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# An adaptive moving total least squares method for curve fitting

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ABSTRACT

The moving least squares (MLS) method and the moving total least squares (MTLS) method have been developed to deal with the measured data contaminated with random error. The local approximants of MLS method only take into account the error of dependent variable, whereas MTLS method considers the errors of all the variables, which determines the local approximants in the sense of the total least squares. MTLS method is more reasonable than MLS method for dealing with errors-in-variables (EIV) model. But because of the weight function with compact support, it is complicated to choose fitting method for the best performance. This paper presents an Adaptive Moving Total Least Squares (AMTLS) method for EIV model. In AMTLS method, a parameter $\lambda$ associated with the direction of local approximants is introduced. MLS method and MTLS method can be considered as special cases of AMTLS method. Curve fitting examples are given to prove the better performance of AMTLS method than MLS method and MTLS method.

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## 1. Introduction

The moving least square (MLS) as an approximation method has been introduced by Shepard [1] in the lowest order case and generalized to higher degree by Lancaster and Salkauskas [2]. The object of those works is to provide an alternative to classic interpolation for approximating a function from its values given at irregularly spaced points by using weighted least square approximations. The MLS approximation is an important method to form the shape function in the meshless methods [3]. It is evolved from the ordinary least squares method, and the corresponding meshless method, in which the shape function is obtained with the MLS approximation, can achieve a very precise solution [4,5]. Now wide range of applications can be found in the framework of function approximation and surface construction [6]. The MLS approximation has been largely documented in the literature and used by many scholars for optimization problems. Among them, Breitkopf et al. [7] and Naceur et al. [8] have presented an extended approach of pattern search algorithms with a fixed pattern panned and zoomed in a continuous manner across the design space. More recently, MLS method for the numerical solution has been applied especially in the engineering literatures for the prediction of machined surface quality and directed projecting onto point clouds [9,10].

As a fitting technology, MLS is one way for building the regression model. This method starts with a weighted least squares formulation for an arbitrary fixed point, and then move this point over the entire parameter domain, where a weighted least squares fit is calculated and evaluated for each measured point individually. But MLS method determines the local approximants in the sense of ordinary least squares (OLS). When errors occur in all of the variables, it makes more sense to determine the local approximants in the sense of total least squares (TLS) [11,12], which is called moving total least squares (MTLS) method [13].

MTLS method is a natural generation of the MLS method for dealing with errors-in-variables (EIV) model in which the errors of all the variables are considered. The TLS approach is tightly related to the maximum likelihood principal component analysis method introduced in chemometrics by Wentzell et al. [14]. In Ref. [13], the TLS

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method based on linear approximation is introduced to the local approximants for determining the coefficients. The parameters of the local approximants are obtained by finding the eigenvector, corresponding to the smallest eigenvalue of a certain symmetric matrix.

In this paper, a curve fitting approach called adaptive moving total least squares (AMTLS) method is proposed for EIV model considering the direction of local approximants. In Section 2, a brief description is given for MLS and MTLS method. AMTLS method is presented in detail in Section 3. And curve fitting examples are given in Section 4 for comparing AMTLS method with MLS and MTLS method. Conclusions are drawn in Section 5.

## 2. MLS method and MTLS method

### 2.1. MLS method

In the MLS approximation, the trial function is

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

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

For the local approximation at $x$, a function is defined as

$$J(x) = \sum_{I=1}^{n} w(x - x_I)\left[\sum_{i=1}^{m} p_i(x_I)a_i(x) - y_I\right]^2 \tag{2}$$

where $(x_I, y_I)$, $I = 1, 2,\ldots, n$ is the discrete point to be fitted. And $w(x - x_I)$ is a weight function which defines the influence domain of $x$ and attributes a weight to each discrete point depending on its position relative to $x$. The weight function should be non-zero over only a small neighborhood of $x_I$ to generate a set of sparse discrete equations. It is positive and its value increases with the decrease of the distance $\|x - x_I\|$ between $x$ and $x_I$. Various ways of choosing such functions can be found in the literature [15–17].

In the influence domain of $x$, the ordinary least squares is used for the local approximation. If the basis function $p_i(x)$, $i = 1, 2,\ldots, m$ is linear, Eq. (2) can be re-written as:

$$J(a,b) = \sum_{I=1}^{n} w(x - x_I)(ax_I + b - y_I)^2 \tag{3}$$

The ordinary least squares method only minimizes the weighted sum of squared distances without considering the error of the independent variable as shown in Fig. 1.

### 2.2. MTLS method

Consider the data $(x_i, y_i)$, $i = 1, 2,\ldots, n$ obtained by measurement for the unknown function $y = f(x)$. Scitovski et al. [13] assume that errors occur in all variables, i.e.

$$y_i = f(x_i + \delta_i) + \varepsilon_i, \quad i = 1, 2, \ldots, n \tag{4}$$

where $\varepsilon_i$, $\delta_i$ are normally distributed random variables with the mean value of zero.

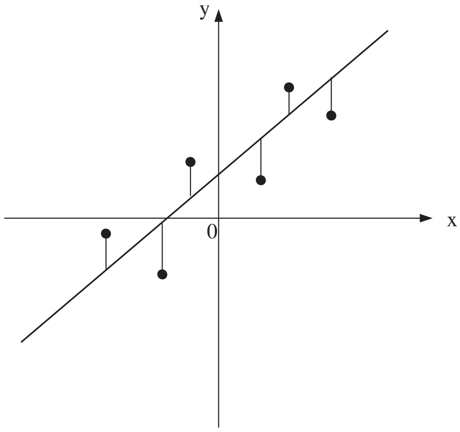


**Fig. 1.** Local approximants of MLS.

When all variables are contaminated, define a function as:

$$J(a,b) = \sum_{I=1}^{n} w(x - x_I)\frac{(ax_I + b - y_I)^2}{a^2 + 1} \tag{5}$$

MTLS method determines the coefficients $a$ and $b$ of Eq. (5) within the influence domain of $x$ in the sense of the total least squares by minimizing the defined function, i.e. by minimizing the weighted sum of squared orthogonal distances as shown in Fig. 2.

## 3. AMTLS method

In this paper, a close attention is paid to the local approximants of MLS and MTLS method. MLS only considers the error of the dependent variable, in which local approximation is carried out in the vertical direction as shown in Fig. 1. MTLS considers the error of all variables at the same time, in which local approximation is carried out in the orthogonal direction as shown in Fig. 2. Generally, MTLS is more reasonable than MLS for dealing

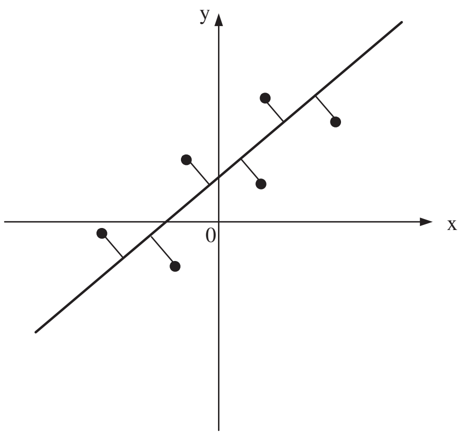


**Fig. 2.** Local approximants of MTLS.

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