Research Report of Intelligent Systems for Medicine Laboratory

Report # ISML/02/2014, May 2014

Modified Moving Least Squares with Polynomial Bases for Scattered Data Approximation

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Abstract

Our overall objective is to develop numerical methods sufficiently robust so that they are effective in the hands of non-specialists, in particular professionals working in the medical and biological fields. One common problem encountered in many fields is the generation of surfaces based on values at irregularly distributed nodes. To tackle such problems, we present a modified, robust Moving Least Squares (MLS) method for scattered data smoothing and approximation. The error functional used in the derivation of the classical MLS approximation is augmented with additional terms based on the coefficients of the polynomial base functions. This allows quadratic polynomial base functions to be used with the same size of the support domain as linear base functions, resulting in better approximation capability. The analysis is supported by several univariate and bivariate examples.

KEYWORDS: Moving Least Squares, random point distribution, scattered data approximation, robust shape function generation

1. INTRODUCTION

Our vision is to enable a surgeon to simulate surgery within the operating theatre in real time, using readily-available computing facilities and to visualize the results immediately. Thus a surgeon would be able to assess the implications of each stage of a surgical procedure, explore possible alternative courses of action or solutions to problems that arise, as events unfold during a complex operation. Achieving this goal requires the creation of an easily-manipulated computational grid, as well as robust, accurate and extremely fast solution methods for the fundamental equations which describe the biomechanical behavior of the subject. The key requirement is that the user – ultimately a surgeon - should not require specialist knowledge in the field of numerical computation, hence the operation of such a system must be robust and reliable, and the results presented to the surgeon must be repeatable, consistent, and within guaranteed bounds of accuracy. A reliable method for interpolating scattered data is required both for visualization and for performing numerical computations (e.g. when using meshless methods [1-5]).

The use of the Moving Least Squares (MLS) method for smoothing and approximating scattered data was proposed by Lancaster and Salkauskas [6]. Since then, due to the smoothness and continuity of the approximation field it generates, the method has been adopted in multiple fields, such as surface definition from points [7], approximation of implicit surfaces [8], animations [9], simulations [2, 10], biomechanics [3, 11], etc.

In most applications a local evaluation of the approximating function is desired, and therefore the compact support domain for each data point (the domain over which the shape function associated with the point is non-zero) is chosen as a sphere or a parallelogram box centered on the point [1, 2, 6]. This simplifies the computing of influence domains for a given point (finding which support domains contain that point). Each data point has an associated dilatation parameter, which characterizes the size of its compact support domain.

Not all node distributions can be used in numerical computations, as shape functions cannot always be computed over the entire problem domain. A valid node distribution is referred to as an “admissible node distribution” [1]. The number of admissible node distributions can be increased by increasing the size of the support domains (the dilatation parameters), but this leads to an increased number of data points inside influence domains, an increased number of shape functions covering a local area, more linearly-dependent shape functions in the local area and increased computational cost.

Higher order polynomial base functions can create better approximations for complex data distributions. Nevertheless, as the degree of the polynomial base function increases, it becomes more difficult to ensure the independence of the shape functions, requiring increased size of the support domains so that more data points are included in the influence domain for each evaluation point.

This paper presents a modified MLS (MMLS) approximation which allows higher order polynomial base functions to be used under the same conditions as lower degree base functions. This is achieved by augmenting the error functional used in the derivation of the MLS shape functions with additional terms based on the coefficients of the polynomial base functions, therefore introducing additional constraints.

The paper is organized as follows: the classical MLS approximation is presented in the next Section; the modified MLS approximation with second order polynomial bases is introduced in Section 3, some properties of the proposed approximation are discussed in Section 4, several univariate and bivariate examples are presented in Section 5, followed by discussion and conclusions in Section 6.

