A trimmed moving total least squares method for curve and surface fitting

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A Trimmed Moving Total Least Squares Method for Curve and Surface Fitting

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Abstract

The Moving Least Squares (MLS) method has been developed for fitting of the measurement data contaminated with errors. The local approximants of the MLS method only take the random errors of the dependent variable into account, whereas the independent variables of measurement data always contain errors. To consider the influence of errors of dependent and independent variables, the Moving Total Least Squares (MTLS) offers a better choice. However, both MLS and MTLS method are sensitive to outliers, which greatly affects the fitting accuracy and robustness. This paper presents an improved method-Trimmed Moving Total Least Squares (TrMTLS) method, in which Total Least Squares (TLS) method with truncation procedure is adopted to determine the local coefficients in the influence domain. This method can deal with outliers and random errors of all variables without setting the threshold or adding small weights subjectively. The numerical simulation and measurement experiments results indicate that the proposed algorithm has better fitting accuracy and robustness compared with the MTLS and MLS method.

Keywords: Moving least squares, Random errors, Outliers, Local approximants

1. Introduction

Various methods of approximation or interpolation of measurement data have been researched in the past decades [1], where MLS method is one of popular methods of approximating a function from a set of some scattered data [2, 3]. The MLS method for smoothing and approximating scattered data was first introduced by Shepard [4] in the lowest order case and generalized to higher degree by Lancaster and Salkauska [5]. The principle of the MLS method is to start with the weighted least squares (WLS) [6] estimation in influence domain at an arbitrary fixed point, and then move the point over the entire parameter domain, where the weighted least squares fitting is calculated and evaluated for each measurement point independently. This method can be regarded as the combination of WLS and piecewise least squares (PLS) [7] in some way. Besides, as a flexible meshless method, there is no need to construct meshes in the domain compared to the finite element method [8]. It has been widely used in many engineering fields. For example, it is known that it formed many meshless methods to solve mathematical and physical problems where traditional calculation methods are not applicable [9-11], such as the element-free Galerkin method [12], the meshless local Petrov-Galerkin [13], and the boundary element free method [14]. In recent years, many scholars have studied and enhanced the moving least squares method [15, 16].

As an approximation method, the MLS method determines local approximants in the sense of ordinary least squares (OLS) method [17], whereas errors always occur to all of the variables. To consider the influence of errors of all variables [18], it makes more accurate to determine the local approximants in the sense of TLS method [17, 19]. For practical engineering problems, the measurement data are usually obtained by uniformly measuring curve and surface. However, since the measurement data are always not enough to express all the curve and surface information, it is necessary to generate new non-measurement points, which may introduce new errors. Besides, outliers are inevitable and will result in a deviation from the measurement data due to the influences from the testing evironment and the instrument itself [20]. MTLS method suffers from the same problem as MLS method and could not be properly applied to curve and surface fitting when outliers occur in the measurement data [21-23].

As mentioned above, the MLS and MTLS method can be greatly influenced by outliers. The fitting results often deviate from the real curve and the performance of fitting is strongly influenced even if only one outlier exists in the measurement data [24, 25]. Therefore, it is critical to avoid or reduce their influence on curve and surface fitting in order to achieve better results for most cases. Some applicable solutions have been proposed [26-28]. One solution is to directly delete the samples which are probably outliers. In this method, a threshold value is set to determine whether the measurement data are outliers , and then the confirmed outliers are deleted from the measurement data before fitting the surface [29-32]. However, the accuracy of this method is directly related to the threshold value. Therefore, it is key to choose the threshold appropriately, which is not an easy job. Another method is to assign small weights to outliers appropriately instead of removing them directly, in which case the negative effects of outliers on the curve and surface reconstruction can be reduced indirectly. However, how to add small weights to outliers is actually a challenging problem, especially when there is more than one outlier in the measurement data. Moreover, although it is clear that their negative influences are relative reduced, it is hard to know what the exact impacts will be generated by these small weights [31].

