Fast Meshless Methods Using RBF-like Domain and Boundary Interpolation

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Abstract: *The Direct Multi-Elliptic Interpolation Method is investigated. The method converts the interpolation problems to special higher order partial differential equations which are solved by using robust multi-level methods. Both domain and boundary version of the method are outlined. Based on carefully chosen partial differential operators, meshless methods are defined, which exhibit strong similarities to the traditional RBF-methods and the method of fundamental solutions. However, the solution of large, full and ill-conditioned algebraic systems is completely avoided.*

Keywords: radial basis functions, multi-elliptic interpolation, boundary interpolation, meshless methods

1 RBF-methods vs. Direct Multi-Elliptic Interpolation

Though the method of radial basis functions (RBFs) [1] exhibits excellent approximation properties in solving scattered data interpolation problems, it has some unpleasant computational drawbacks. If the applied RBFs are globally supported functions, as it is often the case (multiquadrics, thin plate splines, polyharmonic splines etc.), the method leads to a system of algebraic equations with fully populated and severely ill-conditiond (and often non-selfadjoint) matrix, which can cause numerical difficulties when the number of the interpolation points is high.

In fact, as pointed out by several authors, these numerical disadvantages are not so severe than they seem to be. Domain decomposition techniques can reduce the size of the matrix of the system to be solved and make the problem parallelizable. The computational cost of the matrix-vector multiplications can be reduced by fast multipole evaluation techniques. It is also possible to apply compactly supported RBFs as well, which allows to develop multi-level methods. Our approach differs from these methods. We use the idea of the direct multi-elliptic interpolation [2],

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[3], in which the solution of the interpolation problem is defined as a solution of an auxiliary $2m$-order (multi-elliptic) partial differential equation of the form:

$$Lf = 0 \text{ in } \Omega_0 \setminus \{x_1, x_2, ..., x_N\} \tag{1}$$

(in the sense of distributions) .The interpolation conditions

$$f(x_k) = f_k \quad (k = 1, 2, ..., N) \tag{2}$$

are taken into account as special boundary conditions at the interpolation points. Here $x_1, x_2, ..., x_N \in \mathbf{R}^2$ are the given interpolation points and $f_1, f_2, ..., f_N \in \mathbf{R}$ denote the predefined values attached to the interpolation points. Along $\partial\Omega_0$, any regular e.g. Dirichlet boundary condition can be imposed. Note that the above pointwise conditions do *not* destroy the well-posedness of the partial differential equation (1), if the solution is sought in the Sobolev space $H^m(\Omega_0)$ provided that $m \geq 2$, so that the embedding theorem is valid, which is not the case when L is of second order.

With a properly defined operator L, the direct multi-elliptic interpolation can often be rewritten in a variational form. For instance, if L is the biharmonic operator, $L = \Delta\Delta$, then the corresponding (biharmonic) interpolation function is the function of $H_0^2(\Omega_0)$ which has the minimal norm amongst the functions of $H_0^2(\Omega_0)$ satisfying the interpolation conditions (2) with respect to the norm $||f|| := ||\Delta f||_{L_2(\Omega_0)}$ (note that the above seminorm is a norm in the subspace $H_0^2(\Omega_0)$ and equivalent to the original norm of $H^2(\Omega_0)$). The variational formulation makes it easy to analyze the solvability, uniqueness, approximation etc., see [3].

The approach produces an interpolation function which is a slight modification of the polyharmonic splines when L is an iterated Laplacian. Other choices for L lead to other interpolation methods. In general, RBF-like methods are obtained based on the fundamental solution of the applied operator L, since the solution of (1)-(2) (supplied with a regular e.g. Dirichlet boundary condition along $\partial\Omega_0$) can be represented in the form:

$$f(x) = w(x) + \sum_{j=1}^{N} \beta_j \Phi(x - x_j), \tag{3}$$

where w is a function satisfying Eq. (1) everywhere in Ω_0 and Φ is the fundamental solution of L. It should be pointed out that the computation of the a priori unknown coefficients $\beta_1, \beta_2, ..., \beta_N$ is unnecessary in the majority of practical cases. Instead, it is the interpolation function f that should be determined by solving (1)-(2) or the corresponding variational problem. Once f has been determined, the coefficients of the representation (3) can be computed from the equality

$$Lf = \sum_{j=1}^{N} \beta_j \delta_{x_j}, \tag{4}$$

where δ_{x_j} denotes the Dirac distribution concentrated to the point x_j. That is, if one is insisting on the computation of these coefficients, it can be done directly, without solving any additional large, full system of equations.

