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Parameter estimation and outlier detection with different estimation methods

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The best suitable values of unknown parameters are determined by adjustment of observations done more than the number of unknown parameter in applied sciences. Adjustment methods should determine the outlier, that inevitably exists in the observations, while doing estimation of the best appropriate parameter for the unknown parameters. The adjustment is made on the basis of an objective functions with the best parameter estimation from the mathematical model, written for the observations done more than the number of unknown parameters. The most applied methods used for adjustment are Least Square (LS), Least Absolute Values (LAV) and Total Least Square (TLS) Methods. Although there are many advantages of these methods, the LS method also has some disadvantages, such as more affected from gross observation errors in the observation and spread of gross error in other observations. The solution of LAV method and the results obtained with trial and error method for the parameter estimation are less affected by gross observation error; and this method is used successfully in removing the outlier. Besides, with these methods in recent years, the TLS method is used for the adjustment. In this method, the design matrix used for the solution is also erroneous and the residuals of observation and design matrix are calculated together in the solution. In this study, after three adjustment methods have been explained, the parameter estimation and outlier detection are made with using the application data. The success of adjustment methods for parameter estimation and outlier detection had been determined as well by examining the results of these methods.

Key words: Adjustment methods, the parameter estimation, the outlier detection, least square method, least absolute values method, total least square method.

INTRODUCTION

The u-number unknown parameters and the n-number of observation should be equal to each other in order to have a unique solution in a problem. In applied sciences, the basic principle is doing more observations than required in order to provide reliability and to increase the accuracy of observations and the results obtained from the observations. The case of observations number being more than unknown parameters number, different algebraic solutions equal to $\binom{n}{u}$ combination number are obtained. The solution must be done according to the principle in order to obtain the unique unknown parameters. This process is called adjustment, and the principle is called the objective function. The purpose of adjustment is to determine the best suitable (the highest probability) values of unknown parameters without removing any observations from the observation group and to determined the sensitivity and reliability of the certain value of observations and their functions (Wang, 1992).

The success of an adjustment is analyzed with the determination of outlier detection and parameter estimation. Parameter estimation means the determination of u-number of unknown parameters using all of the n-number of observation. The solution, using the adjustment in the parameter estimation, should be obtained with the evaluation of all observations.

The observation group inevitably contains erroneous observations for different reasons and for this reason each observation has a residual value. Since the actual observations and the actual observation residuals are not known, instead of these values, certain observation $\hat{\ell}$

Table 1. The functional model and the objective function of adjustment methods.

Method	Functional Model	Objective function
The least square method	$\ell + v = Ax$	$[Pvv] = \min$.
The least absolute values method	$\ell + v = Ax$	$[P\|v\|] = \min$.
The total least square method	$\ell + v = (A - v_A)x$	$[Pvv; Pv_A v_A] = \min$.

and observation residuals v are used.

Mathematical model done for determination of u-number unknown parameters x with the n-number of observations ℓ is below.

$$\begin{array}{ll} \textit{Functinal model} & \textit{Stochastic model} \\ \hat{\ell}_i = \Phi_i(x_1, x_2, \ldots\ldots\ldots, x_u) & Q_{\ell\ell} = P^{-1}; \quad C_{\ell\ell} = \sigma_0^2 Q_{\ell\ell} \end{array} \tag{1}$$

The linear functional model, also known as Gauss-Morkoff model, is acquired by the linearization of functional model (Vanicek and Wells, 1972; Ghilani and Wolf, 2006). In this model, if $\hat{\ell}$ instead of ℓ and v is used, then mathematical model changes as seen below.

$$E\{\hat{\ell}\} = \ell + v = Ax \qquad Q_{\ell\ell} = P^{-1}; \quad C_{\ell\ell} = \sigma_0^2 Q_{\ell\ell} \tag{2}$$

In Equations (1) and (2), P is the weights matrix of observation, $Q_{\ell\ell}$ is the inverse P weights matrix, $C_{\ell\ell}$ is the variance-covariance matrix of observation, σ_0^2 is a priori variance and A is a design matrix of functional model. The more than required number of observations causes discrepancy among the observations, in this case the solution of problem is not to be unique. The adjustment should be made according to the objective function to obtain a unique solution.

