

Linear regression methods according to objective functions

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The aim of the study is to explain the parameter estimation methods and the regression analysis. The simple linear regression methods grouped according to the objective function are introduced. The numerical solution is achieved for the simple linear regression methods according to objective function of Least Squares and the Least Absolute Value adjustment methods. The success of the applied methods is analyzed using their objective function values.

Key words: Regression Analysis, parameter estimation methods, objective function, least squares method, least absolute value method.

Introduction

In the applied sciences, theoretical relationships between unknown parameters are determined by measurements. Measurement errors affecting the measurement group can exist for many reasons. The number of measurements must be more than the number of unknown parameters to determine the measurement errors. If the numbers of unknown parameters and measurements are taken as u and n , for the significant solution must be $u = n$. In the case of $u < n$, the different solutions number of the problem is equal to the combination $\binom{n}{u}$ [1]. The estimation of unknown parameters, which has the highest probability and the closest to the real value, is obtained from an adjustment calculation according to an objective function. Several estimation methods have been developed for the estimation of unknown parameters [2].

Although it is difficult, to establish a theoretical relationship between independent and dependent unknowns, if there is doubt as regards to a potential relationship, it must be investigated. It was proved in many cases in the literature that relationship equations are of assistance in determining theoretical relationships.

Many science branches use the regression analysis to determine the relationship between unknowns. Regression analysis is a method to determine the functional relationship between independent and dependent unknowns by using measurement. The regression function $y = f(x)$ is obtained from regression analysis, [3-5].

The simple linear regression is the determination of the line equation assuming that the relationship between the unknowns is linear. Simple linear regression transforms to an adjustment problem in case when the measurements number are more than the number of unknowns. Many methods had been developed to determine the simple linear regression equation [6].

This study explains the estimation methods used in determining the unknowns and the simple linear regression function. The success of the simple linear regression methods, classified according to objective functions, is determined using a numerical application.

1. Statistical parameter estimation methods

The process of determining an unknown from the measurement group using a special statistical method is called parameter estimation or prediction. The estimation methods should possess certain characteristics so that the estimation values can represent the statistics of the main set. These characteristics are consistence, unbiased, minimum variance and efficiency and sufficiency [7-8].

The estimation values of unknown parameters are close to the real value as the v residuals. The number of measurements cannot be too many for reasons of speed, time and economy, but it is hoped that the residuals will be small. The more suitable estimation method is one that creates smaller residuals.

Currently, there are many parameter estimation methods. These methods provide direct iterative or conditional solutions. The parameter estimation methods are classified that the Moment, the Maximum Likelihood Estimation, the Least Squares and the Least Absolute Value Methods [8-13]. The most applied ones of these are the Least Squares and the Least Absolute Value Methods.

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1.1. The Least Squares Method

The Least Squares (LS) Method was developed and used by Carl Friedrich Gauss, Adrien-Marie Legendre and Robert Adrain almost simultaneously. The LS method is a parameter estimation method, used widely in engineering and across nearly all fields of science. This method attempts to determine the mathematical relationship between the dependent value and the physical quantity. The optimal method for solving the regression problem is LS method [13-14].

According to the LS method, also known as the L_2 -norm, the estimation of unknown parameters is always unique and easy to implement. The mathematical model of LS method is composed of functional relations between the measurements and unknowns, and the stochastic relationships reflecting the sensitivity of the measurements. The correction equations are formed by the linearized mathematical model.

$$v = Ax - \ell \quad P = Q^{-1} \quad (1)$$

Here, ℓ , A , x , P , Q and v are the measurement value, design matrix, unknown, weight matrix, inverse weight matrix and residuals of the measurements. In case of $n > u$, the LS method should be conducted according to an objective function to find the unique solution from Eq.(1). This objective function minimizes the sum of squared measurement residuals. The mathematical notation of the objective function is $[vv] = \min$. If the measurements possess different sensitivities, this expression becomes $[Pvv] = \min$. [15-17].

