i)}$ is the point representing the regression parameter $(\beta_1^{(i)}, \beta_2^{(i)}, \dots, \beta_N^{(i)})$. The value of $\beta^{(1)}$ is usually specified as an initial guess. Next, each point $\beta^{(i+1)}$ is formed by increasing 5% of the components of $\beta^{(i)}$. The optimization process is iteratively performed through the following steps until the accuracy condition is met [16].

- Sort the points $\beta^{(i)}$ by the function value $f(\beta^{(i)})$ sorted from the smallest to the largest. Furthermore, the value of x_i will be referred to as the worst point.

$$f(\beta^{(1)}) \leq f(\beta^{(2)}) \leq \dots \leq f(\beta^{(N+1)}) \quad (15)$$

- Calculate the average of the best N (x_0) by excluding the value of $\beta^{(N+1)}$

$$\beta^{(0)} = \frac{1}{N} \sum_{i=1}^N \beta^{(i)} \quad (16)$$

- Calculate the reflection ($\beta^{(r)}$) of the worst point against the average point $\beta^{(0)}$ with parameters $\alpha > 0$

$$\beta^{(r)} = \beta^{(0)} + \alpha(\beta^{(0)} - \beta^{(N+1)}) \quad (17)$$

- If $f(\beta^{(1)}) \leq f(\beta^{(r)}) \leq f(\beta^{(N)})$, replace the worst point $\beta^{(N+1)}$ with $\beta^{(r)}$ and repeat back to step 1.

- If $f(\beta^{(r)}) \leq f(\beta^{(1)})$, continue with the expansion step to form the point x_e with $\gamma > 1$

$$\beta^{(e)} = \beta^{(0)} + \gamma(\beta^{(r)} - \beta^{(0)}) \quad (18)$$

If $f(\beta^{(e)}) < f(\beta^{(r)})$, then $(\beta^{(N+1)}) = (\beta^{(e)})$. Otherwise $(\beta^{(N+1)}) = (\beta^{(r)})$. Then go back to step 1.

- If $f(\beta^{(N)}) \leq f(\beta^{(r)})$,

- If $f(\beta^{(N)}) \leq f(\beta^{(r)}) < f(\beta^{(N+1)})$, then perform an external contraction:

$$\beta^{(c)} = \beta^{(0)} + \rho(\beta^{(r)} - \beta^{(0)}) \quad (19)$$

If $f(\beta^{(c)}) \leq f(\beta^{(r)})$, then $\beta^{(N+1)} = \beta^{(c)}$. Otherwise, go to step 7

- If $f(\beta^{(N)}) \geq f(\beta^{(N+1)})$, then perform deep contractions:

$$\beta^{(c)} = \beta^{(0)} + \rho(\beta^{(N+1)} - \beta^{(0)}) \quad (20)$$

If $f(\beta^{(c)}) \leq f(\beta^{(N+1)})$, then $\beta^{(N+1)} = \beta^{(c)}$. Otherwise, go to step 7.

- Perform *shrinkage* on all points except the best point $\beta^{(1)}$ and then return to step 1.

$$\beta^{(i)} = \beta^{(1)} + \sigma(\beta^{(i)} - \beta^{(1)}) \quad (21)$$

Model Evaluation

Pinball loss

Pinball loss is a *loss function* used in quantile regression to measure how well the model predicts certain quantiles of the response variable distribution [15]. This *loss function* is written as formula 2.

$$loss = \tau \sum_{y_t \geq x^t \beta} |y_t - \hat{y}| + (1 - \tau) \sum_{y_t < x^t \beta} |y_t - \hat{y}| \quad (22)$$

Mean Absolute Error (MAE)

MAE is an evaluation matrix used to measure the average absolute error between predicted and actual values in a regression model. MAE provides a direct picture of how much the average of the model predictions deviates from the actual value regardless of the direction of the error [17]. The MAE formula is written in formula 23.

$$MAE = \frac{1}{n} \sum_{i=1}^n |y_i - \hat{y}_i| \quad (23)$$

Research Procedure

The research procedure used RStudio software. The stages are briefly described in **Figure 1**.