In the first part of the study, the mostly used parameter estimation methods, namely, LS, LAV and TLS are explained theoretically. The most applied method in all adjustment methods is Least Square Method which is also known as L_2-norm method. The method explained by Carl Friedrich Gauss in 1795 and announced by Legendre after a short time is used in many sciences and by many scientists till date. The LAV Method, which is also known as L_1-norm, is a long standing method. The written solution of this method is done by Laplace in 1789. This method has been used for the solution of many different problems (Edgeworth, 1887, 1888; Fuchs, 1982; Hawley and Gallagher 1994; Harvey, 1993; Dodge, 1987; 2002; Castillo et al., 2007). TLS Method has been used in the parameter estimation in the recent years. This method was first explained by Golub and Van Loan; and many researches have been done, using this method (Golub and Van Loan, 1980; Van Huffel, 1991; Felus, 2004; Markovsky et al., 2004; Acar et al., 2006; Akyılmaz, 2007).

The success of these methods, using a data set for the application of 3D similarity transformation, is analyzed in the second part of the study.

ADJUSTMENT METHODS

Adjustment, with the help of observations done more than required number, aims to assess the highest possibility of certain values, corrected observations, and sensitivity and reliability of their functions. The solution is done based on the objective function to obtain the estimated values of the unknown parameters by using the mathematical model given by Equation 2. In general, the objective function is formed by minimization of residuals or a function of residuals. The most used adjustment method, their objective functions and functional model are given in Table 1.

The least square (LS) method

The most widely used objective function in geodetic studies is LS method. The reasons to choose this method are: it has simple computation algorithm, no requirement for statistical distribution about the observations, it keeps the initial value of functional and stochastic models, is simple and understandable in terms of the variance-covariance distribution and error statistic (Koch, 1999; Ghilani and Wolf, 2006).

According to LS Method, the solution of a problem is always unique and performed easily. The objective function of LS method, can be shown in different ways as below.

$$\|Pvv\| = [Pvv] = min. \tag{3}$$

The LS method, making the sum of weighted squares of observation residuals to be minimum, gives the most appropriate solution for unknown parameters. If the weight matrix is taken as the inverse of variance-covariance matrix, the LS method solution is the unbiased estimation and minimum variance (Simkooei, 2003).

If the mathematical model, given in equation (2), is solved according to the objective function of LS Method, the following equation is obtained for the unknown parameters.

$$x = \left(A^T PA\right)^{-1} A^T P\ell \tag{4}$$

Considering the mathematical model established in accordance with the LS solution, the residuals, obtained as a result, are affected from all errors of the observations based on the functional model. The most important point in adjustment with LS Method is to assume the observations have the normal distribution. If the observation group has error, observation distribution is not matched with normal distribution. In the LS solution, since the all observations are used in the parameter estimation, even only one outlier in the observation group affected the accuracy and sensitivity of all unknown parameters. Also, the effect of this outlier spreads on all other observation residuals (Huber, 1981; Hampel et al., 1986). For this reason, if there is an outlier in the observation group, the outlier detection, made with the LS Method result, may not be done correctly. In this solution, if a consistent observation is determined as outlier due to the spread of the other observations error, this is called as sinking effect, if an outlier cannot be determined as outlier, this is called as hiding effect (Hekimoğlu, 1997). Both two effects are explained from the functional model with effected of residuals, obtained LS Method. These effects can be understood more clearly than residuals equation. The residuals is obtained in the following form.

$$v = \left(Q_{\hat{\ell}\hat{\ell}} - Q_{\ell\ell}\right)P\ell = -Q_{vv}P\ell \\ v = R\ell \tag{5}$$

The relation between observations and residuals is explained with this equation. The reflection ratio of observation random errors on the observations is shown with redundant matrix R. When this redundant matrix is examined, it is understood that an observation error reflects on not only observation residuals, but also other observation residuals. In addition, a residual occurs with the sum of both observation error and the reflection of other observations errors themselves (Hadi and Siminoff, 1993; Hekimoğlu, 2005).