To avoid setting the threshold or adding small weights subjectively [31, 32], an improved curve and surface fitting approach called TrMTLS method is introduced in this paper. In the influence domain of TrMTLS method, TLS method based on Singular Value Decomposition (SVD) [33] with truncation procedure is adopted for dealing with the outliers and the errors of all variables. It has been proved that the impact of outliers is mitigated and the fitting accuracy is improved. Even if there are no outliers, the results of the improved method are still better than that of MLS and MTLS method. In Section 2, a brief introduction is given for MLS method. TrMTLS method is presented in detail in Section 3. Curve and surface fitting examples including numerical simulation and measurement experiments are given in Section 4 to verify the performance of TrMTLS method. Conclusions are shown in Section 5.

2. MLS method

We first give a brief description of MLS method in this section. To describe the principle of the MLS method, the trial approximation function [34] is defined as

$$u^h(\mathbf{x}) = \sum_{i=1}^{m} p_i(\mathbf{x}) a_i = \mathbf{p}^T(\mathbf{x})\mathbf{a} \tag{1}$$

where $p_i(\mathbf{x})$, i = 1, 2, …, m are the monomial basis functions, a_i are the coefficients of the basis functions and m is the number of terms in the basis functions.

General polynomial basis functions include linear basis function, quadratic basis function, etc., where linear basis functions are widely applied. The listed two common basis functions can be expressed as follows.

Linear basis function:

$$\begin{cases} \mathbf{p}(\mathbf{x}) = (1, x)^T & (m=2) \\ \mathbf{p}(\mathbf{x}) = (1, x, x^2) & (m=3) \end{cases}$$

Quadratic basis function:

$$\begin{cases} \mathbf{p}(\mathbf{x}) = (1, x, x^2)^T & (m=3) \\ \mathbf{p}(\mathbf{x}) = (1, x, y, x^2, xy, y^2)^T & (m=6) \end{cases}$$

At each point of $\mathbf{x}$, an appropriate $\mathbf{a}$ can be chosen so that $u(\mathbf{x})$ is well approximated by $u^h(\mathbf{x})$. To measure the approximation of the function, the approximation function of the discrete weighted L^2 norm can be defined as the following form

$$J = \sum_{I=1}^{n} w(\|\mathbf{x} - \mathbf{x}_I\| / r) \left[\sum_{i=1}^{m} p_i(\mathbf{x}_I) a_i - u(\mathbf{x}_I) \right]^2 \tag{2}$$

where r is the radius of the compact influence domain, and $w(\|\mathbf{x} - \mathbf{x}_I\|/r)$ is a weight function with its value decreasing with the increase of the distance $s = \|\mathbf{x} - \mathbf{x}_I\|$ between $\mathbf{x}$ and $\mathbf{x}_I$. $\mathbf{x}_I$ (I = 1, 2, …, n) is the node in the influence domain of $\mathbf{x}$. Many forms of weight functions have been proposed in previous studies. Commonly used weight functions are the exponential weight function and the spline weight function, etc. The following cubic spline weight function is applied in this paper, which is expressed as equation (3) and shown in Figure 1.

$$w(s) = \begin{cases} \dfrac{2}{3} - 4s^2 + 4s^3 & s \le \dfrac{1}{2} \\ \dfrac{4}{3} - 4s + 4s^2 - \dfrac{4}{3}s^3 & \dfrac{1}{2} < s \le 1 \\ 0 & s > 1 \end{cases} \tag{3}$$

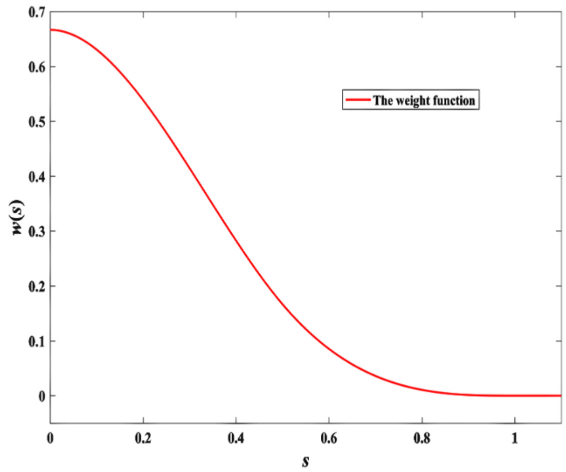


Figure 1. Schematic graph of the cubic spline weight function

In the influence domain of **x**, the coefficients of local approximants are solved by

