

The 1-D Hermite Shepard and MLS method

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Abstract: In many applications, one encounters the problem of approximating 1-D curve and 2-D surfaces from data given on a set of scattered points. Meshless methods strategy is based on some facts: (1) deleting mesh generation and re-meshing, (2) raising smooth degree of solution, (3) localization by using compact support weights. This research presented three generalizations for ancient pseudo interpolation, localization, appending a complete polynomial to the Shepard average weighted approximation and Hermite form of Shepard and MLS method. The new bases for relevant space of approximants are developed and, when evaluated directly, improves the accuracy of evaluation of the fitted method, especially the Hermite type. In this work, we develop some efficient schemes for computing global or local approximation curves and surfaces interpolating a given smooth data. Then we raise the smooth degree of approximation and use of derivatives data. The Hermite Shepard (HSH) is straightforward and efficient.

Keywords: Local and global interpolation, Weighted least square, Singular weights, Local and global support, Discrete weighted inner product, Hermite Shepard method.

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1 Introduction

The struggle for interpolating scattered data in a region bring to exist thoughts the methods based on free of knowledge on previous data location. For example, the meteorology station is not on rectangular, triangular, polygon or regular meshes in a country.

To solve differential equations, is one of the meshless methods applications, specially the PDEs which have high gradient region such as: crack propagation, fragmentation, explosion, elasticity. Meshless methods are widespread to model problems with moving boundaries such as crack growth in solids since changing discontinuities can be represented very easily by modifying only the weighting functions, which is a well-known advantage compared to the classical finite element method. The analysis of these methods are complicated by the finite element or finite difference methods and needs complex mesh generation and mesh refining

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techniques and adaptive methods. Mesh generation have high prices if the number of elements are few. The meshless methods try to substitute mesh dependent methods for putting aside mesh difficulties.

The present method, as an alternative of the finite element method (FEM), can be used successfully for solving differential equations and have some advantages, (1) locality of the method, the elements are called: clouds, windows, supports, neighbourhoods, (2) ability to solve problems defined on a complex domain, (3) flexibility by existing various methods such as weighted residuals. In 1967, Backus and Gilbert described techniques for exploring the collection of all earth models which fit given gross earth data [1].

In 1968, Shepard introduced his meshless method, independent of mesh definition and mesh structure. He benefited from a singular inverse square weight and also pointed to the local and compact support form of these weights. At that time, his method have some disadvantages such as degeneration first derivative and “flat spot” property, and his paper did not have good numerical examples [11]. Here we benefit from the “flat spot” property and extend the Shepard method to a Hermite form. Then, in 1974, McLain [7] presented a computer method for drawing contours for some arbitrary collection of points. The method is based on distance weighted least squares approximation technique with the weights varying with the distance of the scattered data points. In 1981, Lancaster developed the Shepard method and presented moving least squares (MLS) methods. They patterned their method from Taylor expansion and used singular weights, irregular distribution data points, a base such as polynomial, variable coefficients, least square method, etc. [6, 9]. In 1992, Nayroles et al. introduced diffuse element and diffuse approximation method (DEM and DAM) that thoughts as a generalization of FEM tried to remove some limitation of the FEM related to the regularity of the solution and evaluating the derivatives of the unknowns. Their method is similar to the one presented by Lancaster [11], but it seems they did their work independent of Lancaster. They also applied their method for solving some differential equations [10, 4]. In 1994, Belytschko et al. improved DEM derivatives and presented a method called the element free Galerkin method (EFG) and benefited their methods in solving some PDEs. [2]. In 2015, Cao proposed a multiscale MLS algorithm, in which the corresponding scale is changing with the associated given point set. They focus on the multiscale MLS approximation scheme on the unit sphere [3]. Finally, in 2006, Komargodski generalized the MLS method to smoother form and Hermite type [5].

In the present research, we try to improve the numerical results of the Shepard method by using local compact support, variable radius weights and generalizing it into Hermite form by defining and using new base functions. Then, we add a linear combination of simple and complete polynomials to the Shepard method and show better approximation and decrease of the error.

