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Searching for an optimal shape parameter for solving a partial differential equation with the radial basis functions method

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ABSTRACT

This article presents a procedure for searching for an optimal shape parameter for the solution of partial differential equations with the corresponding initial and boundary conditions, where the solution of the problem is unknown. In recent years, radial basis function methods have emerged as alternative computing methods in the scientific computing community.

The numerical solution of partial differential equations has usually been obtained by using finite difference methods, finite element methods (FEMs), boundary elements methods or finite volume methods. In our case, we use the multiquadric radial basis function, Gershgorin's theorem and the Newton method for searching an optimal shape parameter for solving diffusion equations. More cases are presented, the results of which are compared with the results obtained by the FEM.

1. Introduction

Heat and mass transfer in porous media has practical applications in several different areas, such as water pollution, heat transfer, storage of solar energy, drying and the study of moisture migration in soils and construction materials.

The numerical solution of partial differential equations (PDEs) has usually been obtained either by finite difference methods (FDMs) [1], finite element methods (FEMs), finite volume methods (FVMs), etc. These methods require a mesh to support the localized approximations. In recent years, the numerical methods have focused on a concept stemming from radial basis functions (RBFs).

The concept of solving PDEs using RBFs for hyperbolic, parabolic and elliptic PDEs was introduced in [2]. A key feature of the RBFs method is that it does not require a grid. It has been used for modelling radionuclide migration [3], solving moving boundary problems [12] and for many other problems [4]. A few different meshless boundary discretization techniques have been proposed and developed [5–7], which are different but also related to the method proposed in this paper.

The aim of this paper is to present a procedure for searching for an optimal shape parameter for a solution of the PDEs (in our case the diffusion equation) with the corresponding initial and boundary conditions, for which the solution of the problem is unknown.

For comparison purpose, other strategies for selecting good values of the shape parameter are used, such as the statistical tool leave-one-out cross-validation (LOOCV) [8], the greedy algorithm [9] and singular value decomposition (SVD) [10]. Condition numbers can also be calculated by using SVD. The shape parameter is adjusted until the condition number is in the desired range ($10^{13} \leq \kappa(W) \leq 10^{16}$) for double precision computers.

The commonly used RBFs are: linear, cubic, thin-plate spline, Gaussian, and MQ [11]. In our case, the MQ ($\phi(r) = (r^2 + c^2)^{\beta}$, $\beta = 1/2$) type of the RBFs was used. The parameter c is usually called the shape parameter and is a real number.

Some brief information about the RBFs method will also be presented (see the details in [12]). More cases will be presented to illustrate the usefulness of the method.

2. Solving diffusion equation by the RBFs method

This equation describes temperature (density) fluctuations in a material undergoing diffusion:

$$\frac{\partial T}{\partial t} = \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2}. \tag{1}$$

2.1. Initial conditions

The problem is mathematically completely defined when the initial and boundary conditions are specified. The initial condition is presented by

$$T(x, y, 0) = T_0(x, y). \tag{2}$$

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2.2. Boundary conditions

The boundary condition is presented by Neumann (in our case prescribes the heat flow)

$$\frac{\partial T}{\partial x}e_{nx} + \frac{\partial T}{\partial y}e_{ny} = 0, \tag{3}$$

where e_{nx} and e_{ny} are components of the normal to the boundary surface, and Dirichlet boundary conditions:

$$T(x, y) = 0. \tag{4}$$

2.3. Implicit discrete time marching scheme

To time advance the solution, we consider the implicit discrete time marching scheme. Assuming that both the data and evaluation centers are fixed in time. By defining some matrices and terms for governing PDEs and boundary conditions, the solution of time-advanced expansion coefficients, and, consequently, T^{n+1}, are calculated quickly.

The approximate solution is expressed as below:

$$T\left(\mathbf{x}, t_{n+1}\right) = \sum_{j=1}^{N} \alpha_j^{n+1}\Phi_j(\mathbf{x}), \tag{5}$$

where $\alpha_j^{n+1},\ j = 1, \dots, N$, are the unknown coefficients to be determined and $\Phi_j(\mathbf{x}) = \sqrt{(x - x_j)^2 + (y - y_j)^2 + c^2}$ are Hardy's multiquadric functions [13].

We consider the implicit scheme of Eqs.(1) and (3). By substituting Eq.(5) into Eqs.(1) and (3), we obtain:

$$\sum_{j=1}^{N}\left(\frac{\Phi_j(\mathbf{x}_i)}{\triangle t} - \frac{\partial^2\Phi_j(\mathbf{x}_i)}{\partial x^2} - \frac{\partial^2\Phi_j(\mathbf{x}_i)}{\partial y^2}\right)\alpha_j^{n+1} = \frac{T^n(\mathbf{x}_i)}{\triangle t}, i = 1, \dots, N - N_B, \tag{6}$$

$$\sum_{j=1}^{N}\left(\frac{\partial\Phi_j(\mathbf{x}_i)}{\partial x}e_{nx} + \frac{\partial\Phi_j(\mathbf{x}_i)}{\partial y}e_{ny}\right)\alpha_j^{n+1} = 0,\ i = N - N_B + 1, \dots, N, \tag{7}$$

where N_B and N represent the number of points at boundary and all discretized points and $\triangle t$ is a time discretization step.

