

# USE OF PENALIZED WEIGHTED LEAST SQUARE TO OVERCOME CORRELATIONS BETWEEN TWO RESPONSES

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## USE OF PENALIZED WEIGHTED LEAST SQUARE TO OVERCOME CORRELATIONS BETWEEN TWO RESPONSES

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**Abstract.** The non-parametric regression model can consider two correlated responses. However, for these conditions, we cannot use the usual estimation process because there are violations of assumptions. To solve this problem, we use a penalized weighted least square involving knots, smoothing parameters, and weighting in the estimation criteria simultaneously. The estimation process involves a weighted criteria matrix  $\frac{1}{n}$  in the estimation criteria. Estimation results show that the estimated two-response non-parametric regression function with penalized spline is a linear estimation class in  $y$  response observation and depends on the knot point and smoothing parameter. Furthermore, the use of the model on toddler growth data shows some changes in the pattern of weight and height gain. The pattern segmentation that experienced a gradual increase was age 7-43 months for weight and age 6-54 months for height.

**Keywords:** age, height, knots, two responses, weighted penalized, weight.

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## 1. INTRODUCTION

The nonparametric regression is used when we do not have enough information about the relationship patterns that occur in the data. Usually, an easy step to detect the pattern of relationships between responses and predictors is the scatter plot. We can use a nonparametric regression approach when the data plot does not follow a parametric pattern [1]. Some estimators that can be used include spline [2], local polynomial [3], kernel [4], Fourier series [5] and wavelet [6]. Spline estimator has become one of the most developed estimators because it has high flexibility in modeling data. Some spline estimator developments include truncated spline [7], smoothing spline [8], penalized spline [9], robust spline [10], b spline [11], quantile spline [12], multiresponse spline [13], and others.

This article discusses the estimation method of regression parameters in a model that contains two correlated responses. This is very important to study because there are many real data that contain more than one response and correlate with each other. For example, measurements of blood sugar in diabetic patients during the day and night [14] and the child's weight and height [15]. We use penalized weighted least square (PWLS) estimation criteria that involve weighting, knot points and smoothing parameters simultaneously. That is the development of penalized least square which is a standard criterion in the smoothing process. The least square method is used when the data does not experience a violation of the assumption that only involves knots and smoothing parameter. PWLS criteria have been developed by researchers in their use in non-parametric regression models. Some use estimators for smoothing spline [16] and penalized spline [17]. Besides the difference estimator, usually with the use of PWLS by some researchers, it is different in the weighting value used. Some use weighting of the covariance variance matrix [18], number of parameters [19], and bootstrap weighting [20]. However, in simpler conditions, we can use weights based on the number of samples and that can provide accurate estimation results. Therefore, we use the PWLS criterion by

weighting the sample size  $\left(\frac{1}{n}\right)$  in estimating the spline regression coefficient [21].

In this article, the theoretical study that we developed is applied to data on the growth of children under five in South Sulawesi Province. The use of nonparametric regression with PWLS aims to model children's weight and height which are correlated with each other based on age. Modeling of weight and height has been previously investigated using local polynomial regression models [22] and kernel [23] for data on children under five in East Java Province. This article is divided into 4 parts. The second part contains a description of the method used as the theoretical basis of this research. It is related to a nonparametric regression model for two correlated responses. The regression model was estimated using a penalized spline containing knot points and smoothing parameters in controlling the smoothing of the regression curve. The third part contains the results of the study which includes the estimation of nonparametric regression parameters for two responses with PWLS and the application of the model to toddler growth data. In addition to toddler data, the theoretical study that we make here is expected to be one of the reference methods for studying real data that has conditions or assumptions that are in accordance with the method. Furthermore, the fourth section contains a brief conclusion from the results of this study.