$$\mathbf{a} = \mathbf{A}^{-1}(\mathbf{x})\mathbf{B}(\mathbf{x})\mathbf{u} \tag{4}$$

where

$$\mathbf{A}(\mathbf{x}) = \mathbf{P}^T \mathbf{W}(\mathbf{x})\mathbf{P}$$

$$\mathbf{B}(\mathbf{x}) = \mathbf{P}^T \mathbf{W}(\mathbf{x})$$

$$\mathbf{P}=\begin{pmatrix} p_1(\mathbf{x}_1) & p_2(\mathbf{x}_1) & \cdots & p_m(\mathbf{x}_1) \\ p_1(\mathbf{x}_2) & p_2(\mathbf{x}_2) & \cdots & p_m(\mathbf{x}_2) \\ \vdots & \vdots & \ddots & \vdots \\ p_1(\mathbf{x}_n) & p_2(\mathbf{x}_n) & \cdots & p_m(\mathbf{x}_n) \end{pmatrix}$$

$$\mathbf{W}(\mathbf{x}) = diag(w_1(s), w_2(s), \cdots, w_n(s))$$

$$\mathbf{u}=(u(\mathbf{x}_1), u(\mathbf{x}_2), \cdots, u(\mathbf{x}_n))^T$$

The approximation function equation (1) can be rewritten as

$$u^h(\mathbf{x}) = \mathbf{p}^T(\mathbf{x})\mathbf{a} = \mathbf{p}^T(\mathbf{x})\mathbf{A}^{-1}(\mathbf{x})\mathbf{B}(\mathbf{x})\mathbf{u} \tag{5}$$

In this paper, we only consider the linear least squares estimation of influence domain.

3. TrMTLS method

3.1 MTLS method

The TLS method is a method for dealing with errors-in-variables (EIV) model [33, 35] in which errors of all variables are considered. The function model is defined as

$$\mathbf{AX} = \mathbf{B} \tag{6}$$

where

$$\mathbf{A} = \mathbf{A}_1 + \Delta\mathbf{A}$$

$$\mathbf{B} = \mathbf{B}_1 + \Delta\mathbf{B}$$

An augmented matrix is constructed by TLS method based on singular value decomposition

$$\mathbf{C} := [\mathbf{A} \quad \mathbf{B}] = \mathbf{U\Sigma V}^T \tag{7}$$

where $\mathbf{\Sigma} = diag(\sigma_1, \sigma_2, \ldots, \sigma_{n+d})$. Let $\sigma_1 \geq \sigma_2, \ldots, \geq \sigma_{n+d}$ be the singular values of C, and define the partitionings as follows

$$\mathbf{V} := \begin{bmatrix} \mathbf{V}_{11} & \mathbf{V}_{12} \\ \mathbf{V}_{21} & \mathbf{V}_{22} \end{bmatrix} \qquad \mathbf{\Sigma} := \begin{bmatrix} \mathbf{\Sigma}_1 & 0 \\ 0 & \mathbf{\Sigma}_2 \end{bmatrix} \tag{8}$$

When $\mathbf{V}_{22}$ is nonsingular, TLS method solution exists. It is unique only if $\sigma_n \neq \sigma_{n+1}$. On this occasion, the solution of TLS is

$$\hat{\mathbf{X}}_{tls} = -\mathbf{V}_{12}\mathbf{V}_{22}^{-1} \tag{9}$$

To determine parameters of local approximants, TLS method based on SVD is applied to MTLS method. Not only the calculation efficiency is faster, but also the order of the basis function is easier to change. The augmented matrix [33, 36] can be expressed as

$$\mathbf{C}_\mathbf{x} := \mathbf{W}_\mathbf{x}[\mathbf{A} \quad \mathbf{B}] = \mathbf{U}_\mathbf{x}\mathbf{\Sigma}_\mathbf{x}\mathbf{V}_\mathbf{x}^T \tag{10}$$

where $\mathbf{W}_\mathbf{x} = diag(w(\mathbf{x} - \mathbf{x}_1), w(\mathbf{x} - \mathbf{x}_2), \ldots, w(\mathbf{x} - \mathbf{x}_n))$ is the weight matrix. The solution expression of equation (9) is rewritten as

$$\mathbf{a} = -\mathbf{V}_{\mathbf{x}12}\mathbf{V}_{\mathbf{x}22}^{-1} \tag{11}$$

3.2 TrMTLS method

As mentioned above, the MLS and MTLS method are sensitive to the outliers in measurement data. Therefore, the proposed TrMTLS method is a viable alternative method, which can reduce the influence of outliers. In this method, the residual is defined as

$$r(k) = w(y_i - y_{if}) \tag{12}$$

where y_i is the real value, y_{if} is the fitting value and w is the weight value.