2. THE CLASSICAL MLS APPROXIMATION

We will present the classical MLS approximation with polynomial bases using the notations and derivation procedure from [2]. Given n data points (nodes) located at positions $\mathbf{x}_j$ in $\mathbb{R}^d$, $j = 1 .. n$, we can obtain a function $u^h(\mathbf{x})$ that approximates the given scalar values u_j at points $\mathbf{x}_j$ by minimizing the error functional

$$J(\mathbf{x}) = \sum_{j=1}^{n} [(u^h(\mathbf{x}_j) - u_j)^2 \; w(\|\mathbf{x} - \mathbf{x}_j\|)] \tag{1}$$

where the error between the defined function and the given scalar values is weighted using the positive weight function w based on the Euclidian distances between the evaluation point and the positions of the nodes. We use ||.|| as the notation for Euclidian distance.

The function $u^h(\mathbf{x})$ is chosen as a polynomial

$$u^h(\mathbf{x}) = \sum_{i=1}^{m} p_i(\mathbf{x}) a_i(\mathbf{x}) = \mathbf{p}^T(\mathbf{x})\mathbf{a}(\mathbf{x}) \tag{2}$$

where m is the number of terms in the bases $\mathbf{p}(\mathbf{x})$, and $a_i(\mathbf{x})$ are the coefficients that depend on spatial coordinates $\mathbf{x}$ (due to the weight functions which depend on $\mathbf{x}$). For example, commonly used bases and the corresponding coefficients in 2D are:

- linear bases:

$$\mathbf{p}^T(\mathbf{x}) = [1, x, y], \quad \mathbf{a}^T(\mathbf{x}) = [a_1, a_x, a_y] \tag{3}$$

- quadratic bases:

$$\mathbf{p}^T(\mathbf{x}) = [1, x, y, x^2, xy, y^2], \quad \mathbf{a}^T(\mathbf{x}) = [a_1, a_x, a_y, a_{x^2}, a_{xy}, a_{y^2}] \tag{4}$$

The coefficients $a_i(\mathbf{x})$ are obtained by minimizing the weighted least-square functional $J(\mathbf{x})$ given by (1), which can be rewritten in matrix form as:

$$\mathbf{J = (Pa - u)}^T \mathbf{W(Pa - u)} \tag{5}$$

where

$$\mathbf{u}^T = [u_1, u_2, \cdots u_n] \tag{6}$$

$$\mathbf{P} = \begin{bmatrix} p_1(\mathbf{x}_1) & p_2(\mathbf{x}_1) & \cdots & p_m(\mathbf{x}_1) \\ p_1(\mathbf{x}_2) & p_2(\mathbf{x}_2) & \cdots & p_m(\mathbf{x}_2) \\ \vdots & \vdots & \ddots & \vdots \\ p_1(\mathbf{x}_n) & p_2(\mathbf{x}_n) & \cdots & p_m(\mathbf{x}_n) \end{bmatrix} = \begin{bmatrix} \mathbf{p}(\mathbf{x}_1)^T \\ \mathbf{p}(\mathbf{x}_2)^T \\ \vdots \\ \mathbf{p}(\mathbf{x}_n)^T \end{bmatrix} \tag{7}$$

$$\mathbf{W}=\begin{bmatrix} w(\|\mathbf{x}-\mathbf{x}_1\|) & 0 & \cdots & 0 \\ 0 & w(\|\mathbf{x}-\mathbf{x}_2\|) & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & w(\|\mathbf{x}-\mathbf{x}_n\|) \end{bmatrix} \tag{8}$$

We can minimize (5) by setting the partial derivatives of the error functional **J** to zero:

$$\frac{\partial \mathbf{J}}{\partial \mathbf{a}}=\mathbf{P}^T\mathbf{W}\mathbf{P}\mathbf{a}(\mathbf{x})-\mathbf{P}^T\mathbf{W}\mathbf{u}=0 \tag{9}$$

If the square matrix

$$\mathbf{M}=\mathbf{P}^T\mathbf{W}\mathbf{P} \tag{10}$$

also known as the moment matrix, is non-singular, the values of the coefficients at the evaluation point are obtained as:

$$\mathbf{a}(\mathbf{x})=(\mathbf{P}^T\mathbf{W}\mathbf{P})^{-1}\mathbf{P}^T\mathbf{W}\mathbf{u} \tag{11}$$

