TECHNICAL TRANSACTIONS 8/2017
CZASOPISMO TECHNICZNE 8/2017

MECHANICS

DOI: 10.4467/2353737XCT.17.142.6893

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Hermite interpolation of multivariable function given at scattered points

Interpolacja Hermite'a funkcji wielu zmiennych na nieregularnej siatce

Abstract

The paper shows the approach to the interpolation of scattered data which includes not only function values, but also values of derivatives of the function. To this end, an interpolant composed of radial basis functions is used and extended by terms possessing appropriate derivative terms. The latter match the given derivatives. Special attention is paid to the problem of choosing the value of the shape parameter, which is included in radial functions and influences the accuracy and stability of the solution. To validate the method, several numerical tests are carried out in the paper.

Keywords: scattered data interpolation, Hermite interpolation, radial basis functions

Streszczenie

W artykule przedstawiono podejście do interpolacji danych na nieregularnie rozłożonych węzłach. Dane te zawierają nie tylko wartości funkcji, ale również ich pochodne. Do rozwiązania zagadnienia użyto funkcję interpolacyjną złożoną z radialnych funkcji bazowych, powiększoną o człony zawierające odpowiednie pochodne tych funkcji. Pochodne te odpowiadają zadanym pochodnym. Szczególną uwagę położono na problem wyznaczania współczynnika kształtu w funkcjach radialnych. Współczynnik ten warunkuje dokładność i stabilność rozwiązania. Dla sprawdzenia metody przeprowadzono kilka testów numerycznych.

Słowa kluczowe: interpolacja na nieregularnie rozmieszczonych węzłach, interpolacja Hermite'a, radialne funkcje bazowe

1. Introduction

Interpolation methods play an important role in many areas of science, where there exists the need of a prediction on the basis of discrete data. Interpolating functions are also the main point in derivation of numerical schemas for various methods of solving differential equations. Conventional approximation methods allow to interpolate discrete data given on a regular grid or on structured mesh. Moreover, they enable to easily approximate data in two or three dimensions only. To overcome these drawbacks, the so-called meshfree approaches have appeared in recent years [1–3]. They allow to find an interpolating function for data given at scattered nodes, significantly increasing the possibilities of application of such methods.

Instead of polynomials that have been widely used as the basis functions in the interpolation on a mesh-based grid, a kind of functions which depend on data has been introduced in meshfree approaches. They are called radial basis functions (RBFs) since their values depend on the distance between two points in the space. These points can be easily defined in higher dimensional spaces, which does not change the general approach to the solution of the problem. It is a great advantage of the methods based on RBF, which allows to treat multidimensional problems in the same way as in two or three dimensions. An interesting information on this type of functions can be found in [4, 5].

In the present paper, the interpolation of multivariable discrete function is extended according to Hermite idea. We assume that at a node, not only the function value can be given, but also some derivatives can be known. This formulation differs from others that can be found in literature [1, 6], where it has been assumed that at one node there can exist only one degree of freedom, in the form of function value or its derivative. The approach presented in the paper can be especially useful to derive some meshfree methods for the solution of differential equations possessing multiply boundary conditions [7].

2. Hermite interpolation with RBFs

Let us consider a set of scattered nodes $\mathbf{x}_i \in \mathbb{R}^n, i=1,\dots,N$. At each of these nodes a function value $f(\mathbf{x}_i) = f_i$ is given. Moreover, at some of these nodes $\mathbf{x}_k^D, k=1,\dots,N^D$ there are values of derivatives of the function generally denoted by $(D_k f)(\mathbf{x}_k) = Df_k$, where D_k is a differential operator imposed on the function at kth node. For simplicity of the presentation we assume that there can be one derivative value at one node, although one can easily extend the problem to more than one derivative. To find an approximate value of the function at any point different from the given nodes or to analyze the function by tools available in mathematical analysis, an interpolation series involving RBF is introduced in the following form:

