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Review Paper

Moving Least Squares Method and its Improvement: A Concise Review

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Abstract. The concise review systematically summarises the state-of-the-art variants of Moving Least Squares (MLS) method. MLS method is a mathematical tool which could render cogent support in data interpolation, shape construction and formulation of meshfree schemes, particularly due to its flexibility to form complex arithmetic equation. However, the conventional MLS method is suffering to deal with discontinuity of field variables. Varied strategies of overcoming such shortfall are discussed in current work. Although numerous MLS variants were proposed since the introduction of MLS method in numerical/statistical analysis, there is no technical review made on how the methods evolve. The current review is structured according to major strategies on how to improvise MLS method: the modification of weight function, the manipulation of discrete norms, the inclusion of iterative feature for residuals minimising and integration of these strategies for more robust computation. A wide range of advanced MLS variants have been compiled, summarised, and reappraised according to its underlying principle of improvement. In addition, inherent limitation of MLS method and its possible strategy of improvement is discussed too in this article. The current work could render valuable reference to implement and develop advanced MLS schemes, whenever complexity of the specific scientific problems arose.

Keywords: Moving least squares method, Interpolation and optimisation techniques, Shape construction, Meshfree techniques.

1. Introduction

Moving least squares (MLS) method is a mathematical tool proposed by Shepard [1] and Lancaster and Salkauskas [2] to generate surface from a set of scattered data. Since its introduction, MLS has been widely applied in data approximation [3-5], image processing [6-8], and geometry formation [9-12]. The main reason of its robustness in scientific applications could be due to: (i) its deployment of smooth weight function to ensure the continuity of variable fields; (ii) mathematical flexibility to formulate complex arithmetic equation (although polynomial functions are the more popular one); and (iii) its interpolation feature which could be taken as a readily excellent surrogate in many other numerical tools.

Moreover, MLS is one of the most popular approaches to be applied as the guess function in the formulation of finite element method (FEM), and thus evolving FEM to become Diffuse Element Method (DEM) [13]. DEM could be further improvised to form element-free Galerkin [14,15] and meshless local Petrov-Galerkin method [16,17], which are powerful numerical techniques to solve partial differential equations that involve large deformation, such as fracture mechanics, dendritic solidification, and fluid structure interactions. The integration of MLS into other meshfree techniques is extensively reported too, such as in reproducing kernel particle method [18,19], smoothed particle hydrodynamics [20-22], immersed boundary method [23,24], MLS-aided finite element method [25], and local maximum-entropy approximation schemes [26,27].

Nonetheless, MLS may encounter its limitations in some extreme physical problems whenever variable discontinuity might incur, and these include high Peclet number diffusion-convection problem [28] and sharp corner image processing [29,30]. Quite some number of works have been reported on the techniques to improve MLS, yet there is no technical compilation and summary made on these refinements. Therefore, the purpose of the paper is to provide a concise review on the recent available techniques on the improvement MLS for powerful scientific computation.

2. Classical Moving Least Squares Method

Let Ω to be norm vector space while u is the scalar of field variable within Ω . To form an approximation function u^a to relate Ω and u , a succession of polynomial functions P with the associating unknown coefficients α can be used, as shown in Equation (1):

$$u^a = \sum_{j=1}^m P_j(\Omega) \alpha_j = P^T \alpha \quad (1)$$



The discrete norm, J for local approximants can be formed:

$$J = \sum_{i=1}^n W_i R^2 = \sum_{i=1}^n W_i \left[\left(\sum_{j=1}^m P_j(\Omega) \alpha_j \right)_i - u_i \right]^2 \quad (2)$$

where W is the weight function, which will be further described in the next section. R is the residual, which is the discrepancy between the approximated and actual value. The symbol m and n represent the number of guess functions and field variables, respectively. The minimisation of Equation (2) will form a matrix (see Equation (3)), which can be solved to obtain the unknown coefficients.

$$\frac{\partial J}{\partial \mathbf{a}} = 0 \rightarrow \mathbf{A}\mathbf{a} = \mathbf{B} \rightarrow \mathbf{a} = \mathbf{A}^{-1}\mathbf{B} \quad (3)$$

where $\mathbf{A} = \sum_{i=1}^n W_i(\Omega) \mathbf{P}^T(\Omega) \mathbf{P}(\Omega)$ while $\mathbf{B} = \mathbf{P}^T \mathbf{W} \mathbf{u}$.