## 2. RESEARCH METHODS

The regression model that contains two responses means that there are paired data  $(y_{1,i}, y_{2,i})$  which are assumed to be correlated with each other, with the predictor variable  $(x_1, x_2, \dots, x_n)$  which is an unknown form of a relationship pattern. The relationship between variables  $y_{r,i}$  and  $x_i$  follows the nonparametric regression model as follows:

$$y_{r,i} = f_r(x_i) + \varepsilon_{r,i} \quad (1)$$

where  $i=1,2,\dots,n$  is the observed subject,  $r=1,2$  is the number of response variables,  $f_r(x_i)$  is a regression function contained in a Sobolev space,  $\varepsilon$  is the measurement residual which is assumed to be independent of the mean 0 and variance  $\varepsilon$ , which  $\varepsilon_1$  and  $\varepsilon_2$  are correlated.

The function  $f_r(x_i)$  in equation (1) is approximated using segmented polynomial functions like the following equation:

$$f_r(x_i) = \sum_{m=0}^{p+k} \beta_{r,m} g_{r,m}(x_i) \quad (2)$$

where a variable  $\beta_{r,m} = (\beta_{r,0}, \beta_{r,1}, \dots, \beta_{r,(p+k)})^T$  is a regression parameter vector,  $p$  is a regression order,  $k$  is the number of knots and  $g_{r,m} = (g_{r,0}, g_{r,1}, \dots, g_{r,(p+k)})$  is a function that has a definition like the following:

$$g_{r,m}(x_i) = \begin{cases} x_i^m & ; 0 \leq m \leq p \\ (x_i - \tau_{r,(m-p)})_+^p & ; p+1 \leq m \leq p+k, \end{cases} \quad (3)$$

and

$$(x_i - \tau_{r,(m-p)})_+^p = \begin{cases} (x_i - \tau)^p & ; x_i \geq \tau \\ 0 & ; x_i < \tau \end{cases} \quad (4)$$

Based on equations (3) and (4), the function in equation (2) can be stated as follows:

$$f_r(x_i) = \sum_{m=0}^p \beta_{r,m} x_i^m + \sum_{l=1}^k \beta_{r,(p+l)} (x_i - \tau_{r,l})_+^p \quad (5)$$

where  $\tau_{r,l}$  is the knot points of  $l=1,2,\dots,k$  in the  $r^{\text{th}}$  response.

Equation (5) on each response  $r$  can be stated as follows:

$$\underline{f} = \mathbf{X} \underline{\beta} \quad (6)$$

where  $\underline{f} = (f_1, f_2)^T$  and  $\underline{\beta} = (\beta_1, \beta_2)^T$ . The vector  $\underline{f}$  is a regression function in the 1<sup>st</sup> and 2<sup>nd</sup> responses,

with  $f_1 = (f_1(x_1), f_1(x_2), \dots, f_1(x_n))^T$  and  $f_2 = (f_2(x_1), f_2(x_2), \dots, f_2(x_n))^T$ . In the regression coefficient vector  $\underline{\beta}$ , it also contains the regression coefficient vector for the 1<sup>st</sup> and 2<sup>nd</sup> responses with

$\beta_1 = (\beta_{1,0}, \beta_{1,1}, \dots, \beta_{1,(p+k)})^T$  and  $\beta_2 = (\beta_{2,0}, \beta_{2,1}, \dots, \beta_{2,(p+k)})^T$ . For matrix  $\mathbf{X} = \text{diag}(\mathbf{X}_1, \mathbf{X}_2)$  is a predictor matrix that contains knots at the 1<sup>st</sup> and 2<sup>nd</sup> responses.

Furthermore, the non-parametric two response regression model in equation (1) can also be expressed in the form of a vector referring to equation (6), namely:

$$\underline{y} = \mathbf{X} \underline{\beta} + \underline{\varepsilon} \quad (7)$$

Equation (7) can also be written in the form of a matrix as follows:

$$\begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = \begin{bmatrix} \mathbf{X}_1 & \mathbf{0} \\ \mathbf{0} & \mathbf{X}_2 \end{bmatrix} \begin{bmatrix} \beta_1 \\ \beta_2 \end{bmatrix} + \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \end{bmatrix} \quad (8)$$