$$u(\mathbf{x}) = \sum_{j=1}^{N} \alpha_j \varphi(\|\mathbf{x}-\xi\|)\Big|_{\xi=\mathbf{x}_j^I} + \sum_{j=1}^{N^d} \beta_j \left[D_j^{\xi} \varphi(\|\mathbf{x}-\xi\|) \right]_{\xi=\mathbf{x}_j^D} \tag{1}$$

where $\varphi(\|\mathbf{x}-\xi\|)$ denotes RBF function, whose value is depended on the distance between an interpolation point $\mathbf{x}$ and a point ξ, called the center. In the paper the centers coincide with nodes $\mathbf{x}_i$. In Eq. (1) α_j, β_j are interpolation coefficients and D_j^{ξ} denotes the differential operator imposed on the function at $\mathbf{x}_j^d$ node. In this case, the function is considered as the function of ξ variable.

In order to determine the interpolation coefficients, the interpolation conditions are applied for the function:

$$\sum_{j=1}^{N}\alpha_j\varphi(\|\mathbf{x}_i-\xi\|)\Big|_{\xi=\mathbf{x}_j}+\sum_{j=1}^{N^D}\beta_j\left[D_j^{\xi}\varphi(\|\mathbf{x}_i-\xi\|)\right]_{\xi=\mathbf{x}_j^D}=f_i,\ i=1,\ldots,N \tag{2}$$

as well as for its derivatives:

$$\sum_{j=1}^{N}\alpha_j\left[D_j^{\mathbf{x}}\varphi(\|\mathbf{x}-\xi\|)\right]_{\substack{\xi=\mathbf{x}_j\\ \mathbf{x}=\mathbf{x}_i^D}}+\sum_{j=1}^{N^D}\beta_j\left[D_j^{\mathbf{x}}\left[D_j^{\xi}\varphi(\|\mathbf{x}-\xi\|)\right]_{\xi=\mathbf{x}_j^D}\right]_{\mathbf{x}=\mathbf{x}_i^D}=Df_i,\ i=1,\ldots,N^D \tag{3}$$

In Eq.(3) $D_j^{\mathbf{x}}$ denotes the same differential operator as D_j^{ξ} but acting on the radial function viewed as a function of $\mathbf{x}$ variable. It makes the coefficient matrix of the system (2)–(3) a symmetric one, which facilitates its assembling and solution of the problem. This system can be written in a more convenient manner using the following matrix notation:

$$\begin{bmatrix}\boldsymbol{\Phi} & \boldsymbol{\Phi}_{D^{\xi}}\\ \boldsymbol{\Phi}_{D^{\mathbf{x}}} & \boldsymbol{\Phi}_{D^{\mathbf{x}}D^{\xi}}\end{bmatrix}\cdot\begin{bmatrix}\boldsymbol{\alpha}\\ \boldsymbol{\beta}\end{bmatrix}=\begin{bmatrix}\mathbf{f}\\ \mathbf{Df}\end{bmatrix} \tag{4}$$

where:

$$\boldsymbol{\Phi}_{ij}=\varphi(\|\mathbf{x}_i-\xi\|)\Big|_{\xi=\mathbf{x}_j},\quad i,j=1,\ldots,N$$

$$\left(\boldsymbol{\Phi}_{D^{\xi}}\right)_{ij}=\left[D^{\xi}\varphi(\|\mathbf{x}_i-\xi\|)\right]_{\xi=\mathbf{x}_j^D},\quad i=1,\ldots,N,\ j=1,\ldots,N^D$$

$$\left(\boldsymbol{\Phi}_{D^{\mathbf{x}}}\right)_{ij}=\left[D^{\mathbf{x}}\varphi(\|\mathbf{x}-\xi\|)\right]_{\substack{\xi=\mathbf{x}_j\\ \mathbf{x}=\mathbf{x}_i^D}},\quad i=1,\ldots,N^D,\ j=1,\ldots,N$$

$$\left(\boldsymbol{\Phi}_{D^{\mathbf{x}}D^{\xi}}\right)_{ij}=\left[D^{\mathbf{x}}\left[D^{\xi}\varphi(\|\mathbf{x}-\xi\|)\right]_{\xi=\mathbf{x}_j^D}\right]_{\mathbf{x}=\mathbf{x}_j^D},\quad i=1,\ldots,N^D,\ j=1,\ldots,N^D$$