The approximation function can therefore be expressed, based on (2), as:

$$u^h(\mathbf{x})=\mathbf{p}^T(\mathbf{P}^T\mathbf{W}\mathbf{P})^{-1}\mathbf{P}^T\mathbf{W}\mathbf{u}=\sum_{j=1}^{n}\phi_j(\mathbf{x})u_j \tag{12}$$

where the shape functions are defined as:

$$\Phi(\mathbf{x})=\begin{bmatrix}\phi_1(\mathbf{x}) & \cdots & \phi_n(\mathbf{x})\end{bmatrix}=\mathbf{p}^T(\mathbf{P}^T\mathbf{W}\mathbf{P})^{-1}\mathbf{P}^T\mathbf{W} \tag{13}$$

It should be noted that the approximation in equation (12) and the shape functions are not polynomials even if the bases $\mathbf{p}(\mathbf{x})$ are polynomials.

The weight function plays important roles in the formulation of MLS approximation: it provide weightings for the residuals at different nodes within the (compact) support domain and it ensures that nodes enter and leave the influence domain smoothly so that the shape functions satisfy the compatibility condition and the approximation is globally continuous.

As shown by (13) the shape functions can be constructed only if the moment matrix (10) is non-singular. The necessary conditions for the moment matrix to be non-singular depend on the bases used. For linear bases, as in (3), the moment matrix is non-singular as long as in the support domain there are at least 3 non-collinear nodes (in 2D).

For the quadratic bases in (4), the conditions for obtaining a non-singular moment matrix are more complex. At least 6 nodes are needed in the support domain (in 2D), but even if more nodes are included, some nodal distributions can still lead to singular moment matrices (for example nodes distributed on two parallel lines).

In order to avoid the nodal configurations which lead to a singular moment matrix, the usual solution is to enlarge the support domains in order to include more nodes. Other methods have been proposed for handling a singular moment matrix, such as perturbation of nodal positions, coordinate transformation, or the matrix triangularization algorithm (MTA) [2]. These methods were developed in the context of the point interpolation method (PIM), and therefore assume that sufficient nodes exist in the support domain; they also do not ensure the smoothness and continuity of the approximation.

3. A MODIFIED MLS APPROXIMATION METHOD FOR SECOND ORDER POLYNOMIAL BASES

The following derivation will be made for bivariate data, but can be easily extended to higher dimensions. A singular moment matrix basically means that equation (9) used to compute the coefficients $\mathbf{a}(\mathbf{x})$ has multiple solutions, and therefore the functional (1) does not include sufficient constraints to guarantee a unique solution for the given node distribution. Based on this observation we propose to add additional constraints in the functional (1) as:

$$\bar{J}(\mathbf{x}) = \sum_{j=1}^{n} [(u^h(\mathbf{x}_j) - u_j)^2 \; w(\|\mathbf{x} - \mathbf{x}_j\|)] + \mu_{x^2} a_{x^2}^2 + \mu_{xy} a_{xy}^2 + \mu_{y^2} a_{y^2}^2 \tag{14}$$

where

$$\boldsymbol{\mu} = [\mu_{x^2}, \mu_{xy}, \mu_{y^2}] \tag{15}$$

is a vector of positive weights for the additional constraints.

The choice of the additional constraints ensures that, when the classical MLS moment matrix is singular (multiple solutions), we favor the solution having the coefficients for the higher order monomials in the bases equal to zero. This has a similar effect with the procedure of bases terms elimination used in the MTA [2]. By choosing the weights for the additional constraints as small positive numbers we can ensure that the classical MLS solution is almost unchanged when the moment matrix is not singular.