Let $m < N$, where m is the number of nodes in the influence domain, and N is the total number of nodes. Then the truncation procedure estimation [37-39] is

$$\theta_{Tr} = \arg\max\{r_{1:m(r)}^2\} \tag{13}$$

TLS method with truncation procedure is applied for determining the local coefficients in TrMTLS method. In the influence domain of an arbitrary fixed point of TrMTLS method, TLS method based on SVD is firstly adopted for obtaining the coefficients of local approximation. Then, the residuals of all nodes can be obtained by the coefficients of local approximation and appropriate weight function, and the truncation procedure is used to trim a node which the squared residual is the largest. Finally, the local approximation is recalculated to replace the original value by using the TLS method based on SVD. Move the arbitrary fixed point over the entire parameter domain, where the truncation procedure is calculated for each point independently.

To further understand the principle of TrMTLS method, the truncation procedure of influence domain is shown in Figure 2.

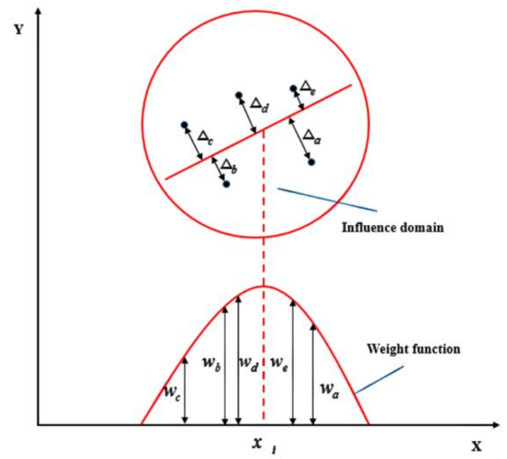


Figure 2. Schematic graph of TrMTLS method

As shown in Figure 2, $\Delta_e < \Delta_b < \Delta_c < \Delta_d < \Delta_a$ and $w_c < w_a < w_b < w_e < w_d$. In the influence domain of x_i, it can be obtained that $w_d\Delta_d$ of the square is the largest, so the node d should be trimmed.

As mentioned above, MLS method only considers the errors of the dependent variable, in which the constraint of local approximation is carried out in the vertical direction. MTLS method can be considered as an improved method for MLS and it takes into account the errors of all variables, in which the constraint of local approximation is carried out in the orthogonal direction. However, they are both sensitive to outliers. Different from MTLS method, TLS method based on SVD with truncation procedure is adopted for dealing with the outliers and the errors of all variables in the influence domain of TrMTLS.

From the previous numerical simulation, it can be found that it is difficult to give appropriate weight function to the nodes in the influence domain before the node with the largest squared residual is trimmed. Here are two ways to solve it: one is to give the weight function to whose value decreases with the increase of the distance between the nodes and the fitting points. The other is to add a same weight value to all nodes in the influence domain. Two ways fit in different circumstances. It can be found that the result of the former way is more accurate when there are obvious outliers in the measurement data, and the latter one is better when there are only unbiased random errors or outliers with not obvious values. We named the former way as unweighted TrMTLS and the other as weighted TrMTLS.

The following procedure, as shown in the flowchart in Figure 3, is carried out in numerical simulation experiments to verify the performance of the improved method:

Step 1: Add the random errors (δ_i, ε_i) and outliers (0, $_{\Delta}y_j$) to the data (x_i, y_i) for getting tested data (x_{im}, y_{im}).

Step 2: Fit the tested data (x_{im}, y_{im}) by MLS, MTLS and unweighted TrMTLS for getting fitting value (x_{if}, y_{if}).

Step 3: Calculate the fitting error s of the theoretical value y_i and fitting value y_{if} by

$$s = \sum_{i=1}^{n} \left| y_i - y_{if} \right| \tag{14}$$

Record the values s_1, s_2, s_3 for MLS, MTLS and TrMTLS respectively.