The described procedure results in the system of equations

$$\mathbf{W} = \begin{bmatrix} W_L \\ W_B \end{bmatrix}[\alpha] = \begin{bmatrix} f \\ 0 \end{bmatrix}, \tag{8}$$

where

$$W_L = \frac{\Phi_j(\mathbf{x}_i)}{\triangle t} - \frac{\partial^2\Phi_j(\mathbf{x}_i)}{\partial x^2} - \frac{\partial^2\Phi_j(\mathbf{x}_i)}{\partial y^2}, \quad \mathbf{x}_i \in X_I, \tag{9}$$

$$W_B = \frac{\partial\Phi_j(\mathbf{x}_i)}{\partial x}e_{nx} + \frac{\partial\Phi_j(\mathbf{x}_i)}{\partial y}e_{ny}, \quad \mathbf{x}_i \in X_B, \tag{10}$$

$$f = \frac{T^n(\mathbf{x}_i)}{\triangle t}, \quad \mathbf{x}_i \in X_I, \tag{11}$$

3. An optimal shape parameter search

Our goal is to define a new method for searching for an optimal shape parameter using a combination of MQ RBF, Gershgorin's theorem (about eigenvalues of matrix) and the Newton iteration for searching the zero of a function.

The accuracy of the calculated optimal shape parameter method is confirmed by other methods which do or do not possess a shape parameter. For instance, we compare the results with those of the FEM. The objective is to confirm the validity and accuracy of our method with other methods.

In an iteration algorithm, we calculate a matrix, **W**, that is constructed from the MQ functions outside the time loop. This matrix, **W**, is defined as the value of the operator, L, on the MQ basis function over $\Omega\backslash\partial\Omega$ and the boundary operator, B, on the MQ basis function on $\partial\Omega$.

Definition 1. Question is a shape parameter, c. Shape parameter is a parameter that MQ function possess, say Hardy's multiquadric functions [13], $\Phi_j(\mathbf{x}) = \sqrt{(x - x_j)^2 + (y - y_j)^2 + c^2}$.

Now we define an algorithm to find an optimal shape over $\Omega\backslash\partial\Omega$. The algorithm is iterative (step-to-step in a loop). Through this iteration the sequence of eigenvalues of each matrix in sequence converge to the eigenvalues of the limit matrix. The very limit matrix, **W**, is positively defined (it is the limit one and the limit matrix is positively defined because its eigenvalues are all positive). The matrices in iteration sequence posses some additional properties that are valuable in proving the validity of the method. For instance, one of the valuable properties of such a matrix is the fact that its eigenvalues are real and different from each other. The function of a matrix is accurately defined with the matrix's spectrum. Our matrices are similar, and influenced by the shape parameter, c. In addition to the shape parameter, the construction of a matrix, as well as the function above, depends on material and geometric properties of the continuum, as does the solution.

We seek for an optimal shape parameter, where the term 'optimal' means the result of the iteration being optimal in a certain sense.

Definition 2. We define an optimal shape parameter to be the value of the shape parameter that is the closest to the minimal eigenvalue of the limit matrix $\mathbf{W}(c)$. Through iteration the sequence of matrices and sequence of eigenvalues converge to a diagonal matrix and, respectively, eigenvalues converge to limit eigenvalues, which is equal to the eigenvalues of limit matrix. Consequently, the shape parameter is close to the eigenvalue as much as desired.

Theorem 3. *Minimum of diagonal matrix's elements equals the optimal shape parameter.*

Proof. From the above facts we assert, as Gershgorin intervals shrink, eigenvalues are also close to each other. In a matrix sequence the eigenvalues limit to shape parameter, which is also a diagonal element. As intervals shrink, the values outer of diagonal tend to zero. In a limit, therefore, a diagonal matrix is derived. Diagonal parameters are also eigenvalues, their value a simple function of optimal shape parameter.

An alternative definition: an optimal shape parameter could also be the sum of limit eigenvalues. The eigenvalues of the limit matrix (and the limit of the eigenvalues sequence) lie on the main diagonal; since shape parameter, c, is the function of RBF (and not of the differential operator).

Gedankexperimnet 1. We perform a gedankexperimnet to confirm the above reasoning. Take a matrix and use the Gershgorin's theorem about eigenvalues of the square matrix that states how the eigenvalues of the matrix are distributed across the $\mathbb{C}$ plane, and (in our case) along the real, $\mathbb{R}$ axes. This fact enables us to calculate shape parameter through the contemporary experiment. Initialize some shape parameter. We use an iterative algorithm of the functions of matrices and of shapes. Through the iteration the rows of matrix (say 2-norm) decrease as function $F(x)$ is applied to the matrix. We examine Gershgorins intervals. The smallest Gershgorins interval gives us an estimate of how much the smallest (not necessary but plausible) eigenvalue differs from a diagonal element of the matrix (a function of the estimated shape parameter). Such an interval comes from the limit of the sequence. In the limit matrix all eigenvalues lie on the matrix diagonal. Since the matrix is diagonal, the Gershgorins norms all vanish. We iterate the shape-parameter loop