Using compactly supported radial basis functions to solve partial differential equations

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Abstract

When applied to solving partial differential equations by either Rayleigh–Ritz or collocation techniques, compactly supported radial basis functions may replace other meshless tools like multiquadrics. They generate sparse and well–conditioned matrices, and we give a survey over the current theoretical results known in this area, as far as they seem to be relevant for boundary element techniques.

1 Introduction

As special instances of meshless methods [1], applications of radial basis functions (RBF) have gained quite some importance over the past years. They have been successfully applied to a large variety of problems [1-7, 17-21, 23-28, 32-34, 39, 45, 55, 61, 66-68], especially as tools for collocation [32, 33] and the Dual Reciprocity Method (DRM) [3, 4, 5, 18, 20, 30, 31, 40, 41]. Unfortunately, the mathematical theory of RBF [35-38] lagged back behind the numerical applications to PDE for quite some time, but recently there was some progress [15, 59] towards a solid underpinning of numerical algorithms using RBF's for solving PDE's. We shall provide a short account of such results.

Furthermore, the construction of compactly supported radial basis functions (CSRBF) by Wendland, Wu and Schaback [46, 56, 62] based on a toolkit by Wu and Schaback [53] made it possible to overcome the non–sparsity of the matrices arising from radial basis function techniques. But

[1]Partially supported by the DFG

the proper choice of the support radius and the smoothness of such functions seems to require some skill and experience on the user's side. We shall provide some guidelines based on numerical experiments.

2 Radial basis functions

A scalar function $\phi : \mathbb{R}_{\geq 0} \to \mathbb{R}$ may be used as a radial basis function (RBF) by forming a space

$$S_X := \text{ span } \{\phi(\|\cdot - x_j\|_2) \ : \ 1 \leq j \leq M\} \tag{1}$$

for each finite set $X := \left\{x_j \in \mathbb{R}^d : 1 \leq j \leq M\right\}$ of scattered "centers". The advantage is that a simple univariate function serves to create a space of multivariate functions, and that the space can be controlled directly by centers, without any triangulation. It is easy to implement numerical algorithms acting on such spaces, and if ϕ is compactly supported or decays quickly towards infinity, the basis functions $\phi(\|\cdot - x_j\|_2)$ for distant centers are only weakly coupled.

A space like S_X can serve for collocation, numerical integration or Rayleigh–Ritz techniques, because it can be seen as a discretization of the space in which the actual solution lies. We shall explain this in the next section. Some RBFs require to add polynomials of some order m (= degree - 1) to the space (1), but we shall ignore details here. Typical cases of radial basis functions are provided in Table 1, where $F(h)$ stands for the standard approximation order attained for interpolation problems, measured in terms of the maximal distance h from any point of a compact domain to its nearest center. Some comments will be given later.

Table 1. All entries are modulo factors that are independent of r and h, but possible dependent on parameters of Φ.

$\Phi(x) = \phi(r), r = \|x\|_2$	m	$F(h)$
$(-1)^{\lceil \beta/2 \rceil} r^\beta, \quad \beta \in \mathbb{R}_{>0} \setminus 2\mathbb{N}$ thin-plate splines	$\lceil \beta/2 \rceil$	$h^{\beta/2}$ [65]
$(-1)^{1+\beta/2} r^\beta \log r, \quad \beta \in 2\mathbb{N}$ thin-plate splines	$\beta/2 + 1$	$h^{\beta/2}$ [65]
$(-1)^{\lceil \beta/2 \rceil} (\gamma^2 + r^2)^{\beta/2}, \ \beta \in \mathbb{R} \setminus 2\mathbb{N}_{>0}$ Multiquadrics	$\lceil \beta/2 \rceil$ if $\beta > 0$	$e^{-\delta/h}$ $\delta > 0$ [37]
$e^{-\beta r^2}, \quad \beta > 0$ Gaussians	0	$e^{-\delta/h^2}$ $\delta > 0$ [37]
$\left(2\pi^{d/2}/\Gamma(k)\right) K_{k-d/2}(r)(r/2)^{k-d/2}$ $2k > d$ Sobolev splines	0	$h^{k-d/2}$ as in [65]
$(1-r)_+^4(1+4r)$ $d \leq 3$ Wendland function	0	$h^{3/2}$ [58]