The paper is arranged as follows: In Section 2, the Shepard and the MLS method and our Hermite improvement idea are set out. In Section 3, some univariate numerical results are considered to show the ability of the method. We explain some generalization and developments in the concluding remark.

2 Shepard and MLS method

It is assumed that a real function $u: \bar{\Omega} \subset \mathbb{R}^d \rightarrow \mathbb{R}$ is to be approximated, its values $u(\mathbf{x}_i) = u_i$ at the points $\mathbf{x}_i \in \bar{\Omega}$, $i = 0, 1, \dots, N$, are given, and N is the number of interpolation nodes. The domain $\bar{\Omega}$ is assumed to be the closure of a simply connected subset Ω of \mathbb{R}^d . For ease of presentation, we shall first assume a 1-D case; then we will find that the results satisfy any number of variables. We show that global approximation u , is an extension of the function u based on N available information. So, the singular points are introduced into the weight functions employed to ensure the interpolation conditions. The analysis is illustrated with examples of univariate problems, and the graphs are conveyed qualitative information that shows progress in the accuracy of the method. First, let $\hat{\mathbf{x}} \in \Omega$ be an arbitrary and fixed point,

$$w_j(\hat{\mathbf{x}}) = w(\hat{\mathbf{x}}, \mathbf{x}_j) = \|\hat{\mathbf{x}} - \mathbf{x}_j\|^{-k}, \quad k = 1, 2, 3, \dots \quad (1)$$

be a weight, and a singularity is located at j -th point, it is global support, the inverse of any number power, even function, symmetric and a local support form of weight can be prepared. Then the normalized base functions is defined as follows:

$$v_i(\hat{\mathbf{x}}) = \frac{w_i(\hat{\mathbf{x}})}{\sum_{k=1}^n w_k(\hat{\mathbf{x}})}, \quad i = 0, 1, 2, \dots, N \quad (2)$$

The above average weight has some properties as:

- 1) Interpolation property at the points \mathbf{x}_i and at the limiting value $v_i(\mathbf{x}_j) = \delta_{i,j}$ for $i, j = 0, 1, \dots, N$.
- 2) $0 \leq v_i(\mathbf{x}_j) \leq 1$, $i, j = 0, 1, \dots, N$.
- 3) $\sum_{i=0}^N v_i(\mathbf{x}) = 1$, $\forall \mathbf{x} \in \bar{\Omega}$.
- 4) For 1-D case, $\lim_{x \rightarrow \infty} v_i(\mathbf{x}) = \frac{1}{N+1}$, where for a large number of points, the limits degenerate.
- 5) $\nabla v_i(\mathbf{x}_j) = 0$, for $i, j = 0, 1, \dots, N$. This property is a crucial disadvantage and is a barrier to the growing order of approximation.
- 6) $v_i \in C^\infty$, this property shows an infinite smooth approximation, but for the FEM, the higher smooth degree has plenty of computational tasks. However, the pure Shepard method does not have good accuracy.
- 7) v_i is an even function with respect to its center.

Using the above explanation, the Shepard method follows as the average weighted of the f_i

$$Su(\mathbf{x}) = \tilde{u}(\mathbf{x}) = \sum_{i=0}^N u_i v_i(\mathbf{x}), \quad (3)$$

where $Su(\mathbf{x}_i) = u_i$, $u_{min} \leq Su(\mathbf{x}) \leq u_{max}$, $Su'(\mathbf{x}_i) = 0$, $Su \in C^\infty$.

For 2-D problems let, $(x_i, y_j, u_{i,j})$, for $i = 0, 1, \dots, N$, $j = 0, 1, \dots, M$, be the given data, $u_{i,j} = u(x_i, y_j)$,

$$w_{i,j}(x, y) = \frac{1}{\|(x, y) - (x_i, y_j)\|^k}, \quad (4)$$

Then we can define 2-D normalized Shepard base functions

$$v_{i,j}(x, y) = \frac{w_{i,j}(x, y)}{\sum_{i=0}^N \sum_{j=0}^M w_{i,j}(x, y)}, \quad (5)$$