Step 4: Calculate the value $|s_2 - s_3|/s_2$. If $|s_2 - s_3|/s_2 > \psi/100$, perform step 5; otherwise, step 5 is skipped.

Step 5: Fit the tested data (x_{im}, y_{im}) using weighted TrMTLS for getting fitting value (x_{if}, y_{if}), then recalculate the sum of errors to replace the previous and record the new value of s_3.

Step 6: Repeat Step 1 − Step5 for 10000 times.

Step 7: Average the recorded values of s_1, s_2 and s_3, and take them as the final value of MLS, MTLS and TrMTLS.

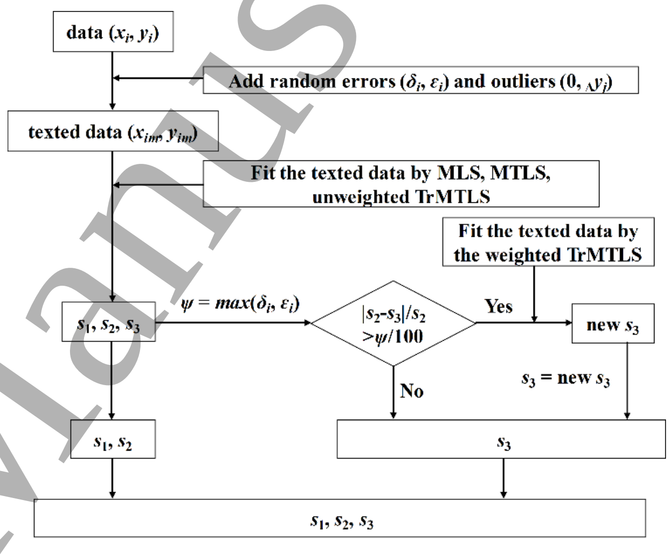


Figure 3. The simulation flowchart of the TrMTLS method

4. Case Study

In this section, four examples are given to verify the performance of TrMTLS method. MLS method and MTLS method are also applied to make a comparison.

Example 1.

Consider the aspheric profile function

$$y = \frac{cx^2}{1+\sqrt{1-(1+k)c^2x^2}} \tag{15}$$

where c = 1/1083 is the reciprocal of the curvature radius of the base vertex and k = − 1.5 is the constant of the quadric surface. Select a uniformly distributed set of points (x_i, y_i), i = 1, 2, …, n determined by equation (15). Then, the random errors (δ_i, ε_i) and outliers (0, $_{\Delta}y_j$) are added to the points (x_i, y_i), forming a set of tested data (x_{im}, y_{im}). In this section, normally distributed random errors with a zero mean are added. Outliers are generated by adding $_\Delta y_j$ to some points of the dependent variable. E_j, j = 1, 2, 3, 4 are outliers as shown in Figure 4. The fitting performance is characterized by equation (14).

Let n = 61 and $d = (max(x) - min(x))/5$ in Example 1. Figure 4 shows the fitting curves by using MLS, MTLS and TrMTLS. The sum of errors for these three methods are listed in Table 1.

Table 1. The sum of errors s of three methods for Example 1

variance		s		
δ_i	ε_i	s_1	s_2	s_3
0.000001	0.001	0.508742	0.570558	0.048801
0.00001	0.001	0.508678	0.570478	0.048792
0.0001	0.001	0.508798	0.570637	0.048815
0.001	0.001	0.508779	0.570605	0.048783
0.001	0.0001	0.508130	0.568753	0.046874
0.001	0.00001	0.508135	0.568739	0.047012
0.001	0.000001	0.508133	0.568737	0.047013

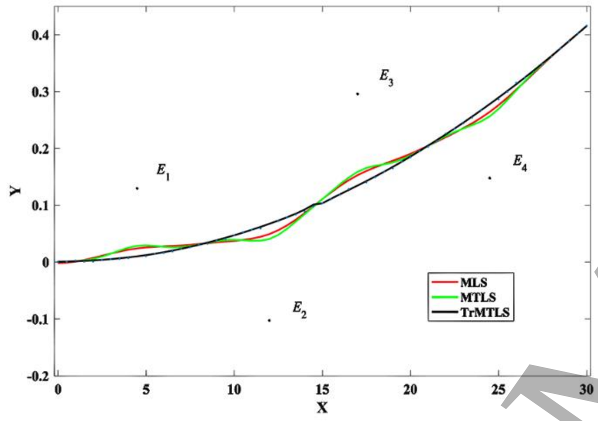


Figure 4. Fitting the aspheric profile curve by MLS, MTLS and TrMTLS method

Example 2.