It is assumed that the measurements have a normal distribution in the LS method however, this is not always true. The distribution of measurements can deviate from the normal distribution due to the inevitable existence of measurement errors. The LS method allows the measurement errors to spread to the other measurement residuals. In this case, an un-erroneous measurement can be determined as erroneous due to the spreading effect of the other measurement errors. This is called the sinking effect of the LS method. Likewise, an erroneous measurement may be identified as un-erroneous as it spreads its error to the other measures and this is known as the hiding effect of the LS method. The sinking and hiding effects are the drawbacks of the LS method [18-21].

1.2. The Least Absolute Value Method

The Least Absolute Value (LAV) Method, also known as the L_1 -norm method, is a longstanding parameter estimation method [13,22-24]. The mathematical model of the LAV Method is formed in similar to the LS Method. The objective function of this method is taken as $[|v|] = \min$. If the measurement possesses different sensitiveness, the objective function is taken as $[P|v|] = \min$. However, the direct solution is not possible except in special cases. The solution is achieved using either trial and error or transforming to linear programming [25].

The number of different solution is equal to $\binom{n}{u}$ combination for the mathematical model given in Eq. (2). In these solutions, different u -number measurements are used each time. One of these solutions is best suited to the objective function of LAV method. Only, u -number of measurements are used in the parameter estimation of the LAV method. These measurements are considered un-erroneous and the residuals are taken as zero; the other measurements, not used in estimation of unknown parameters, v residuals are calculated only for the other measurements. The parameters estimation of the LAV Method is not unique. However, the LAV Method result is almost never affected by measurement errors, which is the most important advantage of the method. Thus, LAV Method is usually used in eliminating the measurement errors within the measurement group [1].

2. Regression Analysis and the Regression Function Determination

Regression problems were first considered in the 18th century by Legendre and Gauss. The methodology was used almost exclusively in the physical sciences until the late 19th century. Even though the real relationship between the dependent and independent variables cannot be detected exactly with regression analysis, the relation function, obtained from the regression analysis, explains the relationship that is closest to the real one. The regression function determination has two-stages. In the first stage, the type of relationship between the variables is determined. Then, the regression functions are determined by calculation method selected according to the relationship type in the second stage. The relationship between the independent and dependent variables can be such; linear, curvilinear, polynomial, quadratic or logarithmic [3,26]. In this study, the linear regression equations will be obtained from the variables.

If the relationship between dependent and independent unknown parameters is linear, the process of the line equation determination is called a linear regression. There are three types of linear regression; simple, multiple and nonlinear regression. Simple linear regression (SLR) determines the relationship between the independent and dependent variables by linear function [5]. The SLR equation is as follows;

$$y_i = ax_i + b \quad (2)$$

SLR analysis has been applied across all the applied sciences because it is a simple functional model [6, 27-30].

2.1. Simple Linear Regression Methods

SLR methods can be classified according to whether there are erroneous measurements and objective function of adjustment method [29, 31]. In this study, the SLR according to the objective functions of LS and LAV methods are examined.

2.1.1. SLR Methods according to the Objective Function of LS Adjustment

SLR method according to the LS method gives the most appropriate solution for unknown parameters by minimizing the sum of the squared distances between a given (x, y) measurement and the determined regression line. This distance can be in the direction of the x axis, y axis, perpendicular or a specific angle to the regression line. The linearized functional equation between the measurements and unknown parameters is given in Eq. (2). The correction equation is obtained by rearranging the functional model as Eq. (1).

$$v = Ax - \ell \quad (3)$$

The unknown parameters of the SLR are found by solving the correction equation according to the LS objective function. The same solution can be found directly using the arithmetic means (\bar{x}, \bar{y}) and variances (S_{xx}, S_{yy}) and covariance, (S_{xy}) of (x, y) measurements.