3 Generalized interpolation

The range of applications of radial basis functions is extremely large, and we confine ourselves here to a still rather general setting where the application wants to solve a linear operator equation

$$Lu = f, \quad L : U \to F, \quad u \in U,$$

where $f \in F$ is given and $u \in U$ has to be constructed. In case of problems with boundary conditions, we put the boundary conditions either into the space U or into the operator L, turning it into a pair (D, R) of a differential and a boundary operator, respectively, and using suitable product spaces for U and F. Examples will follow later.

We then assume that the operator equation is discretized by picking N linear functionals $\lambda_1, \ldots, \lambda_N$ and trying to solve the system

$$\lambda_j(u_h) = f_j \in \mathbb{R}, \ 1 \le j \le N \tag{2}$$

where now u_h is sought in a finite subspace $U_h \subset U$. It should be clear that collocation takes the above form, where the functionals are evaluations of differential operators on points in the interior of some domain, plus functionals evaluating boundary value operators on (possibly only parts of) the boundary of the domain. We allow any kind of linear functionals, and thus one can handle rather exotic cases, mixing various differential or integral operators in a single problem. Furthermore, certain additional conditions like conservation laws can be written that way, and additional properties like ellipticity of the underlying problem are irrelevant. The generality of the setting is possible because the RBF approach has some built–in regularization that allows to handle ill–posed problems without regarding the ill–posedness. We cannot dwell on this subject here, but it can be seen as both an advantage and a drawback, depending on the user's viewpoint.

The simplest case of collocation is pure interpolation at the centers, i.e. $\lambda_j = \delta_{x_j}$ for the same centers x_j as used in the definition of S_X. Then we get the symmetric matrix $A_X = (\phi(\|x_k - x_j\|_2))_{1 \le j,k \le N}$ and require it to be nonsingular. If this matrix is positive definite for **all** choices and **all** numbers N of pairwise distinct centers x_j in $X := \{x_j \in \mathbb{R}^d \ : \ 1 \le j \le N\} \subset \mathbb{R}^d$, the radial basis function ϕ is called (strictly) *positive definite* (SPD) on $\mathbb{R}^d$. This is a rather strong property for a scalar function, and the theory of radial basis functions is focused around the construction of such functions with additional properties. Gaussians and inverse multiquadrics (multiquadrics of Table 1 with $\beta < 0$) even have this property for **all** space dimensions d, but due to a well–known characterization of such functions via complete monotonicity [38, 54], there are no compactly supported radial functions that work for all space dimensions. The construction of compactly supported strictly positive definite radial basis functions (CS–SPD–RBF) for restricted space dimensions was done in 1995 by Wu [62] and Wendland [56], providing functions that can be chosen to suit any space dimension and any smoothness requirement. Surprisingly, these functions are piecewise polynomials, and Wendland's construction provided functions with minimal degrees under the above conditions. See Table 2 for a list, and note that the matrix A_X will be sparse and positive definite in case of CS–SPD–RBF. In Table 2 we have used the cut-off function $(r)_+$ which is defined to be r if $r \geq 0$ and to be zero elsewhere. Furthermore, d denotes the maximal possible space dimension, i.e. if you want to work on R^ℓ, you have to pick a basis function with table entry $d \geq \ell$.

Table 2. SPD($\mathbb{R}^d$) Wendland functions $p_{d,k}$ with native spaces $W_2^{d/2+k+1/2}(\mathbb{R}^d)$

d	k	$p_{d,k}$	
1	0	$(1-r)_+$	C^0
1	1	$(1-r)_+^3\,(3r+1)$	C^2
1	2	$(1-r)_+^5\,(8r^2+5r+1)$	C^4
3	0	$(1-r)_+^2$	C^0
3	1	$(1-r)_+^4\,(4r+1)$	C^2
3	2	$(1-r)_+^6\,(35r^2+18r+3)$	C^4
3	3	$(1-r)_+^8\,(32r^3+25r^2+8r+1)$	C^6
5	0	$(1-r)_+^3$	C^0
5	1	$(1-r)_+^5\,(5r+1)$	C^2
5	2	$(1-r)_+^7\,(16r^2+7r+1)$	C^4