The new functional can be rewritten in the matrix form as

$$\bar{\mathbf{J}} = (\mathbf{Pa} - \mathbf{u})^T \mathbf{W}(\mathbf{Pa} - \mathbf{u}) + \mathbf{a}^T \mathbf{Ha} \tag{16}$$

where **H** is a matrix with all elements equal to zero except the last 3 diagonal entries, equal to $\boldsymbol{\mu}$:

$$\mathbf{H} = \begin{bmatrix} \mathbf{O}_{33} & \mathbf{O}_{33} \\ \mathbf{O}_{33} & diag(\boldsymbol{\mu}) \end{bmatrix} \tag{17}$$

Following the same solution method as before, the minimization of the modified functional gives:

$$\frac{\partial \bar{\mathbf{J}}}{\partial \mathbf{a}} = [\mathbf{P}^T \mathbf{WP} + \mathbf{H}]\mathbf{a}(\mathbf{x}) - \mathbf{P}^T \mathbf{Wu} = 0 \tag{18}$$

Therefore, as long as the modified moment matrix

$$\bar{\mathbf{M}} = \mathbf{P}^T \mathbf{WP} + \mathbf{H} = \mathbf{M} + \mathbf{H} \tag{19}$$

is non-singular, the new coefficients can be computed as:

$$\mathbf{a}(\mathbf{x}) = (\mathbf{P}^T \mathbf{WP} + \mathbf{H})^{-1} \mathbf{P}^T \mathbf{Wu} \tag{20}$$

The modified approximant becomes

$$\bar{u}^h(\mathbf{x}) = \mathbf{p}^T (\mathbf{P}^T \mathbf{WP} + \mathbf{H})^{-1} \mathbf{P}^T \mathbf{Wu} = \sum_{j=1}^{n} \bar{\phi}_j(\mathbf{x}) u_j \tag{21}$$

with the new shape functions:

$$\bar{\Phi} = \left[\bar{\phi}_1(\mathbf{x}) \quad \cdots \quad \bar{\phi}_n(\mathbf{x}) \right] = \mathbf{p}^T (\mathbf{P}^T \mathbf{WP} + \mathbf{H})^{-1} \mathbf{P}^T \mathbf{W} \tag{22}$$

4. PROPERTIES OF THE MODIFIED MLS APPROXIMATION

In this section we demonstrate some useful and important properties of the proposed modified MLS.

4.1. Acceptable nodal distribution

We will consider a nodal distribution as acceptable only if the moment matrix is non-singular, allowing the computation of shape functions at any point in the domain.

Lemma 1: A nodal distribution which is acceptable for the classical MLS method with linear bases is also acceptable for the new modified MLS method with quadratic bases.

Proof:

The moment matrix given by (19) can be rewritten as:

$$\bar{\mathbf{M}} = \bar{\mathbf{P}}^T \bar{\mathbf{W}} \bar{\mathbf{P}} \tag{23}$$

with

$$\bar{\mathbf{P}} = \begin{bmatrix} 1 & x_1 & y_1 & x_1^2 & x_1 y_1 & y_1^2 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & x_n & y_n & x_n^2 & x_n y_n & y_n^2 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} \tag{24}$$

and

$$\bar{\mathbf{W}} = \begin{bmatrix} \mathbf{W} & \mathbf{O}_{n3} \\ \mathbf{O}_{3n} & diag(\boldsymbol{\mu}) \end{bmatrix} \tag{25}$$

Equation (23) can be further transformed into:

$$\bar{\mathbf{M}} = \bar{\mathbf{P}}^T \mathbf{Y}^T \mathbf{Y} \bar{\mathbf{P}} = \mathbf{R}^T \mathbf{R} \tag{26}$$

where

$$\mathbf{Y} = sqrt(\mathbf{W}), \quad \mathbf{R} = \mathbf{Y}\bar{\mathbf{P}}\,. \tag{27}$$