And then, the 2-D Shepard interpolant is defined as follows:

$$\tilde{u}(x, y) = \sum_{i=0}^N \sum_{j=0}^M u_{i,j} v_{i,j}(x, y), \quad (6)$$

In application, we may prefer weights that differ from one introduced before this. When the number of nodes n is significant, it had better delete the role of far nodes by localizing the weights and saving smooth degree of the weights. Therefore, we need weights of the following properties:

- 1) Let support of the weight w_i be a connected and compact set $\bar{\Omega}_i$, $\mathbf{x}_i \in \Omega_i$, $w_i(\mathbf{x}) > 0, \forall \mathbf{x} \in \Omega_i$ and $w_i \in C^\infty(\Omega_i \setminus \{\mathbf{x}_i\})$.
- 2) $\forall \mathbf{x} \in \Omega_i$, there are $k \geq 3$ nodes $\mathbf{x}_j, j = 1, 2, \dots, k$, such that $\mathbf{x} \in \cap_{j=1}^k \Omega_{i_j}$, the value of k is related to the final system and final matrix and must be determined so that the last system has a unique solution.

In most applications, open ball and open interval with a size of the influence radius ρ and center \mathbf{x}_i is gotten as support Ω_i , such as:

$$1) \quad w_\rho(\|\mathbf{x} - \mathbf{x}_j\|) = w\left(\frac{\|\mathbf{x} - \mathbf{x}_j\|}{\rho}\right) = \begin{cases} \frac{\rho^2}{\|\mathbf{x} - \mathbf{x}_j\|^2} & \|\mathbf{x} - \mathbf{x}_j\| \leq \frac{\rho}{3} \\ \frac{9^3}{8^2} \left(\frac{\|\mathbf{x} - \mathbf{x}_j\|}{\rho} - 1\right)^2 & \frac{\rho}{3} \leq \|\mathbf{x} - \mathbf{x}_j\| \leq \rho \\ 0 & \|\mathbf{x} - \mathbf{x}_j\| \geq \rho \end{cases} \quad (7a)$$

$$2) \quad w_\rho(\|\mathbf{x} - \mathbf{x}_j\|) = w\left(\frac{\|\mathbf{x} - \mathbf{x}_j\|}{\rho}\right) = \begin{cases} \frac{\rho}{\|\mathbf{x} - \mathbf{x}_j\|} & \|\mathbf{x} - \mathbf{x}_j\| \leq \frac{\rho}{3} \\ \frac{27}{4} \left(\frac{\|\mathbf{x} - \mathbf{x}_j\|}{\rho} - 1\right)^2 & \frac{\rho}{3} \leq \|\mathbf{x} - \mathbf{x}_j\| \leq \rho \\ 0 & \|\mathbf{x} - \mathbf{x}_j\| \geq \rho \end{cases} \quad (7b)$$

$$3) \quad w_\rho(\|\mathbf{x} - \mathbf{x}_j\|) = \begin{cases} \frac{\rho \cos(\frac{\pi}{2\rho}\|\mathbf{x} - \mathbf{x}_j\|)}{\|\mathbf{x} - \mathbf{x}_j\|} & \|\mathbf{x} - \mathbf{x}_j\| \leq \rho \\ 0 & \|\mathbf{x} - \mathbf{x}_j\| \geq \rho \end{cases} \quad (7c)$$

The moving least square method (MLS), is a generalization of the Shepard method to the higher-order and numerical results show better results. The most part of the accuracy of the Shepard and MLS method is directly related to the weight function (WF) and its radius of support denoted by ρ or dilation parameter. Here during fitting a problem, ρ is constant, but advanced methods and adaptive methods such as h-refinement FEM [8], need the variable size of the WF support. In fact, the WF can be seen as a generalization and reforming of a regular element in FEM.