There is an intrinsic relation of SPD–RBF's to reproducing kernel Hilbert spaces, but there is no room here to give details [52]. In short, one can introduce an inner product $(.,.)_\phi$ such that

$$(\phi(\|\cdot - x\|_2), \phi(\|\cdot - y\|_2)) = \phi(\|x-y\|_2)$$

holds, and then the matrix A_X is a Gramian. The linear hull of all spaces S_X can be completed to form a Hilbert space called the *native* space for ϕ, and a very natural application of RBF techniques would be the case where the bilinear form $a(.,.)$ of a Rayleigh–Ritz setting coincides with the above inner product in the native space. However, such cases are somewhat difficult to handle in full generality, because (for instance) the standard bilinear form for second–order elliptic problems lives in Sobolev space $W_2^1(\mathbb{R}^2)$ containing discontinuous functions and having the natural radial (Bessel) basis function $K_0(r)$ with a logarithmic singularity. Research in this direction is still in its early stages, concentrating on spaces with higher regularity.

For the theoretical analysis of RBF's, the study of these native spaces is of quite some importance. Error bounds normally are first derived for functions in the native space, and are then moved over to other spaces [48]. The generalized RBF interpolation setting can be proven to be optimal in at least three different aspects, and therefore the attained error bounds ([57]

for Wendland's functions in Sobolev spaces) are optimal with respect to all other linear recovery processes based on the same data and working in the same space of functions. We cannot say much more here, and we refer the reader to survey articles on RBF theory [9, 43, 44, 47, 50, 52].

4 Collocation

For applications, the generalization from pure interpolation to collocation requires to replace the point evaluation functionals δ_{x_j} by general functionals λ_j that are continuous on the native space. It is not easy to tell directly which functionals have this property with respect to a given ϕ, but a rule–of–thumb [52] allows any functional λ that can be continuously applied to one argument of $\phi(\|x-y\|_2)$ and be approximated by finitely supported functionals (e.g. differential operator evaluations by finite differences, or integrals by quadrature formulae). But even if the functionals and ϕ are chosen to match, the matrix $A = \left(\lambda_j^y \phi(\|y-x_k\|_2)\right)_{1\le j,k\le N}$ where λ_j^y stands for the evaluation of λ_j with respect to the variable y, is not symmetric and not necessarily nonsingular. We call this an *unsymmetric* collocation, because the functionals δ_{x_k} providing the functions $\phi(\|\cdot - x_k\|_2)) = \delta_{x_k}^y \phi(\|\cdot - y\|_2))$ of the space S_X differ from the collocation functionals λ_j. A *symmetric* collocation [63] drops δ_{x_k} altogether and works with the span of functions $\lambda_k^y \phi(\|\cdot - y\|_2))$ to get a symmetric matrix $A_\Lambda = \left(\lambda_j^x \lambda_k^y \phi(\|y-x\|_2)\right)_{1\le j,k\le N}$ which can be proven to be positive definite whenever the functionals λ_j are linearly independent and continuous in the native space.

The unsymmetric collocation technique for RBF was introduced by Kansa [32, 33] and successfully used by various other authors. e.g. [7, 8, 19, 34]. However, a recent example [29] showed that it may fail in some specially constructed cases which are, fortunately, rare to find. Kansa's technique has the advantage of a wider applicability, because more functionals are allowable for a given RBF, but it still lacks proven error bounds, even for elliptic model problems. This is a challenging research area with little or no progress in the unsymmetric case.

On the other side, symmetric collocation has been investigated recently by Franke and Schaback [15, 16], giving error bounds and criteria for the proper choice of ϕ for a given collocation setting defined by functionals λ_j. A different and independent approach was made by Wu [64]. We cannot provide details here, but the theoretical approximation order roughly is at least the order $F(h)$ given in Table 1 reduced by the order of differentiation involved in the functionals, where h is the density of centers in the sense

$$h = \sup_{y\in\Omega} \min_{1\le j\le N} \|y - x_j\|_2$$

if we work in a bounded domain Ω and use collocation with values of differential operators (order zero allowed for boundary values) at centers x_j. Recent results [51] in the interpolation case suggest to replace $F(h)$ by $(F(h))^2$ in the interior of the domain, and this is the order that is observable there.