Based on the matrix rank properties, because $\mathbf{Y}$ is a diagonal matrix with non-zero (positive) diagonal elements (based on (25), (27), the positive $\mathbf{W}$ and $\boldsymbol{\mu}$):

$$rank(\mathbf{R}) = rank(\bar{\mathbf{P}})\,. \tag{28}$$

From (26):

$$rank(\bar{\mathbf{M}}) = rank(\mathbf{R}^T \mathbf{R}) = rank(\mathbf{R}) \tag{29}$$

and therefore, by combining (28) and (29):

$$rank(\bar{\mathbf{M}}) = rank(\bar{\mathbf{P}})\,. \tag{30}$$

Equation (30) shows that in order for the modified moment matrix to be non-singular, matrix $\bar{\mathbf{P}}$ needs to have full rank (6 in our case). Based on its definition (24), matrix $\bar{\mathbf{P}}$ has full rank only if matrix

$$\mathbf{P}_1 = \begin{bmatrix} 1 & x_1 & y_1 \\ \vdots & \vdots & \vdots \\ 1 & x_n & y_n \end{bmatrix} \tag{31}$$

has full rank. This condition is the same as the condition needed for the classical MLS method with linear bases to have a non-singular moment matrix: the support domain needs to contain at least 3 non-collinear nodes.

This demonstration can be easily extended to 3D, where the moment matrix is non-singular if the support domain contains at least 4 non-coplanar nodes.

These restrictions on nodal distribution are a lot less severe than the restrictions for the classical MLS method with quadratic bases. The shape functions can be computed based on a reduced number of nodes, allowing smaller support domains and increased computational efficiency of the method.

4.2. Continuity of approximation

One of the major advantages of MLS approximation is its compatibility, which means the approximation field function is continuous and smooth in the entire problem domain.

Lemma 2: Let $w^j(\mathbf{x}) = w(\|\mathbf{x} - \mathbf{x}_j\|) \in C^l(\Omega)$ (derivatives up to order l are continuous). If $\boldsymbol{\mu}$ is a constant vector and the moment matrix $\bar{\mathbf{M}}$ is invertible at every point of Ω, then $\bar{u}^h(\mathbf{x}) \in C^l(\Omega)$

Proof:

From Equation (21), the approximation $\bar{u}^h(\mathbf{x})$ on the whole problem domain is a span of all shape functions. Therefore, like for traditional MLS, the smoothness (or the order of continuity) of the approximation equals the smoothness of the shape functions, which is determined by the functions with the minimum order of continuity in (22). Following the assumption that the moment matrix $\mathbf{P}^T\mathbf{W}\mathbf{P} + \mathbf{H}$ is non-singular and since the monomials in the bases have C^∞ continuity, the smoothness of the shape functions is determined by the weight function and the vector $\boldsymbol{\mu}$ (which defines matrix $\mathbf{H}$). As a constant, $\boldsymbol{\mu}$ has C^{∞} continuity, therefore the smoothness of the approximation function is solely determined by the smoothness of the weight functions, similar with the classical MLS approximation.

5. NUMERICAL EXPERIMENTS

The modified MLS (MMLS) method has been implemented in Matlab for 1D and 2D. A quartic weight function with a circular domain was used:

$$w(s) = \begin{cases} 1 - 6s^2 + 8s^3 - 3s^4 & , s \leq 1 \\ 0 & , s > 1 \end{cases} \tag{32}$$