Figure 1. Research flow chart

The detailed research steps can be explained as follows:

1. Data preprocessing is done by handling missing values of unrecorded rainfall values. The handling is done by taking the average between one day before and after the missing data to maintain the data pattern and reduce bias.
2. Data *exploration* was conducted on rainfall variables to gain an initial understanding of the data structure and distribution characteristics.
3. The dataset division is done by dividing the training data by 80% and the test data by 20%.
4. Specification of the quantile regression model is done by selecting quantile values that represent the upper part of the distribution, such as $\tau = 0.75, 0.85,$ and $0.95,$ to capture the extreme characteristics of rainfall.
5. Estimation of quantile regression parameters using Simplex and Nelder-Mead optimization methods separately on training data.
6. Evaluation of model *performance* is carried out based on quantitative indicators such as the level of prediction accuracy against test data using *Mean Absolute Error* (MAE) and *Pinball Loss* terk which are common metrics in quantile regression.
7. The selection of the best model is done by assessing the effectiveness of both optimization methods in the context of rainfall quantile distribution.
8. Interpretation of the contribution of each predictor variable.

3. RESULTS

Data Exploration

Data exploration was conducted after handling 20 rows of missing values. Exploration includes a time series plot of daily rainfall in Bogor City for 365 days which can be seen in Figure 2.

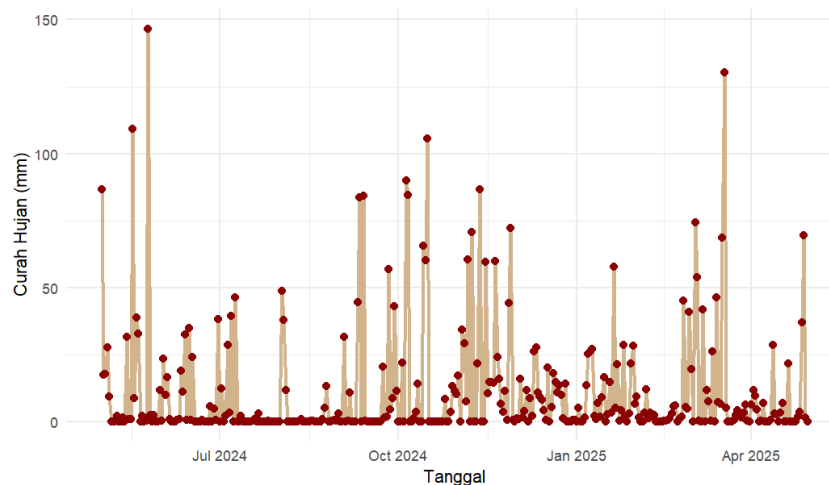


Figure 2. Daily Rainfall of Bogor City on May 1st, 2024-April 30th, 2025

Figure 2 shows significant fluctuations in daily rainfall, with some extreme rainfall events peaking above 100 mm, as is evident in the periods around October-November 2024 and March 2025. The daily rainfall data for Bogor City shows some notable extreme values. This can lead to violations of classical assumptions in linear regression, such as normality and homoscedasticity. Therefore, quantile regression modeling was chosen because it is more resistant to outliers and is able to capture the characteristics of the relationship between variables at different quantile levels.

Quantile Regression Modeling with Simplex Method

Estimation of quantile regression parameters using *Simplex Method* optimization was conducted with 3 quantiles, namely quantiles 0.75, 0.85, and 0.95. Iteration of the algorithm is carried out until the minimum *pinball loss* value is obtained, namely 6.24 for quantile 0.75; 5.48 for quantile 0.85; and 3.21 for quantile 0.95. A summary of the parameter estimation results for each quantile in the training data is presented in **Table 2**.