Let

$$\tilde{u}(x) = \sum_{i=1}^m a_i(x) b^i(x), \quad (8)$$

where $b^i(x) = x^{i-1}$, for $i = 1, 2, \dots, m$, and if $m = 1$, Eq. (8) tend to the Shepard method [11, 6]. Let,

$$J(a_1, a_2, \dots, a_m) = \sum_{k=0}^N w_k(x) (\sum_{j=1}^m a_j(x) b^j(x) - u_k)^2, \quad (9)$$

Minimizing the functional (9) w. r. t variable coefficients $a_i(x)$, tend to the following systems

$$\begin{bmatrix} 1 & \dots & 1 \\ x_0 & \dots & x_N \\ x^{m-1}_0 & \dots & x^{m-1}_N \end{bmatrix} \begin{bmatrix} w_0 & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & w_N \end{bmatrix} \begin{bmatrix} 1 & x_0 & x_0^{m-1} \\ \vdots & \vdots & \vdots \\ 1 & x_N & x_N^{m-1} \end{bmatrix} \begin{bmatrix} a_0(x) \\ \vdots \\ a_N(x) \end{bmatrix} = \begin{bmatrix} 1 & \dots & 1 \\ x_0 & \dots & x_N \\ x^{m-1}_0 & \dots & x^{m-1}_N \end{bmatrix} \begin{bmatrix} w_0 & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & w_N \end{bmatrix} \begin{bmatrix} u_0 \\ \vdots \\ u_N \end{bmatrix}, \quad (10a)$$

$$\mathbf{BW}(x)\mathbf{B}^T \mathbf{a}(x) = \mathbf{BW}(x)\mathbf{U}, \quad (10b)$$

If $\mathbf{A}(x)\mathbf{a}(x) = \mathbf{F}(x)\mathbf{U}$ or $\mathbf{a}(x) = \mathbf{A}^{-1}(x)\mathbf{F}(x)\mathbf{U}$, then the Eq. (8) can be rewritten as

$$\tilde{u}(x) = \sum_{i=1}^m a_i(x) b^i(x) = \{b^1(x), b^2(x), \dots, b^m(x)\} \cdot \mathbf{a}(x) = \{b^1(x), b^2(x), \dots, b^m(x)\} \cdot \mathbf{A}^{-1}(x) \mathbf{F}(x) \mathbf{U}, \quad (11)$$

The Eq. (11) is Lancaster's extension of the Shepard method and is a reformulation of Taylor expansion.

3 Hermite Shepard and mls method

In this study, we present a way of generalizing the method to enable Hermite type interpolation, namely, interpolation or approximation to derivatives data.

In our research, we show a positive effect of radius ρ of WF on the method's accuracy. Then we try to extend the Shepard basis functions by adding some elements of some polynomial basis up to a specified degree, and we see better results. Changing the basis in which the Shepard space is expressed can significantly improve the conditioning of these systems resulting and enhance the accuracy of the solution. The change of basis, locality of WF support, and afterwards using Hermite type basis functions improve the accuracy of evaluation and reduce significance errors. In the Hermite Shepard method, we intelligently change the "flat spot" disadvantage of the pure Shepard [6, 5] into an encouraging property.

If in Eq. (3), we get

$$h_j(x) = v_j(x), \tilde{h}_j(x) = (x - x_j)v_j(x), \quad (12)$$

Based on the Shepard base functions properties denoted in the previous section [11,7,6,1,5], we have the following conditions:

$$h_j(x_i) = \delta_{i,j}, \quad h'_j(x_i) = 0, \quad \tilde{h}_j(x_i) = 0, \quad \tilde{h}'_j(x_i) = \delta_{i,j}, \quad (13)$$

Now, by using the above base functions (12) we can define the 1-D Hermite Shepard approximation

$$\tilde{u}_{HSh}(x) = \sum_{i=0}^N (u_i h_i(x) + u'_i \tilde{h}_i(x)), \quad (14)$$

which is a simple generalization and tricky. We can extend (14) to 2-D and higher-dimensional space.