Least absolute values (LAV) method

The LAV method gives an estimation of unknown parameters by making the sum of weighted absolute of observation residuals to be minimum. The objective function is like that:

$$\|pv\| = [P|v|] = min. \tag{6}$$

The LAV Method is also an unbiased estimate like The LS Method (Yetkin and Inal, 2010). The mathematical model is written as equation (2) for The LAV method and this model is solved with the objective function of the LAV method. However, the direct solution is not possible except in special case according to the objective function. (Bektaş, 2005). The solution is done with either trial and error or converting into the problem linear programming. There is $\binom{n}{u}$ combination number different solution of a linear equation system, obtained with *n*-number of observations and *u*-number of unknown parameters, with LAV method. In these solutions, different u-number observations are used in each time. One of these solutions is suitable to the objective function. If the freedom degree $f = (n-u)$ is high, by using this method the solution of unknown parameters take too much time and are difficult.

The mathematical model given in Equation (2) is transformed into linear programming for the general solution of LAV Method (Mosteller et al., 1950). All unknown parameters, using constraint equation and the objective function of LAV method, must be positive to obtain the solution with linear programming. The constraint equation and the objective function of LAV method are written as follows.

$$Cx = d \quad \text{The constraint equation} \\ f = b^T x = \min. \quad \text{The objective function} \tag{7}$$

In this case, mathematical model written according to the Equation (2) should be transformed into the linear programming. The new unknown parameters group composed of unknown parameters x and observation residuals v are used in the solution of linear programming. All unknowns should be compulsorily positive in the solution of linear programming. For this reason, unknown parameters of LAV method are designated as the difference of new unknown parameters derived as positive and negative (Schmidt, 2005). Number of unknown parameter in the solution of LAV method with the linear programming is double of *u*-number of unknown parameters and *n*-number of observations residuals.

$$x = x^+ - x^- ; \quad x^+,\ x^- \geq 0 \\ v = v^+ - v^- ; \quad v^+,\ v^- \geq 0$$

The mathematical model given in Equation (2) is transformed into the constraint equation given in Equation (7). Similarly, the objective function of LAV method should be transformed into the objective function of linear programming in the same way.

$$\underbrace{\begin{bmatrix} A & -A & -I & I \end{bmatrix}}_{c} \underbrace{\begin{bmatrix} x^+ \\ x^- \\ v^+ \\ v^- \end{bmatrix}}_{x} = \underbrace{[\ell]}_{d} \tag{8}$$

$$f = b^T x = [p|v|] = p^T v = p^T \begin{bmatrix} v^+ & v^- \end{bmatrix} = \min. \\ b^T = \begin{bmatrix} 0 & 0 & P & P \end{bmatrix}; \quad x = \begin{bmatrix} x^+ \\ x^- \\ v^+ \\ v^- \end{bmatrix} \tag{9}$$

The estimation values of unknown parameters can be calculated by solving according to the principles of linear programming.

The parameter estimation with LAV method is made with the observation number equal to unknown parameters. These observations are not taken as corrected error, and the observations residuals are equal to zero. These are the disadvantages of the method. The residuals occur substantially with their own observation errors in the solution of the LAV method. In other words, the observation error is not spread into the other observation residuals less than in LS method. For this reason, LAV method is generally used in outlier detection (Bektas and Sisman, 2010).