- **SLR according to LS Method when the measurements are erroneous**

It is thought that only (y) measurement (LS $(y|x)$), only (x) measurement (LS $(x|y)$), or both (x, y) measurements are erroneous for the LS methods. The objective functions of these methods $\sum_{i=1}^n v_y^2$, $\sum_{i=1}^n v_x^2$ and $\sum_{i=1}^n v_x^2 + \sum_{i=1}^n v_y^2$ are to minimize in the direction of x axis, y axis and both x and y axis respectively, (Figure 1a, 1b, 1c). The mathematical models according to Eq.(2) are as follows:

$$(y_i + v_{y_i}) = a_1 x_i + b_1; \quad y_i = a_2 (x_i + v_{x_i}) + b_2; \quad (y_i + v_{y_i}) = a_3 (x_i + v_{x_i}) + b_3$$

If the weights of measurement are equal, the coefficients of both (x, y) measurements are erroneous and LS $(y|x)$ methods are to be equal [32]. The coefficients are determined through the following equations for LS $(y|x)$, LS $(x|y)$, and both (x, y) measurements are erroneous, respectively [27, 31]:

$$a_1 = \frac{S_{xy}}{S_{xx}}; \quad b_1 = \bar{y} - a_1 \bar{x} \quad (4)$$

$$a_2 = \frac{S_{yy}}{S_{xy}}; \quad b_2 = \bar{y} - a_2 \bar{x} \quad (5)$$

$$a_3 = a_1 = \frac{S_{xy}}{S_{xx}}; \quad b_3 = b_1 = \bar{y} - a_3 \bar{x} \quad (6)$$

• **Orthogonal LS regression method**

It is thought that the (x, y) measurements are erroneous. The objective function of the method $\sum_{i=1}^n d^2$ is minimized to the sum of squared distances perpendicular to SLR line. The Orthogonal LS regression method is the geometric expression of Total Least Squares method [33]. The coefficients of this method are determined according to the objective function as follows [27, 31, 33].

$$a_4 = \frac{1}{2} \left[a_2 - a_1^{-1} + \text{sign}(S_{xy}) \sqrt{4 + (a_2 - a_1^{-1})^2} \right]; b_4 = \bar{y} - a_4 \bar{x} \tag{7}$$

2.1.2. SLR Methods according to the Objective Function of LAV Adjustment

The SLR methods according to the LAV method give the most appropriate solution for unknown parameters by minimizing the sum of the absolute valued distances between a given (x, y) point and the determined regression line. This distance can be in the direction of x axis, y axis, perpendicular or a specific angle to the regression line. In this solution, the functional equation between the measurements and unknowns is formed according to Eq.(2).

The mathematical model is transformed into the problem linear programming equations because the direct solution for this objective function is not possible except in a special case [1]. The linear programming equations are written as follows:

$$\begin{aligned} Cx = d & \qquad \text{constraint equation} \\ f = b^T x = \min. & \qquad \text{objective function} \end{aligned} \tag{8}$$

In this case, the SLR equations and the objective function should be transformed into linear programming equations. The unknown parameters of the LAV method are composed of unknown parameters and measurement residuals. The unknown parameters of linear programming must be positive. For this reason, the new unknown parameters are rearranged as the difference of the unknown parameters derived as negative and positive [34]. In this situation, the number of unknown parameters is double the initial number of unknown parameters and measurement residuals.

$$\begin{aligned} x &= x^+ - x^-; & x^+, x^- &\geq 0 \\ v &= v^+ - v^-; & v^+, v^- &\geq 0 \end{aligned}$$

The objective function of the LAV method is also transformed into the objective function of linear programming. These equations are:

$$[A \quad -A \quad -I \quad I] \begin{bmatrix} x^+ \\ x^- \\ v^+ \\ v^- \end{bmatrix} = [\ell]; \quad Cx = d \tag{9}$$

$$f = b^T x = [v] = [v^+ - v^-] = \min.; b^T = [0 \quad 0 \quad I \quad I]; \quad x = \begin{bmatrix} x^+ \\ x^- \\ v^+ \\ v^- \end{bmatrix} \tag{10}$$

In this case, the mathematical model given in Eq. (2) and the objective function in LAV method have been transformed into the linear programming equation given in Eq.(8) [1, 16].