For interpolation and symmetric collocation with RBF there are some rules to be suggested:

- Pick ϕ smooth enough such that all collocation functionals can be continuously applied to both arguments of $\phi(\|x-y\|_2)$ [52].
- Additional smoothness of ϕ will improve the attainable discretization error at the expense of increased condition number[49].
- Be careful with "wide" Gaussians or multiquadrics, because these have both an exponentially good error behavior and an exponentially bad condition number[49].
- For compactly supported RBF's, pick the support radius in such a way that each RBF support contains roughly the same number B of centers (for each operator, i.e. separately in the interior and on the boundary). Then the condition depends on B, not on the meshwidth. For fixed B, the error first goes down nicely when data are getting more and more dense, but, from a certain h on, one has to enlarge B to get higher accuracy [50].

The proper choice of scale of the RBF in relation to the data density is another challenging research problem. There are many experimental results for multiquadrics [2, 33, 34], but so far there is no systematic theory. Numerical experiments by Floater/Iske [13, 14] and Fasshauer [10, 12] have demonstrated the feasibility of multiscale techniques, using RBFs of different support scales on data subsets of different densities. In many cases, linear convergence with increasing levels is observed, but the theoretical investigations are still rather limited [11, 22, 42].

5 Rayleigh–Ritz applications

For a bounded domain Ω with C^1-boundary $\partial\Omega$ Wendland [59] considers problems of the form

$$
\begin{aligned}
-\sum_{i,j=1}^{d} \frac{\partial}{\partial x_i}\left(a_{ij}\frac{\partial u}{\partial x_j}\right)(x) + c(x)u(x) &= f(x), \quad x \in \Omega && (3)\\
\sum_{i,j=1}^{d} a_{ij}(x)\frac{\partial u(x)}{\partial x_j}\nu_i(x) + h(x)u(x) &= g(x), \quad x \in \partial\Omega && (4)
\end{aligned}
$$

where $a_{ij}, c \in L_\infty(\Omega)$, $i,j = 1\ldots,n$, $f \in L_2(\Omega)$, $a_{ij}, h \in L_\infty(\partial\Omega)$, $g \in L_2(\partial\Omega)$ and ν denotes the unit normal vector to the boundary $\partial\Omega$. $c \geq 0$

and $h \geq 0$, at least one of them being uniformly bounded away from zero on a subset of nonzero measure of Ω or $\partial\Omega$, respectively.

The corresponding variational problem

$$\text{find } u \in W_2^1(\Omega) \ : \ a(u,v) = F(v) \quad \text{for all } v \in W_2^1(\Omega) \tag{5}$$

excludes worrying about boundary values, and allows to work with the whole Sobolev space $W_2^1(\Omega)$.

Under the strong regularity assumption $u \in W_2^k(\Omega)$ and $\Phi(x) = \phi(\|x\|_2)$ having a Fourier transform $\widehat{\Phi}$ satisfying

$$\widehat{\Phi}(\omega) \sim (1 + \|\omega\|_2)^{-2\beta}. \tag{6}$$

with $\beta \geq k > \frac{d}{2} + m$, the Rayleigh–Ritz–Galerkin solution s of the stiffness system based on ϕ satisfies the error bound

$$\|u - s\|_{W_2^m(\Omega)} \leq C\ h^{k-m}\ \|u\|_{W_2^k(\Omega)}$$

for $h \leq h_0$. These results are best possible as far as the approximation order is concerned. However, this work still is preliminary in the sense that boundary conditions were excluded and sufficient regularity had to be assumed. A second paper [60] uses a multilevel technique to attack discretizations of elliptic problems by RBFs. Here, the proof of error bounds still is missing.