An important special case is the following choice: $L := (\Delta - c^2 I)^m$, where I denotes the identity operator, $m \geq 2$ and $c > 0$ is a scaling constant. Now the corresponding fundamental solution is a rapidly decreasing function which can be regarded 'almost compactly supported'. The size of the 'essential' or 'computational' support can be controlled by the factor c.

The main advantage of this approach is twofold. First, the solution and even the generation of large, full (and ill-conditioned) algebraic systems are avoided. Second, the corresponding multi-elliptic equation can be solved by using robust, quadtree/octtree-based multi-level solvers, which significantly reduces the computational cost. Note that the domain Ω_0 of the partial differential equation (1) can be defined in a practically arbitrary way. It can be e.g. a circle or a square: the latter fits especially well the quadtree (QT) context. Both the memory requirement and the computational cost can be estimated typically by $\mathcal{O}(N \log N)$, which is far less than that of the original RBF-methods ($\mathcal{O}(N^2)$ and $\mathcal{O}(N^3)$, respectively).

2 Construction of Meshless Methods

As a model problem, let Ω be a sufficiently regular domain in $\mathbf{R}^2$, and consider the 2D Poisson equation

$$\Delta u = f \tag{5}$$

supplied with some usual (Dirichlet, Neumann or mixed) boundary condition. Suppose that we have M points $(x_1, x_2, ...x_M)$ scattered in the domain Ω and $N - M$ points $(x_{M+1}, x_{M+2}, ..., x_N)$ located on the boundary $\Gamma := \partial\Omega$ without having any special structure. The values of the function f are assumed to be given at the points $x_1, x_2, ...x_M$.

2.1 Construction of Particular Solutions

Utilizing the well-known idea of the method of particular solutions, the first step is to construct such a function U which satisfies (5) without requiring the boundary conditions. This can be done by the following straightforward algorithm.
(a) Let Ω_0 be a square containing the domain Ω, and construct a QT subdivision of Ω_0 based on the points $x_1, x_2, ...x_N$.
(b) Perform a direct multi-elliptic (e.g. biharmonic) interpolation to approximate the function f with an arbitrary regular boundary condition along $\partial\Omega_0$.
(c) At the end of the previous step, the function f is defined at each cell center. Now solve Eq. (5) using the same QT cell system, and this results in the desired particular solution U.

2.2 Construction of Boundary Solutions. BEM vs. Direct Multi-Elliptic Boundary Interpolation

Having obtained a particular solution U, the solution of (5) is expressed as $u = U + v$, where v satisfies the homogeneous equation

$$\Delta v = 0 \tag{6}$$

supplied with a properly modified boundary condition.

The classical tool to solve this problem is the Boundary Element Method. It is well known, however, that one has to face similar computational disadvantages as earlier (large, full systems), and, in order to perform the integrations, a boundary mesh is also needed. To circumvent this, a boundary interpolation technique is applied with a properly chosen partial differential operator L (see [3]). Let

$$L := \Delta(\Delta - c^2 I) \tag{7}$$

which has the fundamental solution $\Phi(x) = -\frac{1}{2\pi c^2}(K_0(cr) + \log cr)$. In other words, the solution of the Laplace equation (6) is approximated by the solution of the (singularly perturbed) fourth order problem:

$$\Delta w - \frac{1}{c^2}\Delta\Delta w = 0 \tag{8}$$

The key issue is to set the scaling constant c in such a way that the size of 'essential support' of the Bessel function appearing in the expression of the fundamental solution of L is in the same order of magnitude than the characteristic distance of the boundary points. This means that Φ becomes (nearly) harmonic far from the origin, i.e. the corresponding boundary interpolation function is (nearly) harmonic outside a narrow vicinity of Γ. It is therefore expected that the boundary interpolation function is a good approximation of the solution of (6).

The implementation of the above boundary interpolation mainly depends on the type of boundary condition.

Dirichlet boundary condition: The values $v(x_k) =: v_k$ $(k = M+1, ..., N)$ are prescribed. Let us apply the same conditions also to the boundary interpolation problem. It turns out that the boundary interpolation function approximates well the solution of (6) provided that the scaling parameter is quasi-optimal. If c is too high, weak singularities are generated at the boundary points and the approximation of boundary condition breaks down. If it is too low, then the approximation of boundary condition is fairly good, but that of the differential equation becomes unsatisfactory. Error estimations can be obtained by the investigation of the equation (7) supplied with the boundary conditions:

$$w|_\Gamma = v|_\Gamma, \quad \frac{\partial w}{\partial n} = \gamma, \tag{9}$$

where the above boundary data are assumed to be sufficiently regular. That is, the Dirichlet data of (6) and (7) are identical. Then the difference of the corresponding solutions can be estimated by

$$||v - w||_{L_2(\Omega)} \leq \frac{const.}{c}(||v||_{H^{1/2}(\Gamma)} + ||\gamma||_{H^{-1/2}(\Gamma)}), \tag{10}$$

i.e. the singularly perturbed solution approximates well the solution of the Laplace equation independently of the Neumann data in (9). A similar estimation holds also with respect to the $H^1(\Omega)$-norm, provided that the boundary data are even more regular.