Note that the matrix size for $\mathbf{A}$ and $\mathbf{B}$ is $m \times m$ and $1 \times m$, respectively. Upon obtaining $\mathbf{a}$, the approximation equation can be formed. The details of the explicit formulation can be found in references such as in the work by Breikopf et al. [31], Liu and Gu [32], Wang [33], and Zhang et al. [34].

3. Manipulation on Weight Function

The weight function (W) can be expressed as a function of the Euclid distance between sampling point ($\mathbf{x}$) and interpolated points ($\mathbf{x}$) within Ω , playing instrumental role in governing the mathematical robustness of MLS [35,36]. The Euclid distance r is normally formed via radial basis function [30,31,37,38]:

$$r = \frac{\|\mathbf{x} - \mathbf{x}_i\|}{h_\Omega} \quad (4)$$

where h_Ω is the size of Ω . However, for problem domain constituted from uneven distribution of nodes, Levin [39] suggested the smoothing of Equation (4) via Equation (5) while Fasshauer [40] complemented Levin's work by proposing various smoothing equations at different approximation order.

$$r = \exp\left(\frac{\|\mathbf{x} - \mathbf{x}_i\|^2}{h_\Omega^2}\right) - 1 \quad (5)$$

Meanwhile the most used equations in the formation of weight function are cubic spline function, quartic spline function, and exponential function, which can be described from Equation (6.1) to Equation (6.3), respectively. These equations will form a symmetrical bell shape.

$$W_i = \begin{cases} 2/3 - 4r_i^2 + 4r_i^3 & r_i \leq 0.5 \\ 4/3 - 4r_i + 4r_i^2 - (4/3)r_i^3 & 0.5 < r_i \leq 1.0 \end{cases} \quad (6.1)$$

$$W_i = 1 - 6r_i^2 + 8r_i^3 - 3r_i^4 \quad (6.2)$$

$$W_i = \exp\left(-\left(\frac{r_i}{\beta}\right)^2\right) \quad (6.3)$$

where β is the shape parameter [32]. Note that W_i is always zero when r is more than 1. To deal with some problem with abrupt change of variable gradient, non-symmetrical W_i can be applied. For instance, Armentano and Durán [41] have proposed the general non-symmetrical equations respectively as in Equation (7):

$$W_i = \begin{cases} \frac{\exp(\chi_1(x_i - \mathbf{x})^2) - \exp(\chi_1)}{1 - \exp(\chi_1)} & -R < x_i - \mathbf{x} < 0 \\ \frac{\exp(\chi_2(x_i - \mathbf{x})^2) - \exp(\chi_2)}{1 - \exp(\chi_2)} & 0 \leq x_i - \mathbf{x} < R \end{cases} \quad (7)$$

where χ_1 and χ_2 are the user-defined integers. Authors would like to refer to the work of Breikopf et al. [31] and Most and Bucher [42] which explains systematically on the formation of non-symmetrical W_i . The mathematical evaluation on the quality of randomly distribution nodes using condition number is discussed too in detail in the work of Zuppa [43].

Li et al. [30] was the first to suggest a doubly weighted weight function ($\hat{W}_i$) for effective simulation and optimisation of structural mechanics, in which the equation has been shown as in Equation (8). More recently, Zheng et al. [44] derived a variation of $\hat{W}_i$ to resolve the outlier of data as shown in Equation (9):

$$\hat{W}_i = W_i \exp(d_i) \quad (8)$$

$$\hat{W}_i = \begin{cases} W_i \left(\frac{1}{1 + \text{core}(r_i)} \right) & , r_i \in \vartheta \\ W_i(1) & , r_i \in \mathbf{x} \setminus \vartheta \end{cases} \quad (9)$$



where

$$\text{core}(r_i) = \sum_{j=1}^{M_i} u_{ij} \left| \frac{\partial \tilde{y}_i^h}{\partial x_i} - \frac{\tilde{y}_i^h - \hat{y}_i^h}{\|\tilde{x}_i - \hat{x}_i\|} \right| \quad (10)$$

In Equation (8), d_i represents the local distance between the nodal coordinates with the most probable failure point; meanwhile in Equation (9), ϑ is the outlier's data set, while the function $\text{core}(r_i)$ is devised to minimise the disturbance of noise to the normal data (see Eq. (10)). $\gamma_i^h = y_i^h - e_i$ (e_i denotes the outlier which could be zero), while u_{ij} is the unit direction vector for $\|\tilde{x}_i - \hat{x}_i\|$. The method will become a conventional MLS if there is no outlier in the data set, i.e. $e_i = 0 \rightarrow \text{core}(r_i) = 0$.