$\boldsymbol{\alpha}$, $\boldsymbol{\beta}$ and $\mathbf{f}$, $\mathbf{Df}$ are vectors containing appropriate interpolation coefficients, function values and the derivatives, respectively.

To determine interpolation coefficients, the system (4) has to be solved yielding

$$\begin{bmatrix}\boldsymbol{\alpha}\\ \boldsymbol{\beta}\end{bmatrix}=\begin{bmatrix}\boldsymbol{\Phi} & \boldsymbol{\Phi}_{D^{\xi}}\\ \boldsymbol{\Phi}_{D^{\mathbf{x}}} & \boldsymbol{\Phi}_{D^{\mathbf{x}}D^{\xi}}\end{bmatrix}^{-1}\cdot\begin{bmatrix}\mathbf{f}\\ \mathbf{Df}\end{bmatrix} \tag{5}$$

The problem of solvability of the system depends on the type of RBF used and it is not studied in detail in the paper. In some cases, the interpolant (1) should be augmented by a polynomial term to ensure the inversion of the system matrix. Some notes on this issue can be found in [1]. For problems analyzed in the paper the system (5) has had unique solutions.

2.1. Accuracy and conditioning of the problem

The most popular RBFs, listed in Table 1, contain shape parameter c. The shape parameter has a significant influence on accuracy. A larger value of this parameter should theoretically make the solution more accurate but leads to an ill-conditioned system, which may not be accurately solved. Therefore, the choice of the appropriate value of c is an important issue in using RBF based methods.

Table 1. Examples of radial basis functions

Name	RBF
Multiquadric	$(r^2+c^2)^{1/2}$, $c \geq 0$
Inverse multiquadric	$(r^2+c^2)^{-1/2}$, $c > 0$
Gaussian	e^{-r^2/c^2}, $c>0$

So far there is no general approach to this end and this value is assumed mostly on the basis of numerical experiments or researchers' experience [1]. Recently, in [8] an algorithm based on a heuristic kind has been proposed, which relates accuracy to condition number of the system of equations and number of significant digits assumed for the computation. It enables to automate the choice of the value of shape parameter. The algorithm searches for the largest value of c, which makes the exponent of the condition number of the interpolation matrix close to the number of significant digits but does not exceed this number. In the case of RBF, it ensures acceptable accuracy and stable solution of Eq. (4). The main condition, which the algorithm is based on, is as follows:

$$\log 10\ \kappa(\overline{\Phi}) \in [r_l, r_u] \Rightarrow c^* \tag{6}$$

where $\kappa(\overline{\Phi})$ denotes the condition number of the system matrix from Eq. (4) and r_l and r_u are lower and upper bound of a range associated with the number of significant digits. Usually r_u is 16, when one operates double precision and r_l is a little less. Note that $\kappa(\overline{\Phi})$ depends on the value of c. Defining a loop, where the value of c is increased or decreased to fulfil Eq. (6) one can determine the quasi optimal value of shape parameter c^*.