The generalization of the Hermite method to the MLS can be gotten by using the following minimization functional

$$J(a_1, a_2, \dots, a_m) = \sum_{k=0}^N w_k(x) \{ (\sum_{j=1}^m a_j(x) b^j(x) - u_k)^2 + (\sum_{j=1}^m a_j(x) b^{j'}(x) - u'_k)^2 \}, \quad (15)$$

The above functional is convex and have a unique minimum. If we differentiate J with respect to the coefficients a_i , the following systems attain

$$\frac{\partial J}{\partial a_i} = 0 = 2 \sum_{k=0}^N w_k(x) \{ b^i(x) (\sum_{j=1}^m a_j(x) b^j(x) - u_k) + b^{i'}(x) (\sum_{j=1}^m a_j(x) b^{j'}(x) - u'_k) \}, \quad (16)$$

As another struggle and generalization of Shepard method, let a constant add to the Eq. (3) as the following

$$\tilde{u}(x) = \sum_{i=0}^N c_i v_i(x) + \alpha, \quad (17)$$

These unknown coefficients can be determined directly if the number of supporting points is equal to the number of coefficients. We show that this generalization does not affect the final result!

By collocating (17) on all points we have

$$\tilde{u}(x_j) = u_j = \sum_{i=0}^N c_i v_i(x_j) + \alpha = c_j + \alpha, \text{ for } j = 0, 1, \dots, N, \quad (18)$$

Now, we have $N + 1$ equations and $N + 2$ unknowns and need one more equation. We impose an equation $\sum_{i=0}^N c_i = 0$, (19)

This equation is named as "moment or side condition" which helps complete the linear system and symmetricity of the coefficient matrix. This can be viewed either as taking away the extra degree of freedom created by constant part in (17). Given a set of data values $\{u_j\}_{j=0}^N$ corresponding to the nodes $\{x_j\}_{j=0}^N$, the interpolation problem is to find a function of the form (17) satisfying side condition (19) and the interpolation conditions (18).

Thus, in this case, the standard (pointwise) interpolation problem can be written in the matrix form as

$$\begin{bmatrix} 1 & 0 & \cdots & 0 & 1 \\ 0 & \ddots & & \vdots & 1 \\ \vdots & & \ddots & 0 & \vdots \\ 0 & \cdots & 0 & 1 & 1 \\ 1 & 1 & \cdots & 1 & 0 \end{bmatrix} \begin{bmatrix} c_0 \\ c_1 \\ \vdots \\ c_N \\ \alpha \end{bmatrix} = \begin{bmatrix} u_0 \\ u_1 \\ \vdots \\ u_N \\ 0 \end{bmatrix}, \quad (20)$$

which the primary matrix is symmetric, invertible, non-singular and consequently have a unique solution. It is easy to show

$$\sum_{i=0}^N c_i v_i(x_j) + \alpha = \sum_{i=0}^N u_i v_i(x), \quad (21)$$

and this means that adding a base $\{1\}$ to the base $\{v_i(x)\}_{i=0}^N$ is neutral and don't tend to a better approximation. It is easy to know that the Eqs. (17), (3), (6), (8), (11), (14) all generate, interpolate or reproduce constant function $u = 1$. Then as another struggle, we try to append $\{1, x\}$ to the Shepard basis $\{v_i(x)\}_{i=0}^N$ and try to get a better solution, So let, Eq. (17) change into $\tilde{u}(x) = \sum_{i=1}^n c_i v_i(x) + \alpha + \beta x$, after collocating and appending two-moment conditions $\sum_{i=1}^n c_i = 0$, $\sum_{i=1}^n c_i x_i = 0$. As Eq. (17), this equation also generates and interpolate the function $u = 1$ and $= x$. As it can be seen, the fitting by this method and to solve the linear system is very simple and easy. This new basis and enriching method, lead to a computationally inexpensive method. In the immediate section, we show the ability and capability of the method in the immediate section.

In most cases, the systems occurring in fitting problems are often very ill-conditioned, but we reach a better condition and sparse matrix here to have the Kronecker delta property.

4 Numerical computation and discussions

This section shows the HSH method's applicability and enriches the approximation with some numerical examples.