In this example, we consider the oscillation function

$$y = e^{ax}\sin(bx) \tag{16}$$

where a = 1/30, b = 0.4. The data are obtained by the same way that is introduced in Example 1 and are still fitted by three methods. Let n = 161 and $d = (max(x) - min(x)) \times 2/25$ in Example 2. The fitting results and curves are shown in Table 2 and Figure 5 respectively.

Table 2. The sum of errors s of three methods for Example 2

variance		s		
δ_i	ε_i	s_1	s_2	s_3
0.000001	0.001	2.614597	2.047388	0.959902
0.00001	0.001	2.614645	2.047429	0.959945
0.0001	0.001	2.614580	2.047395	0.959946
0.001	0.001	2.614596	2.047389	0.960077
0.001	0.0001	2.614229	2.046992	0.960275
0.001	0.00001	2.614255	2.047021	0.960309
0.001	0.000001	2.614258	2.047030	0.960295

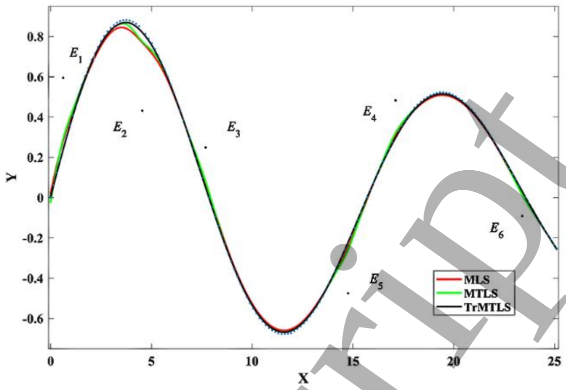


Figure 5. Fitting the oscillation curve by MLS, MTLS and TrMTLS method

Example 3.

In this example, we consider the following function

$$z = (x^2 - y^2)^2 \tag{17}$$

defined on the region $\Omega = [-1, 1] \times [-1, 1]$. Taking a uniformly distributed set of points, the region is divided into a 33 by 33 regular node grids. The data are obtained by the same way in Example 1 & 2. The fitting results using these three methods are shown in Table 3 and the fitted surfaces are shown in Figure 6.

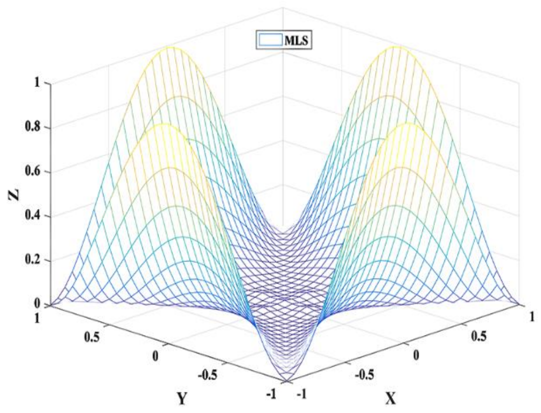
Let n = 1089 and $d = (max(x) + max(y))/10$ in Example 3. The fitting performance is characterized by the sum of errors between the theoretical value and the fitting value

$$s = \sum_{i=1}^{n} \left| z_i - z_{if} \right| \tag{18}$$

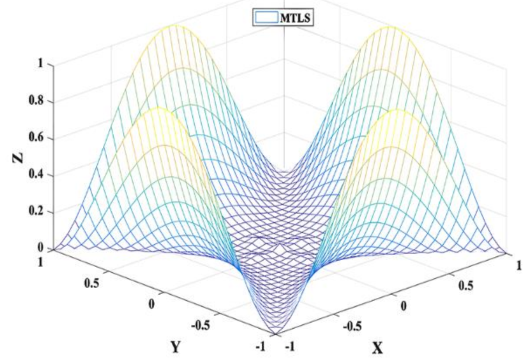
where z_i and z_{if} are the theoretical value and the fitting value.

