A Survey of Data Fitting Based on Moving Least Squares

Lin Shaofu[1,a], Xia Sibin[2,b]

[1]Beijing Institute of Smart City, Beijing University of Technology, Beijing, China

[2]Department of Informatics, Beijing University of Technology, Beijing, China

E-mail: [a]linshaofu@bjut.edu.cn, [b]xsbwork@126.com

Keywords: Data Fitting; Moving Least Squares; Meshless Method.

Abstract: Moving least squares(MLS) is a common method of data fitting, and it has a high degree of flexibility and precision that is significantly better than other fitting methods. This paper introduces the principle of MLS, enumerates the important research progress in recent years at home and abroad, and analyzes the advantages of the method applied in data fitting tasks. MLS also has problems such as susceptibility equations, support domain and weight function selection relying on empirical judgment. The researchers put forward some strategies for the problem, but they have not solved it fundamentally. For the future research direction, this paper suggests that the researchers should study in depth from the mathematical theory, convergence, error analysis and performance comparison of MLS method and its improved methods.

1. Introduction

Whether in engineering or social science research, researchers always encounter mathematical model construction problems based on real data. It is hoped that the mathematical model can be used to extract some features behind the appearance of the image, even the essence of the data that is, fitting the real data to obtain a fitting function that can reflect the characteristics of the data. Generally speaking, the data obtained through measurement, statistics and other methods naturally have certain errors, and the various expression methods have different ability to express the error, which will directly affect the accuracy of the data characteristics reflected by the fitting function[1].

The most common method of data fitting is the least squares(LS) fitting method, which is a meshless method that finds the best function match for the data by minimizing the sum of the squares of the errors. There are some problems in LS fitting method, including the fitting result is too dependent on the establishment of the fitting function, and the ill-posed equation is easy to be generated in the solution [2]. In order to overcome these problems, some scholars have made technical improvements. The moving least squares(MLS) method is one of the improved methods, which has far better fitting flexibility than LS method. MLS is widely supported in data fitting and meshless methods because it has good mathematical theory and inherits the advantages of least squares fitting numerical precision.

2. Principle of MLS

MLS method is mainly divided into a MLS approximation method and a MLS interpolation method. MLS method has two major improvements compared to the least squares method[3]: First, MLS does not use polynomials or other nonlinear functions as fitting functions. The fitting function is composed with a basis function p(x) and a coefficient vector α(x). Where α(x) is a function of the known node x, and different basis functions can be used to obtain different fitting precisions. Secondly, MLS method introduces the concept of compact branching, that is, the value y at the point x is considered to be affected only by the nodes in the subdomain near the point x, which is called the support domain or the influence region of the point x. Supporting nodes outside the domain has no effect on the value of x. nodes which outside the supporting domain has no effect on the value of x. The weight function w(d) is defined on the support domain, indicating the size of the x affected by the nodes in the supported domain. The setting of the weight function and the support domain range during the fitting process will affect the smoothness of the fitted curve or surface. If the weight function is taken as a constant in the entire node region, MLS method degenerates to LS method.

2.1 MLS Approximation

Set the fitting function f(x) of the fitted region to:

$$f(x) = \sum_{i=1}^{m} p_i(x) \cdot a_i(x) = \mathrm{p}^{\mathrm{T}}(x) \cdot \alpha(x) \quad (1)$$

In the above formula, $\mathrm{p}(x)^{\mathrm{T}} = [p_1(x), p_2(x), p_3(x), \dots, p_m(x)]$ is basis function, m is order of the basis function, $\alpha(x) = [a_1(x), a_2(x), a_3(x), \dots, a_m(x)]^T$ is coefficient vector. The coefficient is only related to the coordinates of node x. For the accuracy of the fitting results, we can set different basis functions, such as: For one-dimensional areas:

Linear basis function $\mathrm{p}(x)^{\mathrm{T}} = [1, x]$

Second order basis function $\mathrm{p}(x)^{\mathrm{T}} = [1, x, x^2]$

For two-dimensional areas:

Linear basis function $\mathrm{p}(x)^{\mathrm{T}} = [1, x_1, x_2]$

Second order basis function

$$\mathrm{p}(x)^{\mathrm{T}} = [1, x_1, x_2, {x_1}^2, {x_2}^2, x_1 \cdot x_2]$$

For nodes in the fitted region such as $[x_1, x_2, \dots, x_n]$, calculate the squared term of the error about each true value and the fitted value , and multiply the corresponding weight to obtain the objective function of MLS approximation in the point x support domain:

$$J = \sum_{l=1}^{n} w(x - x_l)[f(x) - y_l]^2 = \sum_{l=1}^{n} w(x - x_l)[\mathrm{p}^{\mathrm{T}}(x) \cdot \alpha(x) - y_l]^2 \quad (2)$$

Where n is the number of nodes in the support domain, x is the node coordinate to be sought, $f(x)$ is the fitting function, y_l is the node value at $x = x_l$, and $w(x - x_l)$ is the weight of node x_l in the current support domain. To find the coefficient α(x), we need to derive the formula (2), namely:

$$\frac{\partial J}{\partial \alpha} = \left(\sum_{l=1}^{n} w(x - x_l)\mathrm{p}(x_l)\mathrm{p}^T(x_l)\right) \cdot \alpha(x) - [w(x - x_1), \dots, w(x - x_n)] \cdot [y_1, y_2, \dots, y_n] \quad (3)$$

Find the minimum value of the derivative function, it can get:

$$\left(\sum_{l=1}^{n} w(x - x_l)\mathrm{p}(x_l)\mathrm{p}^T(x_l)\right) \cdot \alpha(x) - [w(x - x_1), \dots, w(x - x_n)] \cdot [y_1, y_2, \dots, y_n] = 0 \quad (4)$$

$$\alpha(x) = \left(\sum_{l=1}^{n} w(x - x_l)\mathrm{p}(x_l)\mathrm{p}^T(x_l)\right)^{-1} \cdot [w(x - x_1), \dots, w(x - x_n)] \cdot [y_1, y_2, \dots, y_n] \quad (5)$$

Substituting equation (5) into equation (1), the fitted value of the solution node can be obtained.

2.2 MLS Interpolation

Data fitting with interpolation conditions requires that the fit function must pass through some of the nodes for a given discrete data point. The following MLS interpolation fitting method is given in REFERENCE [4]:

Assuming that the interpolation condition is (x_s, y_s),s = {1,2,3, … , t} ⊆ {1,2,3, … , n}, then MLS interpolation fit function is

$$F(x) = f(x) - \sum_{s=1}^{t} k_s(x)\beta_s \quad (6)$$

Where $f(x)$ is MLS approximation fitting function formula (1), $k_s(x) = \prod_{\substack{j=1 \\ s \neq j}}^{t} \frac{(x - x_j)}{(x_s - x_j)}$, $\beta_s = f(x_s) - y_s$.

In fact, this interpolation method is based on the approximation method, and the fitting value of the interpolation point is corrected, so that the fitting value of the interpolation point is the same as the real value. It is found that MLS interpolation method has higher precision than the approximation method. When the interpolation method is applied to form the shape function of the meshless method, the advantage that the preset boundary condition can be directly applied to the fitting process is obtained. However, it is obvious that the interpolation method is more computationally intensive than the approximation method, and it is necessary to evaluate this cost in actual use[5].

2.3 Weight Function

The weight function plays a crucial role in MLS method. The weight function $w(d)$ in MLS method is non-negative, and $w(d)$ is always greater than 0 when the known node is in the support domain, and all outside the support domain is 0. Generally, the circular range is selected as the support domain, and the radius is denoted by r. In the weight function, $d = \frac{||x-x_i||_2}{r}$ is generally set, where x is the coordinate of the point to be determined, and x_i is the coordinates of a known node. $w(d)$ monotonically decreases with the increase of d, and C^1 order is continuous in the support domain.