Table 2. Simplex Optimization Modeling Coefficients

Variable	Quantiles					
	0.75		0.85		0.95	
	Coef	SE	Coef	SE	Coef	SE
Intercept	-2.35	40.035	-5.39	69.353	-3.9	168.317
X ₁	-2.79	1.518	-4.71	1.996	-9.79	5.987
X ₂	1.08	0.294	1.76	0.374	3.75	0.783
X ₃	-0.09	0.654	0.72	0.908	1.16	2.440
X ₄	1.18	1.230	2.69	2.286	1.95	5.671

The variables X₂ and X₄ exert a positive influence on extreme rainfall, indicated by positive coefficient values at each quantile. In contrast, variable X₁ shows a consistent and stronger negative influence at higher quantiles, with a negative coefficient that gets larger in absolute terms from quantile 0.75 to 0.95. Meanwhile, the variable X₃ shows a small and inconsistent coefficient between

quantile 0.75 and quantiles 0.85 and 0.95. This may indicate that the influence of X3 on extreme rainfall is not very strong or stable at the quantile level.

Quantile Regression Modeling with Nelder-Mead Method

As an alternative to the Simplex method, quantile regression is also estimated using the *Nelder-Mead* optimization algorithm with *default* parameters: $\alpha = 1$, $\gamma = 2$, $\rho = 0.5$, $\sigma = 0.5$. Iterations of the algorithm were performed until the minimum *pinball loss* values were obtained, namely 6.24 for quantile 0.75; 5.49 for quantile 0.85; and 3.31 for quantile 0.95. The estimation results of the Nelder-Mead optimization coefficients on the training data are shown in **Table 3**. In general, the parameter estimation results with the Nelder-Mead method show a very similar pattern to the Simplex method, both in terms of the direction of influence and its magnitude.

Table 3. Nelder-Mead Optimization Modeling Coefficients

Variable	Quantiles					
	0.75		0.85		0.95	
	Coef	SE	Coef	SE	Coef	SE
Intercept	-0.142	2.806	-0.116	6.285	-1.95	6.658
X ₁	-2.80	0.881	-4.80	0.982	-9.75	3.198
X ₂	1.06	0.263	1.74	0.295	3.67	0.991
X ₃	-0.104	0.662	0.651	1.168	1.58	3.214
X ₄	1.03	1.281	2.37	2.123	2.31	5.418

The variable X1 continues to show a significant negative effect across all quantiles, similar to the pattern in the simplex. This reinforces the finding that X1 has a strong influence on extreme rainfall intensity. Similarly, variables X2 and X4 consistently show a positive influence with the same pattern as the *Simplex* method. Then the variable X3 still has inconsistency in the sign of the coefficient in some quantiles.

4. DISCUSSIONS

Two evaluation metrics are used to assess the accuracy of quantile regression modeling results, namely *Pinball Loss* and *Mean Absolute Error* (MAE). The evaluation results show that the lowest *Pinball Loss* and the highest MAE are found at quantile 0.95. This difference can be explained through the characteristics of each metric that are shown in **Table 4**.

Table 4. Nelder-Mead Optimization Modeling Coefficients

Optimization	Evaluation Metrics	Quantiles		
		0.75	0.85	0.95
Simplex	Pinball Loss (training data)	6.24	5.48	3.21
	Pinball Loss (test data)	7.75	6.51	3.95
	MAE (training data)	14.06	19.45	44.72
	MAE (test data)	18.89	25.42	59.45
Nelder-Mead	Pinball Loss (training data)	6.24	5.49	3.31
	Pinball Loss (test data)	7.76	6.53	4.02
	MAE (training data)	14	19.49	46.93
	MAE (test data)	18.83	25.46	60.68

Pinball Loss considers the direction of the prediction error at a particular quantile. At quantile 0.95, *overprediction* is more tolerable than *underprediction* because this quantile focuses on predicting very extreme values [18]. In contrast, *MAE* calculates the average absolute error regardless of the quantile position. Therefore, the MAE value increases significantly at extreme quantiles that are difficult to predict.