Table 3. The sum of errors s of three methods for Example 3

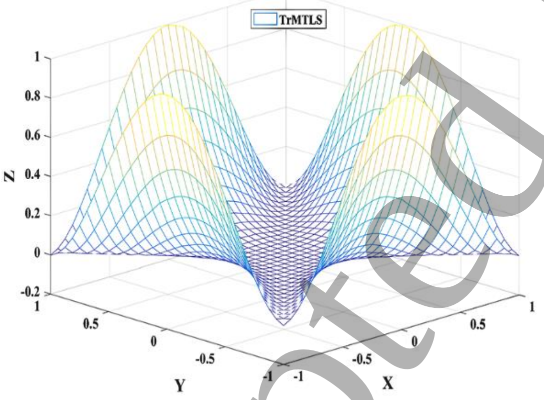
variance		s		
σ_x, σ_y	σ_z	s_1	s_2	s_3
0.000001	0.001	8.267936	4.924211	3.702649
0.00001	0.001	8.267709	4.924068	3.727679
0.0001	0.001	8.268510	4.924925	3.702433
0.001	0.001	8.293442	5.010912	3.971687
0.001	0.0001	8.283595	4.994708	3.708152
0.001	0.00001	8.290440	5.006132	3.733076
0.001	0.000001	8.276531	4.991401	3.708305



(*a*) MLS method



(*b*) MTLS method



(*c*) TrMTLS method

Figure 6. Fitting the surface in Example 3 by three methods

It can be seen from example 1 to example 3 that MTLS and MLS method are sensitive to outliers. Compared with these two methods, the improved algorithm TrMTLS can obviously acquire better results. Even when there are no outliers, the results of the improved method are still better. The function of example 1 is taken as an example to illustrate the performance of TrMTLS method when the data only contain random errors.

The fitting results and curves are shown in Table 4 and Figure 7 respectively. As shown in Figure 7, all of the three methods have provided a nice approximation. From the results of Table 4, the improved method is more accurate than the other two methods.

Table 4. The sum of errors *s* of three methods for Example 1

variance		*s*		
δ_i	ε_i	s_1	s_2	s_3
0.000001	0.001	0.07553	0.0435786	0.0435782
0.00001	0.001	0.07539	0.0434438	0.0434435
0.0001	0.001	0.07540	0.0434348	0.0434345
0.001	0.001	0.07556	0.0436147	0.0436143
0.001	0.0001	0.07440	0.0416549	0.0416548
0.001	0.00001	0.07440	0.0416153	0.0416152
0.001	0.000001	0.07441	0.0416154	0.0416153

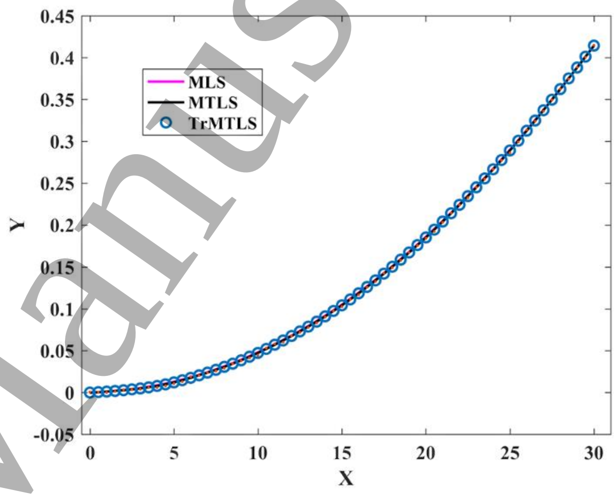


Figure 7. Fitting the curve in Example 1 by MLS, MTLS and TrMTLS method

Example 4.