- **SLR Method according to LAV Method when the measurements are erroneous**

It is thought that only the (y) measurement (LAV ($y|x$)), only the (x) measurement (LAV ($x|y$)), or both (x, y) measurements are erroneous for the LAV Method. These methods $\sum_{i=1}^n |v_y|$, $\sum_{i=1}^n |v_x|$ and $\sum_{i=1}^n |v_y| + \sum_{i=1}^n |v_x|$ are to minimize in the direction of the y axis, x axis and both x and y axes, respectively, (Figures 1a, 1b, 1c). The mathematical models according to Eq.(2) are as follows:

$$(y_i + v_{y_i}) = a_5 x_i + b_5; \quad y_i = a_6 (x_i + v_{x_i}) + b_6; \quad (y_i + v_{y_i}) = a_7 (x_i + v_{x_i}) + b_7$$

The coefficients of these methods are determined according to Eqs. (9) and (10).

- **Orthogonal LAV regression method**

It is thought that the (x, y) measurements are erroneous. The objective function of the method $\sum_{i=1}^n |d|$ is minimized to the sum of the absolute distances perpendicular to the SLR line. (Figure 1d.). The mathematical model is written according to Eq.(2) as follows:

$$y_i + v_{y_i} = a_8 (x_i + v_{x_i}) + b_8$$

The coefficients of this method are determined according to the Eqs. (9) and (10).

- **Bisector (the LS method bisector) regression**

This is the line that obtained of bisects the angle between LS ($y|x$) and LS($x|y$). The objective function of this method $\sum_{i=1}^n |d|$ is minimized from the sum of absolute distances perpendicular to bisector line (Fig. 1e).

The mathematical model is written according to Eq.(2) as follows:

$$y_i + v_{y_i} = a_9 (x_i + v_{x_i}) + b_9$$

The coefficients of this method are determined according to the Eqs. (9) and (10) or through direct solution equations [27, 31].

$$a_9 = (a_1 + a_2)^{-1} \left(a_1 a_2 - 1 + \sqrt{(1 + a_1^2)(1 + a_2^2)} \right); b_9 = \bar{y} - a_9 \bar{x} \quad (11)$$

- **Reduced major axis (RMA) regression**

The method is also called the geometric mean regression. The objective function of this method $\sum_{i=1}^n |v_x v_y|$ is minimized to the sum of absolute product of residuals in the directions of the x and y axis (Figure 1f). The mathematical model is written according to Eq.(2) as follows:

$$y_i + v_{y_i} = a_{10} (x_i + v_{x_i}) + b_{10}$$

The coefficients of this method are determined according to Eqs. (9) and (10) or through direct solution equations [27, 31].

$$a_{10} = \text{Sign}(S_{xy}) \sqrt{\frac{S_{yy}}{S_{xx}}}; b_{10} = \bar{y} - a_{10} \bar{x} \quad (12)$$