The *Simplex* and *Nelder-Mead* methods show similar performance in quantile regression with not too different Pinball Loss and MAE values. However, *Simplex* is slightly superior. This suggests that *Simplex* is more accurate and stable in quantile estimation, although both can find fairly optimal model parameters. Visualization of regression coefficients and 95% confidence intervals at quantiles 0.75, 0.85, and 0.95 (using the *Simplex* method) shows the influence of each variable on extreme rainfall intensity at different quantile levels.

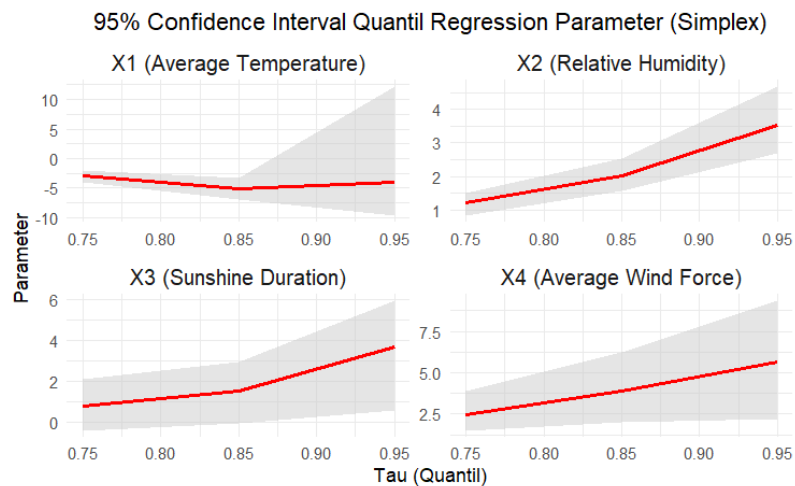


Figure 3. 95% confidence interval plot of quantile regression coefficients (Simplex)

Figure 3 shows that relative humidity and average wind force have a significant positive effect on rainfall in Bogor City. High humidity triggers the formation of rain clouds at sea which are then pushed by the wind to land, increasing the potential for heavy rainfall in a short duration [19]. Average daily temperature has a significant negative effect at quantiles 0.75 and 0.85, but not at quantile 0.95. This is because extreme rainfall in Bogor City generally occurs in the afternoon to evening, while the daytime is hot with long sunshine duration, especially in the transitional season.

This also explains why the sunshine duration variable does not have a significant effect in the 0.75-0.95 quantile range [20], [21].

5. CONCLUSION

This study shows that the Simplex optimization method provides better performance than the Nelder-Mead method in estimating quantile regression parameters for modeling extreme rainfall in Bogor City. Based on the modeling results at quantiles 0.75, 0.85, and 0.95, the Simplex method consistently produced lower Pinball Loss and Mean Absolute Error (MAE) values. The Pinball Loss ranged from 3.95 to 7.75, while the MAE ranged from 18.89 to 59.45. These lower error values show that the Simplex method fits the target quantiles more closely and produces smaller prediction errors, which explains its better accuracy and stability.

The quantile regression models also revealed that average humidity and average wind speed had a consistent positive effect on extreme rainfall intensity, while average temperature had a negative effect across all quantiles. Sunshine duration showed less consistent results and its influence was not as strong. These findings indicate that the selected meteorological variables were relevant for modeling rainfall extremes in Bogor.

These results can be useful as a reference for government or related agencies in improving early warning systems and planning for rainfall-related disasters. For further research, it is recommended to expand the observation period and consider additional variables, such as rainy season indicators or atmospheric pressure, in order to develop a more accurate and comprehensive model.

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