6 Homogenization in the interior (DRM)

Let us consider a standard elliptic model problem

$$\begin{array}{lll} Lu = f & f \text{ in } \Omega \subset \mathbb{R}^d & L : W_\Omega \to L_\Omega \\ Bu = g & \text{in } \partial\Omega & B : W_\Omega \to W_{\partial\Omega} \\ u \approx u_h & u_h \in S_h \subset W_\Omega. & \end{array}$$

in certain Hilbert spaces. We assume that the map R from the data $(f, g) \in L_\Omega \times W_{\partial\Omega}$ back to the solution $u \in W_\Omega$ is linear and bounded. This means that the problem can be solved stably in the above setting.

Radial basis functions can be used in two ways to solve such a problem via homogenization. Going over to a homogeneous problem in the interior is called the Dual Reciprocity Method (DRM) [3, 4, 5, 18, 20, 30, 40, 41]. We outline the computational steps here:

1. Approximate f well in L_Ω by some f_0 in Ω, but make sure that you know explicitly some u_0 with $Lu_0 = f_0$. This is easily achieved by using various RBFs, because one can either start with some ϕ and find ψ with
$$L(\psi(\|\cdot - x\|)) = \phi(\|\cdot - x\|), \tag{7}$$
or start with some ψ and apply L to get ϕ via (7).

2. Evaluate the boundary values $g_0 := Bu_0$ and pose the homogeneous problem $Lu_1 = 0$ in Ω, $Bu_1 = g - g_0$ in $\partial\Omega$. Using a BEM technique, one gets a function u_2 that satisfies $Lu_2 = 0$ exactly, but with disturbed boundary values $Bu_2 = g_2$, such that $\|g - g_0 - g_2\|$ is small in $W_{\partial\Omega}$.

3. Compose the final numerical solution by $u_3 := u_0 + u_2$.

The error analysis takes $u_4 := u - u_0 - u_2$ and gets $Lu_4 = f - f_0$ in Ω, $Bu_4 = g - g_0 - g_2$ in $\partial\Omega$. By our assumption on the stable solvability of the problem, we get an error bound. But any special application must make sure that the approximations lie in the correct spaces and have small errors in the correct norms. This sometimes causes problems and requires quite some theoretical work [20, 31]. But, at least in principle, the basic identity (7) for RBFs makes this approach feasible.

7 Homogenization on the boundary

There is a complementary technique that homogenizes on the boundary. For a BEM audience, this is hardly an advantage, but we have in mind to use CS-RBF with zero boundary values in the interior of the domain, and thus want to go over to a **sparse** problem that is inhomogeneous in the interior, but has homogeneous boundary data. We assume the same setting as above, but now the steps are

1. Solve the problem approximately by invertible RBFs, but just on and near the boundary. This yields functions $u_0 \in W_\Omega, f_0 \in L_\Omega, g_0 \in W_{\partial\Omega}$ such that $Lu_0 = f_0, Bu_0 =: g_0$, where $g_1 := g - g_0$ is small in $W_{\partial\Omega}$. Of course, the function $f - f_0$ will not be small in the interior, but we correct this in the following step.

2. We now suggest to use invertible CS-RBF to solve the problem $Lu_1 = f_1 := f - f_0 \in L, Bu_1 = 0 \in W_\Omega$. In practice, we will get a function $u_2 \in W_\Omega$ such that $Lu_2 = f_2 \sim f - f_0$ and $Bu_2 = g_2$, where $f - f_0 - f_2$ and g_2 are small in L_Ω and $W_{\partial\Omega}$, respectively.

Now we consider $u_3 := u_0 + u_2$ to be an approximation of the solution u, and we get $L(u - u_3) = f - f_0 - f_2$, $B(u - u_3) = g - g_0 - g_2 = g_1 - g_2$, and again we can use the stable solvability to conclude that the result must be a good approximation to the solution.

Let us compare these two approaches.

- The classical DRM has the advantage of reducing the problem by one dimension, but the system on the boundary usually has a non–sparse matrix, even if CS–RBF are used there.

- Homogenization on the boundary can make use of sparsity in both subproblems, but the system in the interior cannot be reduced by one dimension. And, there is no practical experience so far.

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