where *s* is the normalized distance

$$s_j = \frac{\left\| \mathbf{x} - \boldsymbol{x}_j \right\|}{R_j} \tag{33}$$

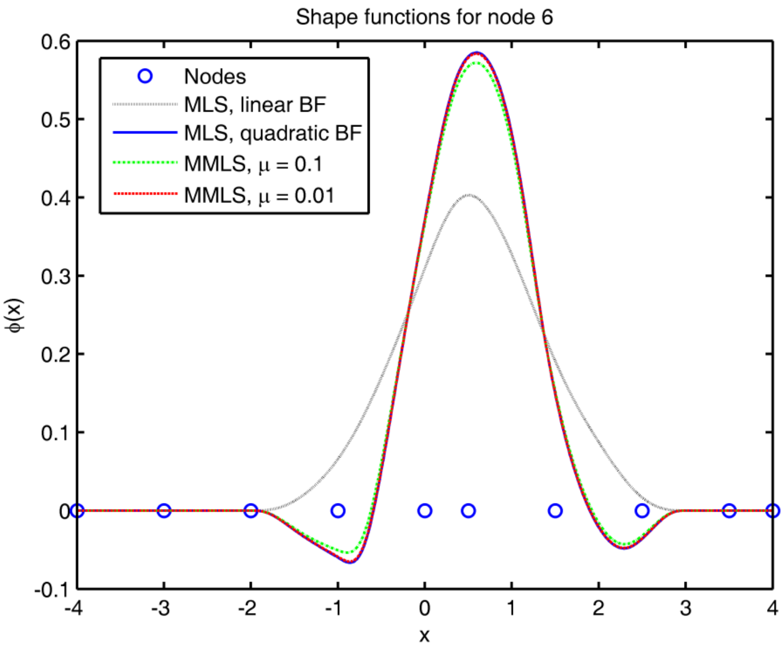
and R_j is the radius of influence domain of node $\mathbf{x}_j$ [2]. For simplicity, in our implementations we used the same weights for all the additional constraints

$$\mu_{x^2} = \mu_{xy} = \mu_{y^2} = \mu \tag{34}$$

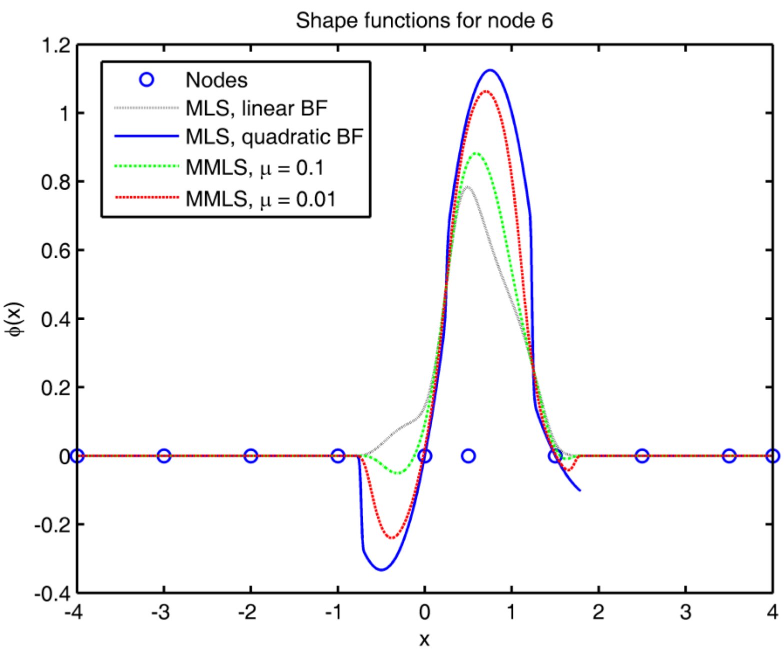
and a constant radius of influence for all nodes $R_j = R$ (as we used nodal distributions with an almost constant density of nodes within the domain).

5.1. MLS and modified MLS (MMLS) shape functions in 1D

A comparison between the MLS and the MMLS shape functions is presented in Figure 1 for different values of μ and *R*. For the radius of influence, the larger value (*R*=2.5) was chosen such that more than 3 nodes are in the support domain of any point in the interval, while the lower value (*R*=1.3) only ensures that 2 nodes are in the support domain of any point in the interval. For small radius of influence *R* the classical MLS with quadratic base functions has singular moment matrix for parts of the domain, while the modified MLS does not have such problem. The value of the weight parameter μ influences the shape functions: the smaller the value, the closer the MMLS shape functions are to those of the classical MLS with quadratic base functions (when these exist).



a)



b)

Figure 1. MLS and MMLS shape functions comparison for node 6. a) R = 2.5. b) R = 1.3; the classical MLS with quadratic base functions (BF) has singular moment matrix for part of the domain.