4. Manipulation on Discrete Form

For better removal of outlier and noise in data, the discrete norm as in Equation (2) can be further modified by adding more constraints before the minimisation as in Equation (3). Lei et al. [45] discovered that MLS only considers the total residuals of data without taking the local errors into account, and this will make MLS prone to the errors-in-variables problem. Thus, they modified Equation (2) to become Equation (11) for 1D highly non-linear problem which may involve trigonometric function.

$$J = \sum_{i=1}^n W_i \frac{\lambda^2 \alpha_2^2 + 1}{\alpha_2^2 + 1} (\alpha_1 + \alpha_2 x - \alpha_3)^2 \quad (11)$$

where λ is the user-controlled coefficient, while α_1 , α_2 , and α_3 are MLS coefficients.

Furthermore, for studies which involve irregular node distance, singularity of matrix may happen, and this will disrupt the MLS analysis. Joldes et al. [46] added in more constraints for J as shown in Equation (12) to minimise the probability of encountering matrix singularity:

$$J = \sum_{i=1}^n W_i \left[\left(\sum_{j=1}^m (P_j(\Omega) \alpha_j) \right)_i - u_i \right]^2 + \left(\sum_{j=1}^m (w_j \alpha_j) \right) \quad (12)$$

where w is the additional weight function for computing α . Their works evidenced that the application of Equation (12) in data approximation will result in a lower root mean square error compared with the classical MLS. Joldes et al. [46] also deployed a constant value for w across j and indeed there will be a lot of investigation can be done in the future if the w is varied with α_j . Similar modification effort was reported by Matinfar and Pourabd [47], in which the index of α in the constraint terms as in Equation (12) is upscaled. Although the constraints would grant MLS method with higher ability to solve non-linear integral equation with irregular nodal distributions, it incurs a longer CPU time and computational burden [47]. A more complicated constraints are reported too by Wang et al. [48]. Meanwhile Levin [49] solved the problem by downscaling the index for residual as 1 and replacing the removed residuals with Hardy's multiquadric function as shown in Equation (13). The method is named as moving least- H_d approximation.

$$J = \sum_{i=1}^n W_i H_d R \quad (13)$$

In Equation (13), t is the distance between the nodes, which H_d can be mathematically described as:

$$H_d = \sqrt{t^2 + \lambda^2} \quad (14)$$

The variable gradient can be included as one of the constrain as well, as reported by Liu and Gu [32], Komagodski and Levin [50], and Lee et al. [51]. MLS with a constraint is named as Hermite-type MLS, while its discrete norm can be written as in Equation (15).

$$J = \sum_{i=1}^n W_i \left[\left(\sum_{j=1}^m (P_j(\Omega) \alpha_j) \right)_i - u_i \right]^2 + \sum_{i=1}^n W_i \left[\left(\sum_{j=1}^m \left(\frac{\partial P_j(\Omega)}{\partial \Omega} \alpha_j \right) \right) - \frac{\partial u_i}{\partial \Omega} \right]^2 \quad (15)$$

As the field gradient transpires during computation of Hermite-type MLS, this method is more suitable to be applied in the meshfree techniques, especially during solving partial differential equations with Neumann boundary condition.

5. Iterative Moving Least Squares Method

Another alternative of MLS improvement is enforcing the continuous reduction of residuals via iteration process. One of the iterative MLS method was proposed by Fasshauer and Zhang [52], in which α is continuously updated upon the calculation of residuals, as shown in Equation (16).

$$\begin{aligned} (u^0)^0 &= (P^T \mathbf{a})^0; R^0 = (P^T \mathbf{a})^0 - (u^0)^0 = (P^T \mathbf{a})^{n/2} \\ (P^T \mathbf{a})^n &= (P^T \mathbf{a})^n + (P^T \mathbf{a})^{n/2} \end{aligned} \quad (16)$$

The iterations required for convergence of Equation (16) can be improved when the weight function or discrete norm is carefully examined. The method may not improve the accuracy if the approximated function is not properly selected.