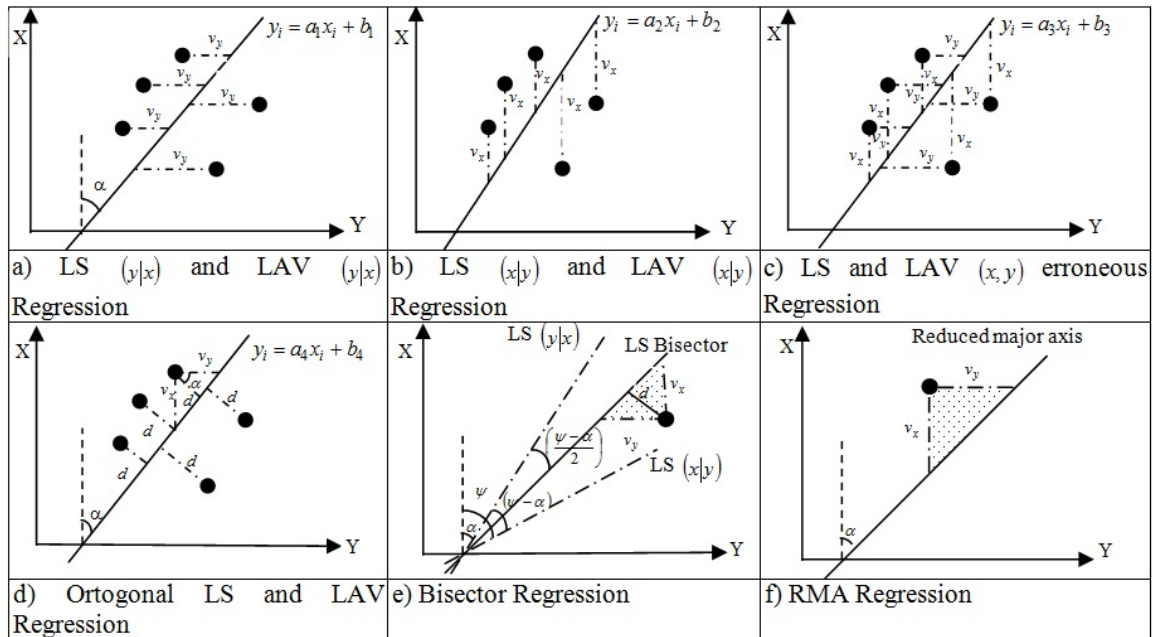


Fig. 1. Simple linear regression methods.

3. Numerical Application

An application was undertaken to determine a SLR regression line equation for the (x, y) measurements. The aim of this application is to investigate the appropriateness of the SLR methods in the light of theoretical explanations. In this application, the LS $(y|x)$, LS $(x|y)$, Orthogonal LS according to the LS objective function; Orthogonal LAV, Bisector and RMA regression methods according to the LAV objective function were used. The values and general distributions of the measurements are given in Tab. 1 and Fig. 2.

Tab. 1. Measurement values

| NN | x | y |
|----|-------|------|
| 1 | 4.75 | 2.20 |
| 2 | 5.50 | 2.02 |
| 3 | 3.45 | 1.10 |
| 4 | 8.25 | 4.04 |
| 5 | 3.25 | 0.52 |
| 6 | 9.30 | 5.78 |
| 7 | 10.00 | 5.40 |
| 8 | 8.20 | 5.20 |
| 9 | 3.25 | 1.50 |
| 10 | 9.50 | 6.48 |
| 11 | 2.40 | 0.80 |
| 12 | 6.50 | 3.33 |
| 13 | 5.20 | 2.75 |
| 14 | 6.40 | 3.75 |
| 15 | 8.80 | 5.03 |

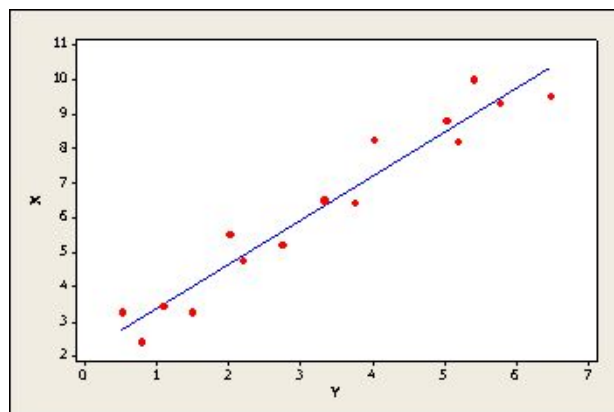


Fig. 2. Distribution of the measurement values.

A program was created for the six methods using MatLab. The SLR equations and the objective function of these methods were determined and the results of methods are given in Table 2.