A commonly used weight function is a spline function, such as a cubic spline function:

$$w(d) = \begin{cases} \frac{2}{3} - 4d^2 + d^3 & d \le \frac{1}{2} \\ \frac{4}{3} - 4d + 4d^2 - \frac{4}{3}d^3 & \frac{1}{2} < d \le 1 \\ 0 & d > 1 \end{cases} \qquad (7)$$

3. Research Status of MLS

In 1981, Lancaster et al. generalized LS method and proposed MLS approximation and MLS interpolation, which were first applied to surface fitting. After years of development, MLS method has extended more and wider research directions and applications, including MLS improved method, MLS method and other meshless methods, and image deformation processing.

For data fitting and meshless methods, MLS method develops more rapidly. Ni Hui et al. proposed a new MLS fitting method with interpolation conditions. This method adds corrections based on the MLS approximation method. Compared with the improvement, the fitting results are better.

Cheng Yumin et al. [6] studied the proposed complex variable MLS method for the two-dimensional data fitting problem. This method reduces the undetermined coefficients in the fitting process, and thus greatly reduces the need for the number of nodes in the tightly supported domain. The utility model has the advantages of less matching points, high precision and fast calculation speed, and is not easy to form an ill-posed equation group. Sun Xinzhi specifically analyzed the approximate error for the complex variable MLS method [7].

Ren Hongping proposed a new method to derive MLS method[8]. This study deduced MLS interpolation method from the perspective of inner product and established an improved MLS interpolation method. The improved formula is simpler than Lancaster's formula and improves computational efficiency.

Yang Jianjun et al. carried out a series of studies, and finally proved that the interpolation precision of MLS normal function is related to the shape of the weight function, the size of the support domain, the form of the basis function and the density of the interpolation points[9]. In addition, the problem of whether the coefficient vector should participate in the derivative operation when MLS method is applied to the meshless method is discussed[10]. The discussion and numerical test are carried out. The conclusion is that the coefficient vector participates in the derivative operation and has no advantage for the solution effect. There are a number of potential problems in the strong meshless method, suggesting that the coefficient vector should not participate in the derivative operation.

Liu Jun[11] used a large number of simulation examples to study the curve and surface fitting and interpolation of MLS method. He calculated the influence of the distribution degree of scatter data, the size of the tight support domain, the selection form of the weight function, the form of the basis function on the accuracy of fitting and interpolation, and the convergence. And some solutions are proposed on how to improve and improve the accuracy of fitting and interpolation near the boundary.

Wei Yifu et al. [12] changed the two norm used in the traditional support domain to the elliptical norm, indirectly increasing the weight of some sample points and expanding the scope of the influence domain, which is more accurate than MLS method.

Fasshauer combines radial basis interpolation and MLS fitting method, and proposes an approximate MLS approximation method[13], and applies this method to the study of partial differential equations. This method not only takes advantage of the radial basis function but also takes into account the advantages of MLS method. After establishing the connection between the two, it is not necessary to solve the linear equations. Later, Fasshauer proposed an iterative method for the method and proved the necessary and sufficient conditions for its convergence.

Wendland takes the thin-plate spline function as an example to analyze the error of the radial basis function in the sobolev space. Using the spherical surface as the template, MLS approximation is obtained [14]. Then Wendland combined the Galerkin method to obtain a meshless method and performed error analysis[15].

In general, in the data fitting application, the development of MLS method is more to improve the accuracy and efficiency of the fitting, and to some extent to compensate for some defects of MLS itself.

4. Advantages of MLS

LS method is the most commonly chosen method for data fitting, and usually uses a polynomial function or a low-order piecewise function to construct a fitting function. When using a polynomial function, increasing the polynomial order appropriately can improve the fitting effect, but the ill-posed equation will appear when fitting, affecting the fitting effect, and even lead to the equation solving failure; when using the low-order piecewise function fitting, first need Set a certain strategy to hardly divide the scatter into several parts, and then use each of the parts to fit LS method. This method avoids the data oscillation that may occur in the polynomial fitting and greatly reduces the risk of the ill-posed equation. However, the continuity and smoothness of the fitted data are affected by segmentation[16].