Neumann boundary condition: Now the values

$$\frac{\partial v}{\partial n}(x_k) =: \delta_k \qquad (k = M+1, ..., N) \tag{11}$$

are prescribed. To correctly approximate this boundary condition in the corresponding boundary interpolation problem, it is expected that a higher order interpolation operator should be used. The straightforward candidate would be $L := \Delta(\Delta - c^2 I)^2$, the fundamental solution of which is again nearly harmonic far from the origin. A surprising negative result is that the corresponding boundary interpolation function fails to approximate the solution of (6), though the approximation of the boundary condition may be very good. To overcome this difficulty, we have borrowed the idea of the method of fundamental solutions [4]. Let us define new, "off-boundary" points $x'_{M+1}, x'_{M+2}, ..., x'_N$ located near the Neumann boundary points $x_{M+1}, x_{M+2}, ..., x_N$ in the outward normal direction. Now define a boundary interpolation function based on these new points with a fourth-order operator defined by (7). Let the interpolation conditions at the points $x'_{M+1}, x'_{M+2}, ..., x'_N$ be of Dirichlet type as follows:

$$v(x'_k) := \alpha_k \qquad (k = M+1, ..., N). \tag{12}$$

The Dirichlet data $\alpha_{M+1}, ..., \alpha_N$ are updated iteratively to enforce the Neumann conditions (11) at the original points $x_{M+1}, ..., x_N$. The simplest strategy is:

$$\alpha_k := v(x_k) + \delta_k \cdot ||x'_k - x_k||. \tag{13}$$

This iteration can be easily incorporated in the multi-level solver of the interpolation problem. Note that the new points $x'_{M+1}, x'_{M+2}, ..., x'_N$ should also be used in the generation of the QT cell system.

The above method mimics the method of fundamental solutions when the locations of the sources are identical to $x'_{M+1}, x'_{M+2}, ..., x'_N$. However, the use of large and full matrices and systems is again avoided. Note also that these strategies can be applied together when a mixed boundary condition is given for Eq. (6) (Dirichlet type on a part of Γ and Neumann type on the remaining part).

3 Further Applications

Biharmonic equations. Now consider the following model problem:

$$\Delta\Delta u = f \qquad u|_\Gamma = u_0, \qquad \frac{\partial u}{\partial n}|_\Gamma = v_0, \tag{14}$$

The idea of the method of particular solutions is again applicable, so that we may assume that the function f is identically zero. Now the solution can be approximated by a boundary interpolation based on the operator $L := \Delta\Delta(\Delta - c^2 I)$, i.e. the solution of the biharmonic equation $\Delta\Delta u = 0$ is approximated by that of the sixth-order equation $\Delta\Delta w - \frac{1}{c^2}\Delta\Delta\Delta w = 0$. Estimations similar to (10) can also be deduced (including also the boundary data of Δw).

Vectorial interpolation. In this type of problems, a vectorial function $\mathbf{v} : \mathbf{R}^2 \to \mathbf{R}^2$ is to be interpolated from pointwise data:

$$\mathbf{v}(x_k) = \mathbf{v}_k \in \mathbf{R}^2 \quad (k = 1, 2, ..., N) \tag{15}$$

In many practical problems, some additional condition is prescribed for $\mathbf{v}$, e.g. rot $\mathbf{v} = 0$ (or div $\mathbf{v} = 0$). Using the potential function (or the stream function, respectively), the interpolation conditions (15) can be reformulated as

$$\text{grad } \phi(x_k) = \mathbf{v}_k \quad (k = 1, 2, ..., N). \tag{16}$$

To construct a multi-elliptic interpolation, the corresponding multi-elliptic operator should be at least of sixth order (according to the fact that the interpolation function is now sought in $H^3(\Omega_0)$). The most natural choice is $L := (\Delta - c^2 I)^3$ with $c \geq 0$.

4 Conclusions

The Direct Multi-Elliptic Interpolation converts the original interpolation problem to an auxiliary multi-elliptic partial differential equation that can - and should - be solved by robust quadtree-based multi-level methods. The resulting interpolation function can be represented in an RBF-like form based on the fundamental solution of the applied partial differential operator. The approach is suitable to define both domain and boundary type truly meshless methods but no large and dense algebraic systems have to be solved.

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