5.2. Approximation accuracy in 1D

Using the same nodal distribution as in the above example we approximated a non-polynomial function, *u(x)=sin(x)*, using MLS and the MMLS, for different values of μ and *R*. The approximation accuracy was determined using the root mean square error

$$RMSE = \sqrt{\frac{\sum_{i=1}^{N}(u(x) - u^h(x))^2}{N}} \quad (35)$$

computed using N=801 points equally distributed in the interval [-4, 4]. The results are presented in Figure 2 and Table 1.

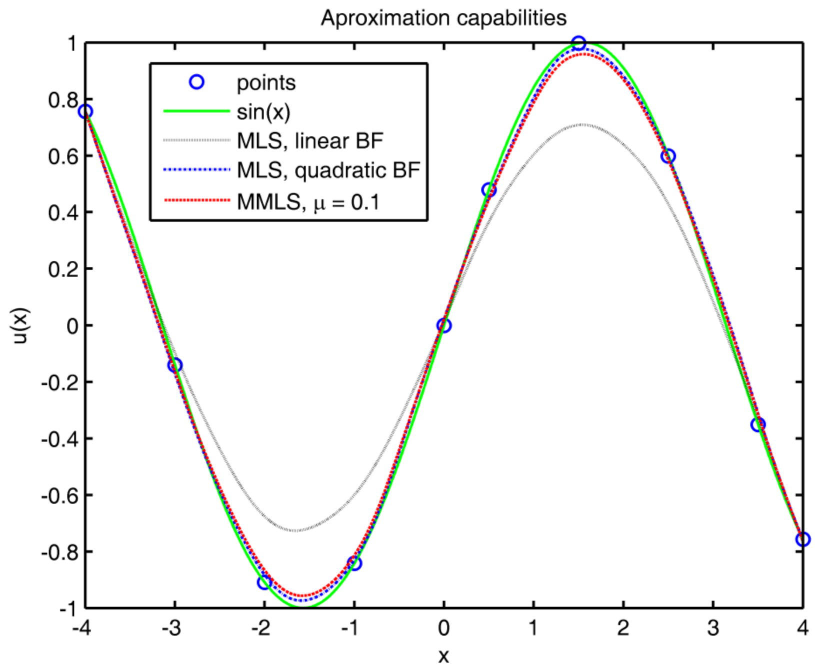


Figure 2. Approximation capability for MLS and MMLS, *R* = 2.5.

Table 1. Root mean square error in approximating *u(x)=sin(x)* using the points presented in Figure 2.

Approximation method	**Radius of nodal influence domain, *R***	
	2.5	**1.3**
MLS, linear BF	0.1765	0.0631
MLS, quadratic BF	0.0297	Singular **M**
MMLS, $\mu = 0.1$	0.0355	0.0545
MMLS, $\mu = 0.01$	0.0301	0.0445

The results show that the approximation accuracy of the MMLS is better than that of the classical MLS with linear base functions, approaching the accuracy of classical MLS with quadratic base functions as the value of parameter μ decreases. Figure 2 clearly shows the advantage of using higher degree base functions in terms of approximation accuracy.

5.3. Approximation accuracy in 2D

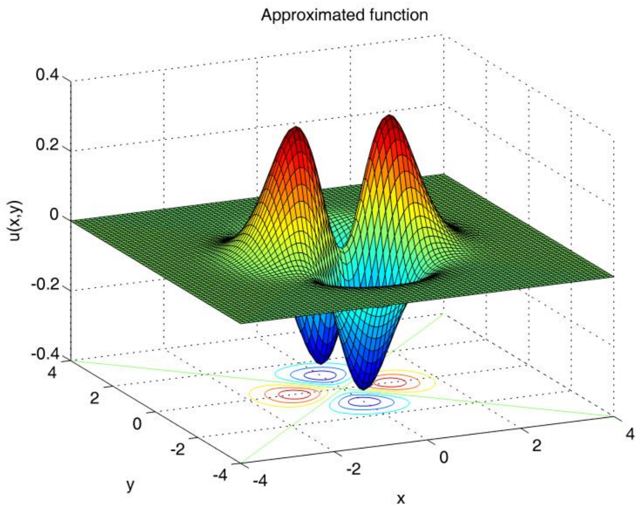
The following function was used for testing the approximation accuracy in 2D:

$$u(x,y) = (x^2 - y^2)e^{-x^2-y^2} \tag{36}$$

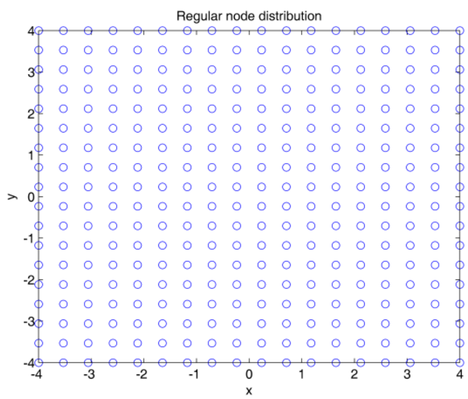
using MLS and the MMLS, for different values of μ and R. The chosen function combines rapid transitions between peaks and dips with almost flat regions over the domain. Both regular and irregular node distributions were used, consisting of 324 nodes, as shown in Figure 3. The RMSE was computed using a regular distribution of N=81*81 points. The results, presented in Table 2, support the conclusions drawn from the univariate results.

Table 2. Root mean square error in approximating $\boldsymbol{u}(\boldsymbol{x},\boldsymbol{y}) = (\boldsymbol{x}^2 - \boldsymbol{y}^2)\boldsymbol{e}^{-x^2-y^2}$ using the nodes presented in Figure 3.

Approximation method	**Regular node distribution**		**Irregular node distribution**	
	Radius of nodal influence domain, *R*			
	1.5	**0.8**	**1.5**	**0.8**
MLS, linear BF	0.0366	0.0136	0.0372	0.0168
MLS, quadratic BF	0.0107	Singular **M**	0.0134	Singular **M**
MMLS, $\mu = 0.1$	0.0158	0.0127	0.0185	0.0162
MMLS, $\mu = 0.001$	0.0108	0.0058	0.0135	0.0091
MMLS, $\mu = 0.0001$	0.0107	0.0053	0.0134	0.0062



a)



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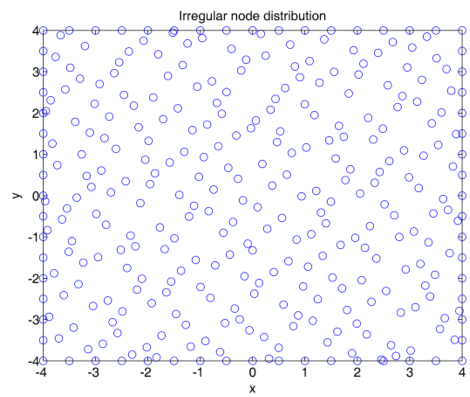

c)

Figure 3. a) Approximated function – eq. (36). b) Regular node distribution. c) Irregular node distribution.

6. DISCUSSION AND CONCLUSSIONS

The modified Moving Least Squares (MMLS) presented in this paper is based on the error functional used in the derivation of the classical MLS approximation augmented with additional terms based on the coefficients of the polynomial base functions. This allows quadratic polynomial base functions to be used with the same size of the support domain as linear base functions, resulting in better approximation capability while maintaining the continuity and smoothness of the approximation.

The numerical examples show that the approximation accuracy of the MMLS is better than that of the classical MLS with linear base functions, approaching the accuracy of classical MLS with quadratic base functions as the value of parameter μ (the weights for the additional constraints) decreases. The important benefit of the proposed method is the ability to provide an approximation for cases when classical MLS with quadratic base functions fails due to a singular moment matrix.

The proposed method has been presented for bivariate functions and quadratic base functions, but can be extended to 3D and higher order polynomial bases.

Acknowledgements: The second author is a recipient of the SIRF scholarship and acknowledges the financial support of the University of Western Australia. The financial support of the Australian Research Council (Discovery Grant No. DP120100402) and the National Health and Medical Research Council (Grant No. APP1063986) is gratefully acknowledged.

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