Compared with LS method, MLS method has the similar localization processing ability as the piecewise function due to the introduction of the concept of compactness. It solves the shortcomings of segmentation, and the data local fitting precision is higher, which ensures the continuity of the fitted data, and the function image is smoother. Meanwhile, the coefficient vector of basis functions and a combination of modes, solve LS method, the selection and combination of various types of experience required basic function dependencies fitting function design, significantly reduce the difficulty of fitting function design. Changing the basis function and weight function can flexibly adjust the data fitting effect. The order of the basis function can affect the fitting precision. Different weight functions can affect the smoothness of the fitted image. The weight function is only related to the calculation point and the nodes in the support domain. When the point is changed, the calculated coefficient vector will also change.

For other improved LS methods, such as weighted LS, the method also uses the concept of weight function, except that the weighted LS weight function range is defined in the entire node space, and the weight and node coordinates There is no functional relationship. For each node to be calculated, it is calculated by the weighted value of all known nodes[17]. When the weight function range of the weighted LS method is reduced to a subfield in the node space, the weight is set to a function related to the node coordinates, that is, MLS method. It can be seen that MLS method is more affected by the nodes in the local area than the weighted LS method, and the reflection of the local data features is more accurate.

Compared with other meshless function forming methods that can be used for data fitting, such as smooth particle method, unit decomposition method, reconstructed kernel particle method and radial basis function method, the values fitted by MLS method Higher precision, this feature is unmatched by other methods[18].

5. Defect of MLS

5.1 Inherent Defect

MLS method achieves a large optimization of the data fitting effect based on LS method, but since it is essentially an improvement of LS method, it also retains the inherent defects of LS method, that is, it is easy to form Morbid or singular equations. The occurrence of this defect is usually related to factors such as too high a base function order, too few nodes in the support domain, and too small a support domain. It can be processed quickly by the basis function reduction and the amplification support domain, but at the same time, partial fitting will be lost. In addition, some studies have adopted the weighted orthogonal function as the basis function[19]. This method avoids the step of finding the inverse of the matrix in the method, and it is not easy to form the ill-posed equations, but the basis function is more complicated, and the problem is not completely solved[20].

5.2 Influence Radius And Weight Function Selection

In MLS method, the influence radius and the weight function have a great influence on the fitting effect. How to choose the appropriate support domain radius and weight function for the fitted data is a difficult problem in actual use. The radius of influence is the radius of the support domain. When the radius r is too small, the matrix generated by the method may be irreversible or even morbid, resulting in inaccurate or even incomprehensible fitting results. When r is too large, there are more nodes in the support domain, and the calculation amount is large. Can not effectively reflect the characteristics. The weight function largely determines the smoothness of the data-fitted image.

The REFERENCE [21] discusses the selection of the influence radius and the weight function, and puts forward some suggestions:

When the order of the basis function is high, in order to ensure that the equations are solvable during the fitting, the support domain needs to contain more linearly independent nodes, that is, a larger influence radius. For the selection of the influence radius, when the nodes are evenly distributed, the radius can be dynamically determined by setting the unit length of the node distribution and the number of base functions and the number of nodes adjacent to the node to be sought.

For the weight function, to ensure that the fitting function is continuous, a smooth continuous function is required. The researchers have proposed a number of expressions of weight functions to choose from, including exponential functions, logarithmic functions, Gaussian functions and spline functions, etc., commonly used as spline functions. The form and order of the weight function are different, and the resulting fitting effect will be different. In general, the higher the order of the weight function of the same kind, the better the fitting accuracy. When the precision is high, the accuracy improvement caused by using higher order weight functions will not be obvious, but the amount of calculation will be larger. Therefore, in actual use, the determination of the order of the weight function requires a trade-off between accuracy and computation.

5.3 Uneven Distribution of Nodes

The data fit validity of MLS method depends on the local nodes. When the nodes are evenly distributed, MLS method can well characterize local features. However, in actual use, there is a situation in which the data distribution is uneven. For such cases, MLS method may not be able to solve the fitting value of the data sparse region under the premise of ensuring high-precision fitting in the dense data region, resulting in a fitted image. There are no value areas such as breakpoints and voids, and abnormally large or very small data is generated in the vicinity of the valueless area, which is inconvenient for data analysis work. At present, there is no targeted solution to this problem, which needs further study.