Example 1:

		Pure Shepard	HSh	$\{1\}$	$\{1, x\}$	$\{1, x, x^2\}$	$\{1, x, x^2, x^3\}$
n	5	0.22658	0.11338	0.22658	0.22458	0.22424	0.2108
	10	0.08806	0.04568	0.088061	0.08642	0.08511	0.082466
	15	0.055601	0.028017	0.055601	0.05463	0.053949	0.052569
	20	0.04098	0.020086	0.04098	0.04038	0.040206	0.039213

Table 1: Error table of approximating the function $u(x) = \sin \pi x e^{-x}$, by Shepard, Hermite Shepard (HSh) method, and the effect of enriching process and adding polynomials on pure Shepard is shown, the weight

function is $w_j(\mathbf{x}) = \frac{1}{(x-x_j)^2}$ which is a global support and singular inverse square weight, it shows that the error column 1 and 3 are equal, this table shows h -refinement is more effective than p -refinement by polynomials i. e error decrease by increasing the nodes, and column table is more effective than rows and increasing the augmented polynomials. This table shows better accuracy of p -refinement and HSh method (14) that tries to raise smooth order of the approximation.

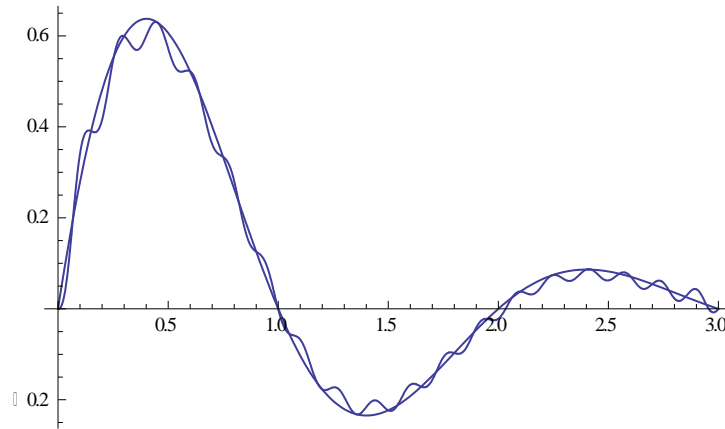


Figure 1-a: The exact function $u(x) = \sin \pi x e^{-x}$ and its approximation, by enriched Shepard method, under conditions: $a = 0, b = 3, n = 20, \sum_{i=1}^n c_i v_i(x) + \sum_{k=0}^3 c_{n+k+1} x^k, w_j(\mathbf{x}) = \frac{1}{(x-x_j)^2}$, which needs improving.

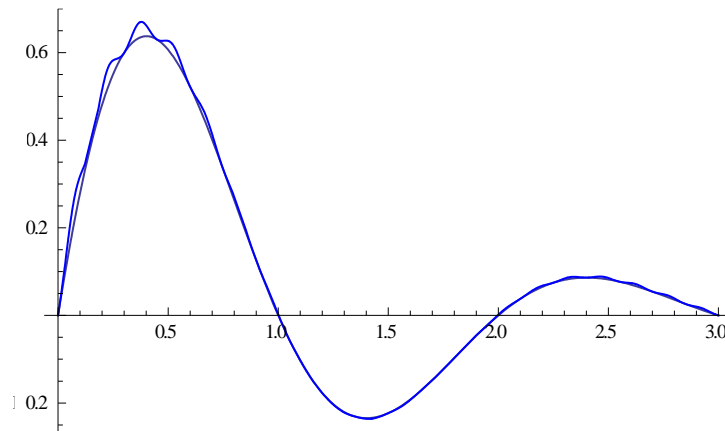


Figure 1-b: The exact function $u(x) = \sin \pi x e^{-x}$ and its approximation, by Hermite Shepard (HSh) method, under conditions: $a = 0, b = 3, n = 20, \sum_{i=1}^n (u_i v_i(x) + u'_i(x - x_j) v_j(x)), w_j(x) = \frac{1}{(x-x_j)^2}$ which is better and higher accuracy than Fig. 1-a.