Tab. 2. The results from the SLR methods.

| Method | Regression Equation | Objective Function Value |
|---------------------------|----------------------------|--------------------------|
| LS _(y x) | $y_i = 0.7339x_i - 1.3094$ | 3.2204 |
| LS _(x y) | $y_i = 0.7812x_i - 1.6080$ | 5.6165 |
| Orthogonal LS Regression | $y_i = 0.7507x_i - 1.4155$ | 2.0763 |
| Orthogonal LAV Regression | $y_i = 0.7868x_i - 1.5374$ | 4.7156 |
| Bisector Regression | $y_i = 0.7573x_i - 1.4570$ | 4.3193 |
| RMA Regression | $y_i = 0.7572x_i - 1.4564$ | 4.3193 |

4. Results

The numerical applications were undertaken using various objective functions to determine the SLR equation. While LS_(y|x), the LS_(x|y) and Orthogonal LS regression methods are used according to the LS objective function, the Orthogonal LAV, Bisector and RMA regression are used according to the LAV objective function. The results obtained from these applications are as follows:

- The objective function values of the Orthogonal LS regression method were smaller than the objective function of the other methods.
- The Bisector regression and the RMA Regression methods from the LAV method solutions determined rather similar objective function value.
- The objective function value of the Bisector and RMA Regression methods was the closest to the objective function value of the Orthogonal LS method.
- It was observed that the most appropriate method was the Orthogonal LS regression method for the LS methods and the Bisector Regression or RMA Regression for the LAV methods.

Furthermore, the objective function values of the other methods were calculated from the results of the methods (Tab. 3).

Tab. 3. Objective function values of the SLR Methods.

| Method | $\sum_{i=1}^n v_y^2$ | $\sum_{i=1}^n v_x^2$ | $\sum_{i=1}^n d^2$ | $\sum_{i=1}^n d $ | $\sum_{i=1}^n v_x v_y $ |
|--------------------------------|----------------------|----------------------|--------------------|--------------------|--------------------------|
| LS _(y x) Regression | 3.2204 | 5.9782 | 2.0929 | 4.7920 | 4.3877 |
| LS _(x y) Regression | 3.4278 | 5.6165 | 2.1286 | 4.8186 | 4.3877 |
| Orthogonal LS Regression | 3.2465 | 5.7602 | 2.0763 | 4.7948 | 4.3244 |
| Orthogonal LAV Regression | 3.6483 | 5.8932 | 2.2533 | 4.7156 | 4.6368 |
| Bisector Regression | 3.2710 | 5.7034 | 2.0788 | 4.3193 | 4.7957 |
| RMA Regression | 3.2706 | 5.7041 | 2.0787 | 4.7957 | 4.3193 |

It was observed in this analysis that the Orthogonal LS regression method, Bisector Regression and RMA Regression decreased the objective functions of the other methods.

5. Discussion and Evaluation

In this study, the determination of the SLR equation was explained using the measurements group. The LS and LAV methods were used for the regression problem which is also an adjustment problem. The theoretical solutions of the SLR methods were explained for parameter estimation methods and a numerical solution was obtained using a measurement group in order to analyze the success levels of the methods.

The smallest objective function value was provided by the Orthogonal LS regression according to the objective function of the LS method. This method also decreased the objective functions of the other SLR methods. The Bisector and RMA Regression methods gave the smallest objective function values with rather similar results according to the objective function of the LAV method. These methods also provided small values for the objective functions of other the SLR methods.

It is known that the LS method is weak to determine the measurement errors although this method is powerful in parameter estimation. The LAV method is a rather strong method to determine

the measurements errors even though it uses an adequate number of measurements and excludes the other measurements for the parameters estimation. If the advantages and disadvantages of these two methods are evaluated, it is obvious that these methods should be used together for better results. In this case, obtain a successful solution to the SLR, it is necessary to first acquire the determination of the measurements errors according to the LAV method and removing them from the measurement group, then, after the unknown parameter estimations are calculated the LS method is used with all the measurement groups.

In the light of this information, the Orthogonal LS Regression method is outstanding according to the LS method with the Bisector and RMA Regression methods being appropriate according to the LAV method. It is recommended that these three methods are used for determination of the SLR equation taking into account the existence of measurement errors within the measurements group.

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