3. Numerical experiments

To validate the method, several numerical experiments have been carried out. Below there are examples of two-variable test functions used in these experiments:

$$f_1(x_1,x_2) = \sin(4x_1)\cdot\cos(5x_2) \tag{7}$$

$$f_2(x_1,x_2)=\frac{3}{4}e^{-1/4\left((9x_1-2)^2+(9x_2-2)^2\right)}+\frac{3}{4}e^{-1/49(9x_1+1)^2-1/10\,(9x_2+1)^2}$$
$$+\frac{3}{4}e^{-1/4\left((9x_1-7)^2+(9x_2-3)^2\right)}-\frac{1}{5}e^{-(9x_1-4)^2-(9x_2-7)^2} \tag{8}$$

To obtain data points, functions (7)–(8) have been discretized with the use of scattered node distributions presented in fig.1

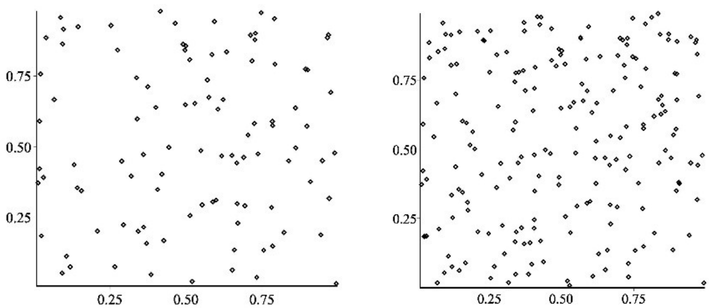

Fig. 1. Scattered node distribution for numerical experiments: $N = 100$ (left), N=200 (right)

At N^D chosen grid points some derivatives of the test functions have been assumed as given data. Accuracy of the approach has been determined by a kind of L_2 error norm in the following form:

$$\delta=\sqrt{\sum_{i=1}^{NN}\left(u_i-f_i\right)^2}\Big/\sqrt{\sum_{i=1}^{NN}\left(f_i\right)^2} \tag{9}$$

where u_i and f_i denote values of the interpolation function and the test one respectively, evaluated at NN regularly distributed points. The obtained results are presented in Tabs. 2 and 3. For comparison, similar results, obtained using classical RBF interpolation (without derivatives) are included in the tables.

Table 2. Results obtained with multiquadrics RBF

		Hermite approach			**classical approach**		
		c^*	$\delta(f_1)$	$\delta(f_2)$	c^*	$\delta(f_1)$	$\delta(f_2)$
$N = 100$	$N^D = 18$	0.60	1.064e-3	3.306e-2	0.70	1.107e-3	5.524e-2
	$N^D = 36$	0.50	1.748e-3	1.328e-2			
$N = 200$	$N^D = 18$	0.40	8.943e-4	4.346e-4	0.45	9.337e-4	1.413e-3
	$N^D = 36$	0.35	9.225e-4	7.095e-4			

Comparing the results of Hermite interpolation with those obtained using classical approach, one can notice that the introduction of information about derivatives in most cases leads to better accuracy of the approximation. It should be taken into account that more information (function and derivative values) increase the dimension of the system matrix from Eq. (4) making this matrix more ill-conditioned. Therefore, the value of the shape parameter has to be smaller to guarantee a stable solution and, finally, the accuracy may not be improved.

Table 3. Results obtained with invers multiquadrics RBF

		Hermite approach			**classical approach**		
		c^*	$\delta(f_1)$	$\delta(f_2)$	c^*	$\delta(f_1)$	$\delta(f_2)$
$N = 100$	$N^D = 18$	0.70	1.040e-3	4.561e-2	0.85	8.022e-4	1.074e-1
	$N^D = 36$	0.65	1.301e-3	4.140e-2			
$N = 200$	$N^D = 18$	0.45	1.443e-3	5.950e-4	0.55	9.002e-4	3.928e-3
	$N^D = 36$	0.45	9.174e-4	7.536e-4			

4. Conclusion

In the paper, the Hermite type interpolation of a function given at scattered nodes has been shown. To this end, an interpolant built with RBFs has been applied. Treating these functions as functions of two vector variables (interpolation point and center), one can obtain symmetric system matrix, which facilitates its assembling and accelerates the solution process. In the paper, special attention is paid to determining appropriate value of the shape parameter included in RBFs. This parameter is determined as a result of a trade-off between accuracy and conditioning of the system of equations following form interpolation conditions. It ensures a stable solution of the problem.

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