Fleishman et al. [29] also devised the iterative algorithm for MLS, but in a sense of gradual addition of data during the iterative process. Upon the inclusion of new data, the residuals shall remain acceptably small. The hike of residuals during the inclusion implies the existence of outliers, and henceforth the outliers are to be excluded for formation of the incumbent MLS equation. In contrast with the idea of the work of Zheng et al. [53], the outliers' data here will be re-computed to form second equation (or more), and the process will be repeated until all the data is fitted. In other words, the heart of node-addition iterative scheme lies



the principle of forward searching algorithm [54]. Such algorithm would be able to path the way to formulate the piecewise MLS as suggested by Li et al. [55]. Combination of these two schemes could mitigate the problem in forming equations for variables with discontinuity in gradient.

6. Composite Moving Least Squares Method

Composite MLS refers to the MLS schemes built upon the combination of the improvement techniques as discussed in the previous sections. Hybrid of the improvement methods shall be an effective strategy to optimise computational accuracy for complex nodes modelling.

For instance, Gois et al. [9] proffered a weight function equation which may produce a sharp edge and a discrete norm with special constraints to interpolate highly nonlinear fluid interface (i.e. an evolving elliptical shape). Their modification can be expressed mathematically as in Equation (17.1) and Equation (17.2).

$$W_i = \left[1 - \left(\frac{\|x - x_i\|^2}{\gamma \Delta h} \right) \right]^4 \quad (17.1)$$

$$J = \sum_{i=1}^n W_i \left[\left(\sum_{j=1}^m (P_j(\Omega) \alpha_j) \right)_i - u_i \right]^2 + K \sum_{i=1}^n W_i \zeta_i^2 \quad (17.2)$$

in which K and γ is to be defined by users while ζ is the normal for the data curve [9]. It is noteworthy that the work has comprised the transient geometrical change, and therefore it involves iterative MLS.

Trask et al. [56] also administered the similar computational techniques by modifying the weight function and imposing constraints on the discrete norms to model a square with sharp corners. Meanwhile Dabboura et al. [57] improvised the Hermite type MLS by upscaling the derivatives of variables to the order of four with modified weight function to solve generalised Kuramoto-Sivashinsky equation. More recently, augmented MLS method has been proposed by Li and Li [58], Wang et al. [59] and Qu et al. [60], in which the polynomial guess function is replaced with fundamental solution of the underlying differential equations. Although the augmented MLS method could produce a more precise results [58], the method is hindered by the availability and complexity of the fundamental solutions [60].

It is also noteworthy to mention here that interpolating MLS method is also a well-known MLS variant, in which the stiffness matrix of A as in Equation (1) is transformed to appear orthogonal order, and this will greatly enhance the computational speed. Its brief mathematical description can be referred in the work of Tey et al. [61]. Nonetheless, the method is more popular only to be applied as the interpolation functions in finite-element-based numerical schemes as it can effectively pre-empt the singularity issue in solving matrix A and facilitate the imposition of essential boundary condition [62]. The numerical works which employed interpolating MLS have been reported by Shen et al. [3], Ren and Cheng [63], and Wang et al. [64–66], to name a few.

Another related variant is complex variable MLS method, in which the number of coefficients of trial functions are reduced by splitting the guess function into real and imaginary part. The method was proposed by Cheng and Li [67], and its mathematical robustness is improved substantially by Ren and Cheng [68] and Li [69]. Most often, complex variable MLS is blended with interpolating MLS for practical applications, forming improved complex variable MLS (ICVMLS). ICVMLS is also more popular to be applied in the integration with meshfree techniques for various physical simulation such as elastodynamic analysis [70], advection-diffusion problem [71], and wave propagation [72].

Although Composite MLS method is more robust by integrating the strength of those MLS variants, it will generally increase the complexity and computational cost during its implementation [53]. Therefore, Composite MLS might not be the most efficient MLS variant, unless the complexity of the interpolation domain calls up the necessity. The strategies deployed to develop these variants of MLS have been further summarised too as in Figure 1.