Example 2:

		Pure Shepard	HSh	{1}	{1, x}	{1, x, x ² }	{1, x, x ² , x ³ }
n	5	0.211316	0.138666	0.211316	0.211596	0.212857	0.196325
	10	0.068418	0.038528	0.068418	0.0687535	0.070834	0.066145
	15	0.039793	0.017512	0.039793	0.040099	0.042043	0.039666
	20	0.028166	0.0099297	0.028166	0.0284342	0.030169	0.0286463

Table 2: Error table of approximating the function $u(x) = \sin \pi x e^{-x}$, by GShM, the effect of the enriching process on pure Shepard is shown, the local, compact and small support singular inverse square weight (7b) is used, the error of column 1 and 2 are equal, $\rho = 1.31 h$, of course, ρ is experimental and is not optimum, Note that in rows 3 and 4, a temporary error grow are seen.

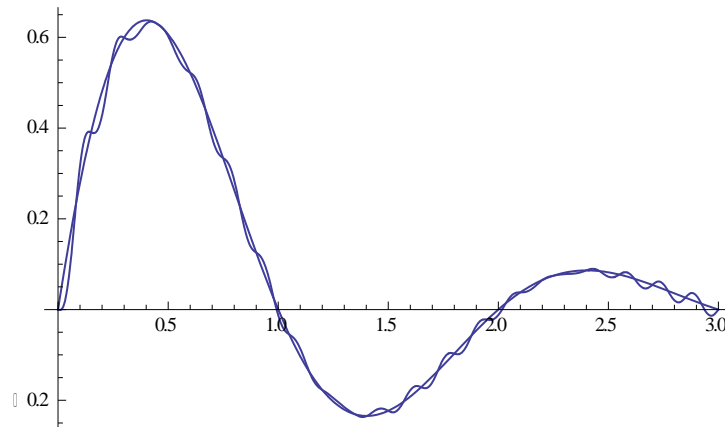


Figure 2-a: The exact function $u(x) = \sin \pi x e^{-x}$ and its approximation, by enriched Shepard method, under conditions: $a = 0, b = 3, n = 20, \sum_{i=1}^n c_i v_i(x) + \sum_{k=0}^3 c_{n+k+1} x^k$, and use of the local compact support WF

(7b), $\rho = 1.01h$ which is better than Fig. 1-a, but needs improving. The parameter 1.01 is experimental and is not optimal.

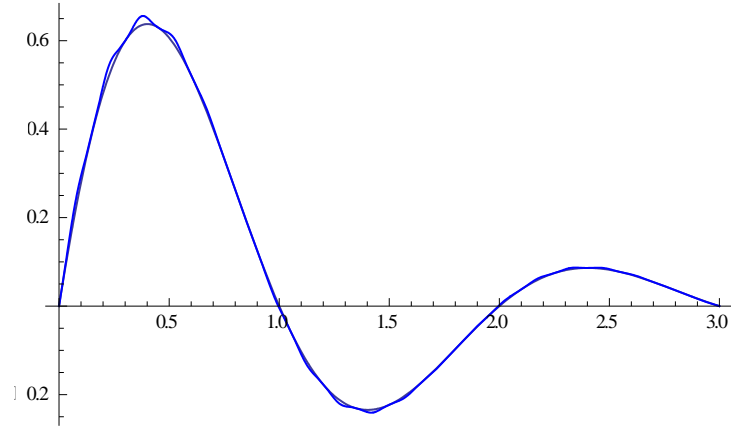


Figure 2-b: The exact function $u(x) = \sin \pi x e^{-x}$ and its approximation, by Hermite Shepard (HSH) method, under conditions: $a = 0$, $b = 3$, $n = 20$, $\sum_{i=1}^n (u_i v_i(x) + u'_i(x - x_j) v_j(x))$, and use of the local compact support WF (7b), $\rho = 1.01h$ which is better and higher accuracy than Fig. 2-a. The parameter 1.01 is experimental and is not optimal.

5 Concluding remarks

The Shepard method is an ancient meshless approximation. It is a particular type and simple form of the MLS method. Our method has been associated with meagre computational cost and simple algorithm. This paper describes Hermite Shepard method (HSH), localization of the WFs and also enrichment polynomial basis approach on Shepard. Experimental results show that this method is enough in computation and complexity algorithms in comparison.

Our method can be generalized to 2-D problems, it can be used for numerical solution to PDEs. Also, we can add polynomials or another linear combination of functions to the HSh.

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