The total least square (TLS) method

The design matrix A formed for the solution of mathematical model is considered to have no error. It is not an accurate approach that design matrix, obtained with errors existed inevitably in the observations, does not include any error. In this case, the errors of design matrix A should be taken into account in the solution. The mathematical model of classical TLS method introduced by Golub and Van Loan in 1980 is given subsequently.

$$\hat{\ell} = \ell + v = (A - v_A)x \tag{10}$$

Here, v_A are the residuals of related elements of design matrix A and v is the observation residual. It is thought that observations residuals v and residuals of design matrix v_A are the independent variables, having the same variance and zero-mean (Akyılmaz, 2007). The mathematical model, given in Equation (10), is solved according to the objective function of TLS method. This objective function is given subsequently.

$$\left\|P\left[v;v_A\right]P\right\| = [Pvv;Pv_A v_A] = min. \quad (11)$$

Although all elements of the design matrix A are erroneous in general solution of the problem, the case of some part of this matrix composed of fixed-coefficients occurs frequently in application. For these fixed-coefficients should not be reduced in the solution of TLS method; the unknown parameters, having fixed-coefficients, are distinguished from other unknown parameters. In this case, design matrix A is divided into two parts, A_1 and A_2. The first part A_1 is for fixed unknown parameters x_1; the second part A_2 is for the other unknown parameters x_2. The elements of A_1 matrix are fixed and known exactly. In this case functional model and the objective function of the TLS method are given as;

$$\begin{aligned} &\ell + v = \left[A_1; A_2 + v_{A_2}\right]\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \\ &\left\|P\left[v; v_{A_2}\right]P\right\| = \min. \end{aligned} \quad (12)$$

The extended matrix $\left[A_1; A_2; \ell\right]$ is obtained with observations ℓ and design matrix A. It should be divided into two parts, the square matrix Q, be $Q^T Q = I$, and the upper triangular matrix R to solve this matrix. This division of extended matrix $\left[A_1; A_2; \ell\right]$ is obtained with the QR factorization. The aim of this division is to distinguish the unknown parameters that should have fixed-coefficient, from other unknown parameters..

$$\left[A_1; A_2; \ell\right] = QR \text{ or } Q^T\left[A_1; A_2; \ell\right] = R\begin{bmatrix} R_{11} & R_{12} & R_{1b} \\ 0 & R_{22} & R_{2b} \end{bmatrix} \quad (13)$$

Here, R_{11}; the sub matrix of the fixed coefficient unknown parameters (the dimension (m_1,m_1)), R_{12}; the sub matrix of the correlation between fixed coefficient unknown parameters and the other unknown parameters (the dimension (m_1,m_2)), R_{22}; the sub matrix of the not fixed coefficient unknown parameters (the dimension (m_2,m_2)), R_{1b}; the sub vector of the fixed coefficient observation ℓ (the dimension (m_1,1)), R_{2b}; the sub vector of not fixed coefficient observation ℓ (the dimension (m_2,1)).

The second part, given in Equation (13), can be written as;

$$\left[R_{22}; R_{2b}\right]P\left(P^{-1}\begin{bmatrix} x_2 \\ -1 \end{bmatrix}\right) \approx 0 \quad (14)$$

The elements of matrix $\left[R_{22}; R_{2b}\right]P$, in this case, are linearly dependent. This matrix is divided into the three matrixes, U, V, Σ, by Singular Value Decomposition (SVD) to take the inverse of non-square linearly dependent. The diagonal elements of Σ and m+1[th] element of V matrix are $\sigma_m > \sigma_{m+1}$ and $v_{m+1,m+1} \neq 0$ in the solution. Here, the calculation of unknown parameters x_2 is made by $v_{m+1} = -1$ should be done for the TLS method solution (Felus, 2004). The unknown parameters x_2, in this case are calculated as;

$$x_2 = -\frac{1}{C_{m_2+1}V_{m_2+1,m_2+1}} C_{1 \cdots m_2}\left[V_{1,m_2+1}, V_{2,m_2+1}, \ldots\ldots, V_{m_2,m_2+1}\right] \quad (15)$$

The unknown parameters x_1 are acquired with the values of unknown parameters x_2 from the first row of the Equation (13).

$$\begin{aligned} &R_{11}x_1 + R_{12}x_2 - R_{1b} \approx 0 \\ &x_1 = R_{11}^{-1}\left(R_{1b} - R_{12}x_2\right) \end{aligned} \quad (16)$$

The most common solution of LS method is to take the observation group and the design matrix as erroneous, namely, TLS method (Acar et al., 2006; Akyılmaz, 2007). It is impossible that the observation errors in observation group do not affect the design matrix. If the errors in observation group are determined better, the unknown parameters can then be estimated better. As a result, the proximity of unknown parameters to the certain value is related with the modeling of error in observation group.