Each element in the equation (8) can be explained by  $y_1 = (y_{1,1}, y_{1,2}, \dots, y_{1,n})^T$  is the 1st response vector,  $y_2 = (y_{2,1}, y_{2,2}, \dots, y_{2,n})^T$  is the 2nd response vector,  $\mathbf{X}_1$  is the  $\mathbf{X}$  matrix for the 1st response and  $\mathbf{X}_2$  is the  $\mathbf{X}$  matrix for the 2nd response.

$$\mathbf{X}_1 = \begin{bmatrix} 1 & x_1^1 & x_1^2 & \cdots & x_1^p & (x_1 - \tau_{1,1})_+^p & \cdots & (x_1 - \tau_{1,k})_+^p \\ 1 & x_2^1 & x_2^2 & \cdots & x_2^p & (x_2 - \tau_{1,1})_+^p & \cdots & (x_2 - \tau_{1,k})_+^p \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & x_n^1 & x_n^2 & \cdots & x_n^p & (x_n - \tau_{1,1})_+^p & \cdots & (x_n - \tau_{1,k})_+^p \end{bmatrix},$$

$$\mathbf{X}_2 = \begin{bmatrix} 1 & x_1^1 & x_1^2 & \cdots & x_1^p & (x_1 - \tau_{2,1})_+^p & \cdots & (x_1 - \tau_{2,k})_+^p \\ 1 & x_2^1 & x_2^2 & \cdots & x_2^p & (x_2 - \tau_{2,1})_+^p & \cdots & (x_2 - \tau_{2,k})_+^p \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & x_n^1 & x_n^2 & \cdots & x_n^p & (x_n - \tau_{2,1})_+^p & \cdots & (x_n - \tau_{2,k})_+^p \end{bmatrix}.$$

Furthermore,  $\beta_1 = (\beta_{1,0}, \beta_{1,1}, \dots, \beta_{1,(p+k)})^T$  is a regression coefficient vector in the 1<sup>st</sup> response and

$\beta_2 = (\beta_{2,0}, \beta_{2,1}, \dots, \beta_{2,(p+k)})^T$  is a regression coefficient vector in the 2<sup>nd</sup> response,  $\varepsilon_1 = (\varepsilon_{1,1}, \varepsilon_{1,2}, \dots, \varepsilon_{1,n})^T$  is an error vector in the 1<sup>st</sup> response and  $\varepsilon_2 = (\varepsilon_{2,1}, \varepsilon_{2,2}, \dots, \varepsilon_{2,n})^T$  is an error vector in the 2<sup>nd</sup> response.

### 3. RESULTS AND DISCUSSION

#### 3.1. Estimation of The Regression Coefficient With Penalized Weighted Least Square

Estimation of parameter  $\underline{\beta}$  as a coefficient in the two-response nonparametric regression model through Penalized Weighted Least Square (PWLS) optimization. The PWLS equation contains the goodness of fit and the penalty functions which can be stated as follows:

$$\mathbf{L} = (2n)^{-1}(\underline{y} - \mathbf{X}\underline{\beta})^T \mathbf{W}(\underline{y} - \mathbf{X}\underline{\beta}) + \lambda \underline{\beta}^T \mathbf{D}\underline{\beta} \quad (9)$$

The goodness of fit function is given by  $(\underline{y} - \mathbf{X}\underline{\beta})^T (\underline{y} - \mathbf{X}\underline{\beta})$  and the penalty function is given by  $\lambda \underline{\beta}^T \mathbf{D}\underline{\beta}$ .

Furthermore, the  $\mathbf{W}$  matrix is a weighted of matrix given by  $\mathbf{W} = \text{diag}\left(\frac{1}{2n}\right)$  of size  $2n \times 2n$  or in the form of a matrix as follows:

$$\mathbf{W} = \begin{bmatrix} \frac{1}{2n}\mathbf{I} & | & \mathbf{0} \\ \hline - & | & - \\ \mathbf{0} & | & \frac{1}{2n}\mathbf{I} \end{bmatrix}$$