An experiment was carried out to further illustrate the performance of TrMTLS method. As shown in Figure 8, the coordinate measuring machine is used to measure the profile of a standard cylinder with a radius of 40.1840 mm. The data of profile are obtained by measuring horizontally fixed cylinder surface with a non-contact displacement sensor KEYENCE LK-G150. Let $n = 950$ and $r = (max(x) - min(x) \times 9/1000$ in Example 4. The repetitive positioning error of X-axis is about 15 μm and the repetitive measurement error of the sensor LK-G150 is about 0.5 μm. All three methods are used to fit the measurement data and the circular regression algorithm based on the least square method is applied to obtain the regression radius. The results of MLS, MTLS and TrMTLS are shown in Table 5. As shown in Figure 9, the fitting curve of the proposed method is shown and the second profile is the local enlargement of a section of the fitting curve. Compared with the other two methods, it can be known that the result of the TrMTLS method is closest to the standard cylindrical radius under the same condition. The experimental result verifies the performance of our proposed method.

Table 5.The radius of three methods for Example 4

variance		R(mm)		
δ_i	ε_i	MLS	MTLS	TrMTLS
0.015	0.0005	40.1578	40.1600	40.1653

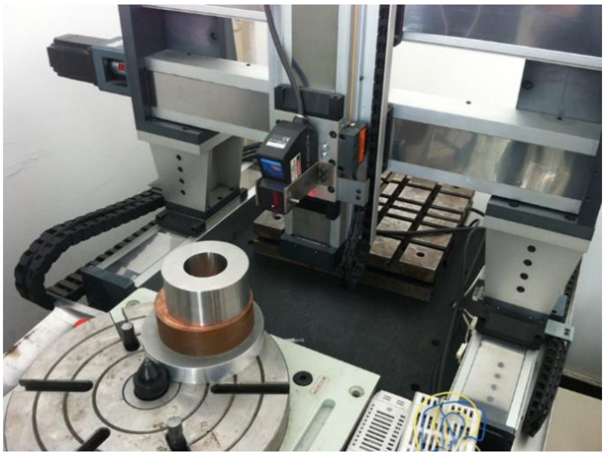


Figure 8. The profile measurement of a standard cylinder by coordinate measuring machine.

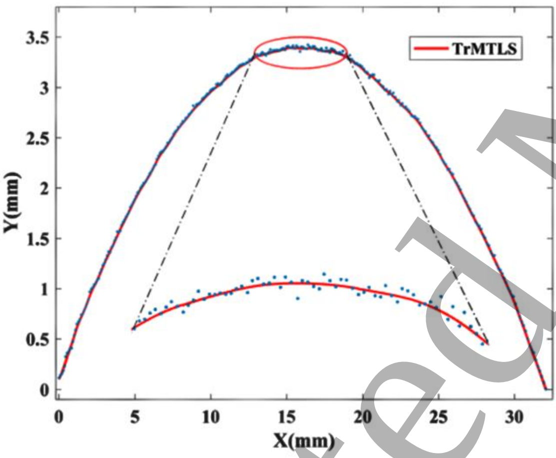


Figure 9. Fitting the profile of standard cylinder in Example 4 by TrMTLS method

As mentioned above, the TrMTLS method can deal with the outliers and the random errors of all variables without setting the threshold or adding small weights subjectively. In all the above examples, TrMTLS method has better fitting accuracy and robustness than the MLS and MTLS method. Most importantly, it is noted that the truncation procedure is employed only once and only one point is trimmed in each influence domain of the TrMTLS method. Although there are multiple outliers in the measurement data, the proposed method can obtain a better result after the truncation procedure is applied in the entire parameter domain independently. Even if there are no outliers, the node with the largest squared residual may be regarded as an outlier. Further research will be carried out to achieve good performance using the TrMTLS method without choosing weight function for trimming the node with the largest squared residual.

5. Conclusions

The advantage of MLS and MTLS method is to obtain the shape function with high order continuity and consistency by employing the basis function with low order and choosing a suitable compact support weight function. They are the popular methods for curve fitting because of their nice approximation properties. However, due to the construction way of the MLS and MTLS method, both of them are sensitive to outliers. To avoid setting the threshold or adding small weights subjectively, an improved curve and surface fitting approach named as TrMTLS method is introduced in this paper. In the influence domain of TrMTLS method, TLS method based on SVD with truncation procedure is adopted for dealing with the outliers and the errors of all variables. To verify the performance of the proposed algorithm, the discrete points generated by numerical simulation and obtained by experimental measurement are fitted by three methods under the same condition. From all the fitting results, it can be seen that the TrMTLS method is more robust and accurate than the MLS and MTLS method, which confirms the validity of the proposed TrMTLS.

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