Numerical application

3D similarity transformation equations are written between common points; the coordinates of these points are known in two coordinate systems and the unknown parameters of coordinate transformation x are calculated from the solution of these equations. Details of 3D similarity transformation can be found in (Ghilani and Wolf, 2006; Acar et al., 2006). In this paper the 3D similarity transformation has been done between two coordinates system to examine the LS, LAV and TLS adjustment methods. In the application, the success of these methods has been analyzed for the parameter estimation and the outlier detection. The common point coordinates are known in 3D I. and II. system, given in Table 2.

The calculated unknown parameters of the LS, LAV, TLS methods by taking the weights of observations equal to each other are given in Table 3.

A few of the observations group consisting of point coordinates have been tainted to examine the success of the outlier detection for the LS, LAV and TLS methods. X and Y coordinates of 2-number point and Z coordinate of 5-number point are increased by 1m., Y coordinate of 3-number point is decreased by 1m. to the tainted observation group has been created from I.system coordinates. The tainted dataset is given in Table 4.

The unknown parameters are calculated by using the LS, LAV, TLS method, and these parameters are given in Table 5. The weights of observations have been taken as equal in this solution.

RESULTS

The application of 3D similarity transformation is done to

Table 2. The common point coordinates.

PN	I. System			II. System		
	X (m)	*Y (m)*	*Z (m)*	*X (m)*	*Y (m)*	*Z (m)*
1	3946.180	1034.600	147.166	3946.140	1034.689	147.182
2	4157.930	1003.780	163.420	4157.923	1004.097	163.418
3	3834.090	1137.090	127.455	3834.054	1137.112	127.477
5	4206.520	1244.190	164.747	4206.420	1244.155	164.684
9	4351.350	1605.400	180.284	4351.514	1605.241	180.217

Table 3. Estimation values of unknown parameters.

Parameters	LS Method	LAV Method	TLS Method
X_0	0.6559	-0.0149	0.6626
Y_0	1.5077	1.9487	1.5257
Z_0	0.6695	0.4846	0.3039
ε_x	0.0000642	0.0000702	0.0001269
ε_y	-0.0001395	-0.0000957	0.0000320
ε_z	0.0002853	0.0004410	0.0002929
κ	0.9997499	0.9998745	0.9997526

Table 4. The tainted point coordinates.

PN	I. System			II. System		
	X (m)	*Y (m)*	*Z (m)*	*X (m)*	*Y (m)*	*Z (m)*
1	3946.180	1034.600	147.166	3946.140	1034.689	147.182
2	4158.930	1004.780	163.420	4157.923	1004.097	163.418
3	3834.090	1136.090	127.455	3834.054	1137.112	127.477
5	4206.520	1244.190	165.747	4206.420	1244.155	164.684
9	4351.350	1605.400	180.284	4351.514	1605.241	180.217

Table 5. Estimation values of unknown parameters with tainted point coordinates.

Parameter	LS Method	LAV Method	TLS Method
X_0	-1.8003	-0.1995	-1.9716
Y_0	6.4996	2.4353	6.6358
Z_0	3.1423	0.4054	4.6545
ε_x	-0.0002742	0.0000795	-0.0005301
ε_y	-0.0008968	-0.0000701	0.0013452
ε_z	0.0015353	0.0005540	0.0015914
κ	0.9999038	0.9998761	1.0000149

examine the success of adjustment methods in the parameter estimation and outlier detection. The parameter estimation is done with the observations group obtaining the real case application in the first part of application. All observations in observation group should be evaluated together and included in the solution at the same proportion for parameter estimation.