In PWLS, there is a matrix  $\mathbf{D}$  as a diagonal matrix  $(0,1)$ , i.e.  $\mathbf{D} = \begin{bmatrix} \mathbf{D}_1 & \mathbf{0} \\ \mathbf{0} & \mathbf{D}_2 \end{bmatrix}$ , where

$\mathbf{D}_1 = \text{diag}(a_{1,11}, \dots, a_{1,pp}, a_{1,(p+1)(p+1)}, a_{1,(p+2)(p+2)}, \dots, a_{1,(p+k+1)(p+k+1)})$  is the  $\mathbf{D}$  matrix in the 1<sup>st</sup> response and

$\mathbf{D}_2 = \text{diag}(a_{2,11}, \dots, a_{2,pp}, a_{2,(p+1)(p+1)}, a_{2,(p+2)(p+2)}, \dots, a_{2,(p+k+1)(p+k+1)})$  is the  $\mathbf{D}$  matrix in the 2<sup>nd</sup> response. Value of

$a_{11} = \dots = a_{pp} = a_{(p+1)(p+1)} = 0$ , and  $a_{(p+2)(p+2)} = \dots = a_{(p+k+1)(p+k+1)} = 1$ .

The estimation process  $\underline{\beta}$  is done by differentiating  $\mathbf{L}$  for  $\underline{\beta}$ .

$$\begin{aligned} \mathbf{L} &= (2n)^{-1}(\underline{y} - \mathbf{X}\underline{\beta})^T \mathbf{W}(\underline{y} - \mathbf{X}\underline{\beta}) + \lambda \underline{\beta}^T \mathbf{D}\underline{\beta} \\ &= (2n)^{-1}(\underline{y}^T - \underline{\beta}^T \mathbf{X}^T) \mathbf{W}(\underline{y} - \mathbf{X}\underline{\beta}) + \lambda \underline{\beta}^T \mathbf{D}\underline{\beta} \\ &= (2n)^{-1}(\underline{y}^T \mathbf{W}\underline{y} - 2\underline{y}^T \mathbf{W}\mathbf{X}\underline{\beta} + \underline{\beta}^T \mathbf{X}^T \mathbf{W}\mathbf{X}\underline{\beta}^T) + \lambda \underline{\beta}^T \mathbf{D}\underline{\beta} \end{aligned}$$

The minimum value of  $\mathbf{L}$  in the equation (9) is obtained when  $\frac{\partial \mathbf{L}}{\partial \underline{\beta}} = \mathbf{0}$  is obtained:

$$\begin{aligned} -2\mathbf{X}^T \mathbf{W}\underline{y} + 2\mathbf{X}^T \mathbf{W}\mathbf{X}\underline{\beta} + 2\lambda \mathbf{D}\underline{\beta} &= \mathbf{0} \\ \mathbf{X}^T \mathbf{W}\mathbf{X}\underline{\beta} + \lambda \mathbf{D}\underline{\beta} &= \mathbf{X}^T \mathbf{W}\underline{y} \\ \hat{\underline{\beta}} &= (\mathbf{X}^T \mathbf{W}\mathbf{X} + \lambda \mathbf{D})^{-1} \mathbf{X}^T \mathbf{W}\underline{y} \end{aligned} \quad (10)$$

As a result, the form of nonparametric regression estimation of two responses with penalized spline becomes as follows:

$$\hat{\underline{f}} = \mathbf{X}\hat{\underline{\beta}}$$

Based on equation (10), it can be written :

$$\hat{\underline{f}} = \mathbf{X}(\mathbf{X}^T \mathbf{W}\mathbf{X} + \lambda \mathbf{D})^{-1} \mathbf{X}^T \mathbf{W}\underline{y} \quad (11)$$

Equation (11) can also be simplified as follows:

$$\hat{\underline{f}} = \mathbf{H}(\lambda)\underline{y}, \text{ where } \mathbf{H}(\lambda) = \mathbf{X}(\mathbf{X}^T \mathbf{W}\mathbf{X} + \lambda \mathbf{D})^{-1} \mathbf{X}^T \mathbf{W}$$