7. Inherent Limitation of Moving Least Squares Method and Its Possible Improvement

The major limitation of MLS is its predefined polynomial approximants, which will obstruct the interpolation for discontinued variable gradient. For sharp features, most probably the scalar field should not be in polynomial relationship with the space at the first place. To put the polynomial equation in order, complex manipulations as examined in the previous section are required. Furthermore, during the computation for a multivariable norm vector space, there will be a spike in number of approximants for formation of accurate MLS equation.

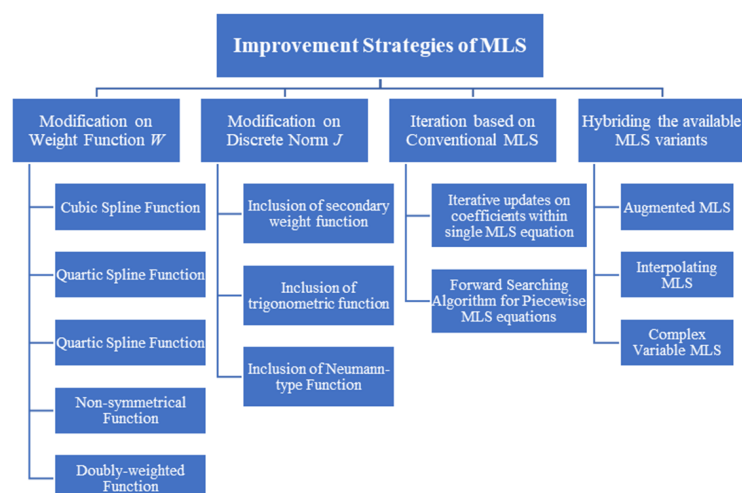


Fig. 1. Summary of strategies in improving MLS method.



To rectify the above issue, the manipulation on the index of the approximants could be a powerful alternative. Tey et al. [73] proposed the Multivariable Power Least Squares Method (MPLSM) which render the possibility to optimise the index of approximants. The method can be further combined with the other MLS improvement methods. The number of approximants can be reduced without sacrificing the accuracy of approximated equations.

Moreover, formulation of reproducing kernel functions (RKF) could be a complementary mathematical tool for MLS method. Instead of taking the least squares operations on the approximated function as shown in Equation (3), the formulation of RKF will take the integration to form continuous polynomials equation(s). The seminal explanation on the mathematical formulation of RKF can be found in the works by Akgül et al. [74], Akgül [75], and Baleanu et al. [76]. MLS and RKF can be combined too to obtain a better prediction accuracy, and this had been reported by Liu et al. [77] and Salehi and Dehghan [78].

In general, the future improvement of MLS method shall not only consider the results accuracy, but also the simplicity of algorithm and compactness of approximated equations. Other possible methods which have the potentials to be blended with MLS methods are partial least squares methods [79,80], principal component regression [81,82], principal covariates regression [83,84], and reduced rank regression [85]. A complete review on these methods can be referred to the work of Kiers and Smilde [86]. Meanwhile, there is no universal or objective “best” MLS variant as the selection of the appropriate variant is highly dependent on the complexity and necessity of the problem domain. There shall be a conciliation between the accuracy and simplicity for efficient interpolation of complex engineering studies such as prediction of solar power [87] and ocean energy [88], optimisation of chemical processes [89,90], and formation of complicated engineering structure [91,92].

8. Concluding Remarks

The current work has revisited the classical MLS and reviewed its improved features made by researchers since its introduction in 1968. The predefined polynomial approximants' function appears to be the inherent limitation for MLS. Besides than the modification of weight function, discrete norms and iterative algorithm, the manipulation on the index of the approximants and integration with other interpolation tools could be the computational alternatives to improve MLS.

Author Contributions

W.Y. Tey initiated the project, conducted the extensive literature review, and drafted the main manuscript text. N.A. Che Sidik and Y. Asako provided technical advice and involved in the scrutiny on the mathematical expressions and discussion. M.W. Muhiedeen and O. Afshar assisted in the enrichment of contents and proofread the manuscript. All authors discussed the results, reviewed, and approved the final version of the manuscript.

Conflict of Interest

The authors declared no potential conflicts of interest with respect to the research, authorship, and publication of this article.

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