The I. system coordinates are transformed into II. system coordinates and the differences are determined between calculated value and measured values for real case application. These differences have been taken as residuals of the point coordinates. The residuals of the point coordinates are given in Table 6. The objective functions, $[Pvv]$ ad $[P|v|]$ values of each method are calculated by using these residuals. When these values have been examined, it is observed that the LS, the TLS

Table 6. The residuals of point coordinate with real case application.

PN	LS Method			LAV Method			TLS Method		
	v_x	v_y	v_z	v_x	v_y	v_z	v_x	v_y	v_z
1	0.024	0.044	0.000	0.000	0.000	0.000	0.024	0.044	-0.006
2	-0.068	-0.236	-0.014	-0.072	-0.316	-0.002	-0.070	-0.237	0.005
3	0.075	0.116	0.008	0.053	0.102	0.000	0.079	0.116	-0.016
5	0.082	0.042	0.025	0.121	-0.016	0.037	0.081	0.042	0.034
9	-0.113	0.036	-0.018	0.000	0.000	0.000	-0.114	0.036	-0.017
$[Pvv]$		0.1056			0.1349			0.1073	
$[P\|v\|]$		0.9006			0.7201			0.9197	

Table 7. The residuals of point coordinate with tainted values.

PN	LS Method			LAV Method			TLS Method		
	v_x	v_y	v_z	v_x	v_y	v_z	v_x	v_y	v_z
1	-0.420	0.213	-0.143	-0.065	0.045	0.000	-0.424	0.204	-0.119
2	0.496	0.656	-0.325	0.861	0.703	0.000	0.477	0.629	-0.403
3	-0.275	-0.553	-0.019	0.000	-0.841	0.000	-0.242	-0.538	0.079
5	-0.046	-0.088	0.758	0.081	0.000	1.039	-0.052	-0.093	0.721
9	0.243	-0.225	-0.270	0.000	0.000	0.000	0.242	-0.202	-0.278
$[Pvv]$		2.1733			3.0351			2.0827	
$[P\|v\|]$		4.7300			3.6340			4.7022	

and the LAV methods have the smallest value for objective function $[Pvv]$ and $[P|v|]$ respectively. This solution has indicated that the methods provide the objective function.

It is observed in the examination of Table 6 that the LS and the TLS methods have estimated unknown parameters, taken as error of all observations; and also the residuals have been calculated for all observations. As for the LAV method, it is observed that the observations, using unknown parameters determination, have not been taken as error. The residuals of these observations are equal to zero. The other observations residuals are calculated.

The point coordinates of I. coordinate system are transformed into the II. coordinate system with the unknown parameters for tainted values in the second part of application. The residuals of point coordinates are determined between calculated value and measured values; and these values are given in Table 7. The comparison has been made between the residuals values and the tainted values of point coordinates to determine the success of LS, LAV and TLS methods for outlier detection.

DISCUSSION AND CONCLUSIONS

At the end of this examination, it is observed that LS and TLS methods calculate nearly the same residuals for all points. The solutions of these methods have distinguished the residuals, corresponding tainted error values to the other errors; however it cannot determine the numerical values precisely. These methods are also observed to have spread the errors of other observation errors in the solution of the tainted observations; especially, residual value v_x of 1-number point is closed to the gross error residuals. The case can be explained with spread of error of LS and TLS method. If the results of TLS and LS methods are compared, it is not been observed that there is meaningfully difference. In the solution of the LAV method, residuals corresponding to all the tainted error values are determined, and also their numerical values are calculated better than the LS and TLS methods. Moreover, this method has not changed the residuals of the other observations.

Finally, if the adjustment methods are evaluated, it is suggested that TLS method is used since all observations are included together in the solution and at the same proportion for the parameter estimation. Although the TLS method has not shown any meaningfully difference from LS method in the 3D similarity transformation application, this model can be modeled the in observation errors better than the LS method. Furthermore, it is suggested that LAV method be used, because it gives quite correct result than the other methods for outlier detection.

The author of this paper suggests, for a successful adjustment, to acquire first the determination of outlier measurements solving based on LAV method and removing them from the observation group, after the unknown parameter estimations are calculated, using the TLS method with all the observation groups.

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