The knot point in matrix  $\mathbf{X}$  is a combination of curves that shows the pattern of changes in curve behavior at different intervals. The lambda parameter  $\lambda$  is a smoothing parameter that controls the smoothness of the function of the data. If  $\lambda$  is large, then the estimation of the function obtained will be smoother, and preferably if  $\lambda$  is small, then the estimate of the function obtained will be even more rough [20]. The choice of knot points and  $\lambda$  parameters is done by trial and error by selecting knot points that are at data intervals in the predictor variables. The best model is a model that comes from optimal knots and lambda. One method used

to select the optimal knot point and optimal lambda is to use the Generalized Cross Validation (GCV) method. The optimum smoothing parameter  $\lambda$  is determined based on the minimum Generalized Cross Validation (GCV) value. The GCV method can be defined as follows:

$$GCV(\tau, \lambda) = \frac{MSE(\tau, \lambda)}{(2n^{-1}tr[\mathbf{I} - \mathbf{H}(\tau, \lambda)])^2} \quad (12)$$

where  $MSE(\tau, \lambda) = 2n^{-1} \sum_{i=1}^n (y_i - \hat{y}_i)^2$  is the mean square error and  $\mathbf{H}(\lambda) = \mathbf{X}(\mathbf{X}^T \mathbf{W} \mathbf{X} + 2\lambda \mathbf{D})^{-1} \mathbf{X}^T \mathbf{W}$  is the hat matrix.

### 3.2 Applications on Toddler Growth Data

The nonparametric regression model with PWLS was applied to the growth data of children under five as measured by weight and height based on the age of the toddler. Figure 1 shows a scatter plot of weight and height data by age.

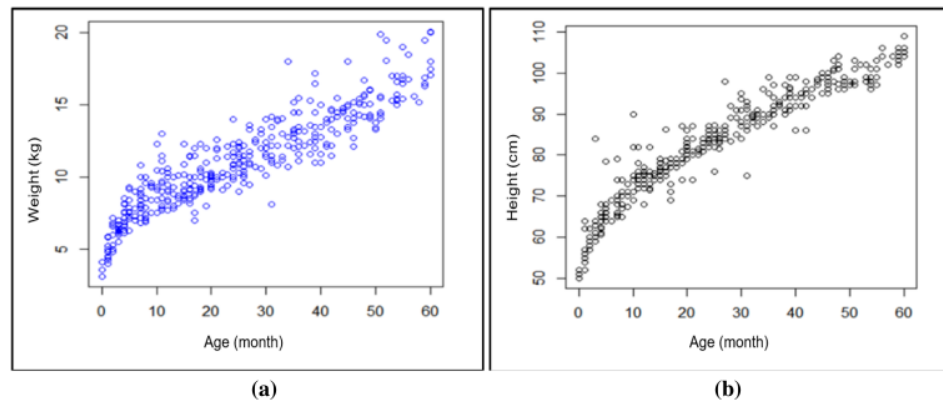


Figure 1. Scatter plot of weight by age (a) and height by age (b)

Based on Figure 1, we can see both data plots of weight and height tend to increase with age. We use nonparametric regression so that we are more flexible in modeling the data. This is due to the placement of knot points that can be selected according to the data. In addition, the involvement of smoothing parameters can also result in a smoother and more accurate estimation of the regression curve.

Next, we tested the correlation between body weight and height and obtained a correlation of 0.8. This means that there is a very strong correlation between the weight and height of toddlers. Therefore, these data were analyzed using PWLS nonparametric regression. The optimal model selection is based on the minimum GCV value and the optimal model has obtained in the second order with 2-knot points. The bi-response nonparametric regression equation with PWLS for the weight factor is as follows:

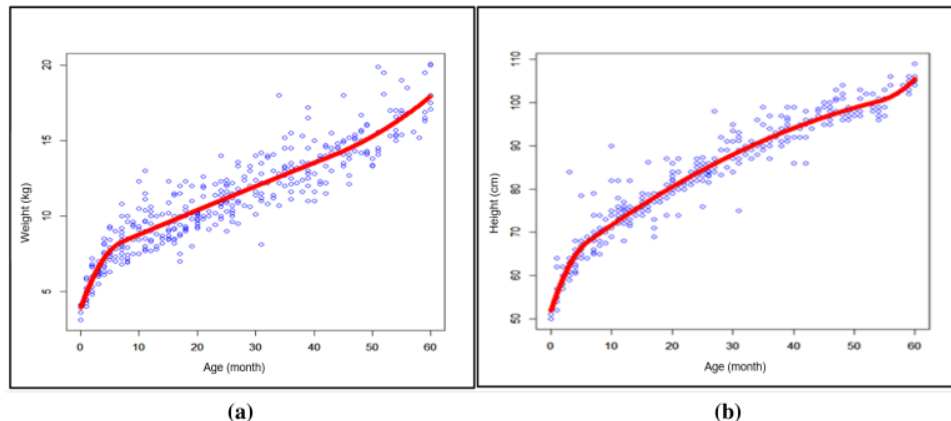
$$\hat{y}_1 = 3,8967 + 1,0871x - 0,0659x^2 + 0,0657(x-7)_+^2 + 0,0049(x-43)_+^2$$

For the height factor, the nonparametric two response regression equation with PWLS is obtained as follows:

$$\hat{y}_2 = 51,8304 + 4,3016x - 0,2745x^2 + 0,2676(x-6)_+^2 + 0,0925(x-54)_+^2$$

The PWLS biresponse nonparametric regression equation for weight and height corresponds to the estimated regression curve shown in Figure 2 below.

Based on Figure 2 (a) and the non-parametric two response regression model with PWLS, the results show that the average body weight increases with the age of the toddler. In general, weight gain in infancy (0-60 months) follows 3 different patterns. For the age of less than 7 months, toddlers experience a very rapid weight gain, then it increases slowly at the age of 7-43 months, and again increases rapidly after the age of 43 months. Furthermore, in Figure 2 (b) for height, the average height also increases with the age of the toddler. The increase in height during toddlerhood follows 3 patterns, namely at the age of less than 6 months, toddlers experience a very rapid increase in height and tend to slow down their growth at the age of 6 to less than 54 months. Furthermore, the height again quickly increased at the age of 54 months and over. These results indicate that changes in weight and height gain are at different age intervals. This indicates that a child's weight and height have different trends at their growing age. Therefore, in the effort to prevent stunting, it is necessary to work on each pattern segmentation that is considered slowing child growth and development.



**Figure 2.** Estimation of two response nonparametric regression curve with PWLS on toddler growth data a) weight and b) height

#### 4. CONCLUSIONS

Data that contains two responses and correlate with each other cannot be modeled using the usual approach in non-parametric regression. This will be very much obtained in real data so that the error will correlate. In this article, we use PWLS criteria in estimating the regression parameters. PWLS considers the goodness of fit and penalty functions. The involvement of weighting, knot point and smoothing parameters can overcome the correlation that occurs in the data. The weighting we use in the goodness of fit function is

$\frac{1}{2n}$ . Of course, other weighting can also be used for other research material. The results of estimating the regression parameters through PWLS show that the model is very dependent on knots, smoothing parameters and weighting used. Therefore, we need to find the optimal parameter values based on the minimum GCV value. In addition to the GCV method, there are several other methods known in nonparametric regression to find optimal parameter values, including Generalized Maximum Likelihood (GML), Unbiased Risk (UBR), and Cross Validation (CV).

The application of the model to toddler growth data, namely weight and height based on the age of the baby, has a different upward trend in the three segments of the pattern of change. Weight increases drastically in newborns up to the age of before 7 months, then increases slowly at the age of 7-43 months, and again increases rapidly at the age of over 43 months. For height, it also increases dramatically in newborns up to the age of 6 months, then the baby's height gain slows down at the age of 6-54 months, and when the age is over 54 months, the toddler's height begins to increase rapidly. Therefore, it is necessary to pay special attention to each segment that shows slowing growth. To avoid stunting, it is recommended to give extra attention to babies aged 6-54 months.

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