6. Conclusion

This paper expounds the principle of MLS method, enumerates the improvement of MLS method by researchers at home and abroad in recent years, and summarizes the advantages of MLS method in data fitting application compared with other data fitting methods. The problem with the use of MLS method is explained.

MLS method and its various improvement methods play an important role in data fitting and meshless method research. At present, there are few studies on the mathematical theory, convergence, error analysis and performance comparison of MLS method and its improved methods. In addition, for the problem that the ill-posed equations of MLS method are difficult to solve, the influence radius and the weight function are selected, the solutions proposed by the researchers still have certain limitations, and further research is needed.

References

[1] Xi Shengfeng. "Research and Application of Data Fitting Program." Journal of Zhejiang University of Technology 31.5(2003): 586-590.(in Chinese)

[2] Vogel, Curtis R. . A Constrained Least Squares Regularization Method for Nonlinear III-Posed Problems. Society for Industrial and Applied Mathematics, 1990.

[3] Zeng Qinghong, and Lu Detang. "Flaw and Surface Fitting Based on Moving Least Squares." Journal of Graphics 25.1(2004): 84-89. (in Chinese)

[4] Ni. Hui, Z. Li, and H. Song. "Moving least square curve and surface fitting with interpolation conditions." International Conference on Computer Application & System Modeling 2010.

[5] Liping, Wang , and R. Hongping . "The Comparative Study about Two Kinds of Moving Least Squares Methods in Surface Fitting." Journal of Taiyuan Normal University (2014).

[6] Cheng, Yumin , and J. Li . "A complex variable meshless method for fracture problems." Science in China Series G 49.1(2006):46-59.

[7] Sun Xinzhi. "Analysis of Complex Variable Least Squares Approximate Errors." Journal of Southwest University (Natural Science Edition) 39.2. (in Chinese)

[8] Ren, Hong Ping, Y. M. Cheng, and W. Zhang. "An interpolating boundary element-free method (IBEFM) for elasticity problems." Science China Physics Mechanics & Astronomy 53.4(2010):758-766.

[9] Yang Jianjun, and Zheng Jianlong. "Interpolation accuracy of moving least squares function." Journal of Changsha University of Science and Technology: Natural Science Edition 6.2 (2009): 67-72. (in Chinese)

[10] Yang Jianjun. "Approximation of the Derivatives of Moving Least Squares Method." Computer Aided Engineering 27.1(2018):28-34. (in Chinese)

[11] Liu Jun. Research on surface fitting and interpolation of moving least squares scatter curve. Diss. Zhejiang University, 2011. (in Chinese)

[12] Wei Yifu, KAWAMURA Yasumi, and Wang Dejun. "Improved moving least squares method and its application in structural reliability analysis." Journal of Shanghai Jiaotong University 52.4(2018): 455-460. (in Chinese)

[13] Fasshauer, Gregory E. "Approximate Moving Least-Squares Approximation: A Fast and Accurate Multivariate Approximation Method." Vienna University of Technology (2003):105--116.

[14] Wendland, Holger . "Moving Least Squares Approximation on the Sphere." Vanderbilt University Press (2001):517-526.

[15] Wendland, Holger . "Computational aspects of radial basis function approximation." Studies in Computational Mathematics 12.12(2005):231-256.

[16] J. Ferguson. and P. A. Staley. Least squares piecewise cubic curve fitting. 1973.

[17] Ruppert, D. , and M. P. Wand . "Multivariate Locally Weighted Least Squares Regression." Annals of Statistics 22.3(1994):1346-1370.

[18] Cheng Yumin. "Research Progress and Review of Moving Least Squares." Computer Aided Engineering 18.2(2009): 5-11. (in Chinese)

[19] Chen Meijuan, and Cheng Yumin. "Improved Moving Least Squares Method." Quarterly Mechanics 24.2 (2003): 266-272. (in Chinese)
[20] Li, Xiaolin , H. Chen , and Y. Wang . Error analysis in Sobolev spaces for the improved moving least-square approximation and the improved element-free Galerkin method.. Elsevier Science Inc. 2015.
[21] Ni Hui. Research on Several Problems in Moving Least Squares Data Fitting. Diss. Zhejiang Sci-Tech University, 2011. (in Chinese)