

RADIAL BASIS FUNCTIONS - SOME RECENT DEVELOPMENTS

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Abstract. Radial basis functions (RBF) is a recent methodology for scattered data interpolation, offering possibilities for meshfree numerical solution of PDEs to spectral accuracy also on irregular domains in any number of dimensions. We briefly introduce RBFs, and then focus on some recent developments, especially with regard to the Gibbs and the Runge phenomena for RBF interpolants. The latter suggests ways to further enhance the RBF methodology for solving PDEs.

1. Introduction. RBFs were introduced by R. Hardy around 1970 [14]. In a much noted 1982 survey [13], the approach was found to be the preferable one of about 30 then known methods. Although unconditional non-singularity of the interpolation problem was known early in some special cases [1], it was the proof in 1986 of guaranteed nonsingularity also in the case used by Hardy [15] which propelled the development of RBFs into one of the most active areas in modern computational mathematics.

In this presentation, we first introduce RBFs as a generalization of cubic splines to multiple dimensions, and then note some results concerning accuracy and conditioning. One of the most striking developments over the last several decades regarding numerical solutions of PDEs has been the increased use of high-order methods. Their primary limitation so far has been difficulties in case of irregular boundaries. RBFs are on the way to become the long sought after opportunity to generalize high-order finite difference (FD) and pseudospectral (PS) methods [4] to such situations. For the first time, freedom from mesh generation, ability to do local refinements, and easy handling of irregular geometries can all be combined with spectral accuracy.

The types of RBFs we are most interested in depend on a scalar *shape parameter*. A good choice for it can greatly improve the final result, but the selection of it has in the past often required a compromise between accuracy, computational cost, and numerical stability. After commenting briefly on these issues, we will present some new results, especially on how insights into the Runge phenomenon for RBFs opens up additional opportunities towards the efficient solution of PDEs.

2. Introduction to RBFs via cubic splines. A standard cubic spline is made up of a different cubic polynomial between each pair of adjacent node points, at which it features a jump in the *third* derivative. If the spacing between the points is h , it is well known that the error will decrease like $O(h^4)$. Convenient generalizations to more space dimensions have in the past been available only if the nodes are lined up in the coordinate directions.

Another way to approach the problem of finding the 1-D cubic spline is the following: At each data location x_i , $i = 1, \dots, n$, place a translate of the function $\phi(x) = |x|^3$, i.e. at x_i the function $\phi(x - x_i) = |x - x_i|^3$. We can then ask if it is possible to form a linear combination of all these functions

$$s(x) = \sum_{k=1}^n \lambda_k \phi(x - x_i) \tag{2.1}$$

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such that this takes the desired function values f_i at the data locations x_i , i.e. such that $s(x_i) = f_i$ holds. This amounts to requiring that the coefficients λ_k satisfy the linear system of equations

$$\begin{bmatrix} \phi(x_1 - x_1) & \phi(x_1 - x_2) & \cdots & \phi(x_1 - x_n) \\ \phi(x_2 - x_1) & \phi(x_2 - x_2) & & \phi(x_2 - x_n) \\ \vdots & & & \vdots \\ \phi(x_n - x_1) & \phi(x_n - x_2) & \cdots & \phi(x_n - x_n) \end{bmatrix} \begin{bmatrix} \lambda_1 \\ \lambda_2 \\ \vdots \\ \lambda_n \end{bmatrix} = \begin{bmatrix} f_1 \\ f_2 \\ \vdots \\ f_n \end{bmatrix} \quad (2.2)$$

The interpolant $s(x)$, as given by (2.1), will become a cubic function between the nodes and, at the nodes, have a jump in the third derivative. We have thus described another way to create an interpolating cubic spline.

2.1. Generalization to multiple dimensions. In 2-D, we can use a *rotated* version of the same radial function. In d dimensions, we can write these rotated basis functions as $\phi(\|\underline{x} - \underline{x}_i\|)$, where $\|\cdot\|$ denotes the standard Euclidean norm. The form of the RBF interpolant and of the linear system that is to be solved has hardly changed from the 1-D case. Instead of (2.1) and (2.2), we now use as interpolant

$$s(\underline{x}) = \sum_{k=1}^n \lambda_k \phi(\|\underline{x} - \underline{x}_k\|) \quad (2.3)$$

with the collocation conditions

$$\begin{bmatrix} \phi(\|\underline{x}_1 - \underline{x}_1\|) & \phi(\|\underline{x}_1 - \underline{x}_2\|) & \cdots & \phi(\|\underline{x}_1 - \underline{x}_n\|) \\ \phi(\|\underline{x}_2 - \underline{x}_1\|) & \phi(\|\underline{x}_2 - \underline{x}_2\|) & & \phi(\|\underline{x}_2 - \underline{x}_n\|) \\ \vdots & & & \vdots \\ \phi(\|\underline{x}_n - \underline{x}_1\|) & \phi(\|\underline{x}_n - \underline{x}_2\|) & \cdots & \phi(\|\underline{x}_n - \underline{x}_n\|) \end{bmatrix} \begin{bmatrix} \lambda_1 \\ \lambda_2 \\ \vdots \\ \lambda_n \end{bmatrix} = \begin{bmatrix} f_1 \\ f_2 \\ \vdots \\ f_n \end{bmatrix}. \quad (2.4)$$

2.2. Different types of radial functions. The error $O(h^4)$ for cubic splines in 1-D will become $O(h^6)$ in the case of quintic splines ($\phi(x) = |x|^5$), and it falls to $O(h^2)$ for linear splines ($\phi(x) = |x|$). The sizes of these errors correspond directly to which derivative of $\phi(x)$ it is that features a jump. This leads to the 'obvious' question: why not choose a $\phi(x)$ which is infinitely differentiable everywhere, such as $\phi(x) = \sqrt{1+x^2}$ (the choice by Hardy)? If we ignore issues related to the Runge phenomenon (see Section 5), the accuracy will in general become spectral, i.e. of the form $O(e^{-c/h})$, where $c > 0$ and h is a typical node spacing [17].

Table 2.1 lists a number of possible choices of radial functions. For the non-smooth ones, the order accuracy surprisingly turns out to improve with the number of dimensions [2]. For the infinitely smooth RBFs, we have also introduced a *shape parameter*, which we denote by ε . For small values of ε , the basis functions become very flat, and for large values, they become sharply spiked (IQ, IMQ, GA) or piecewise linear (MQ). Although both these extremes (ε very small, and ε very large) might seem unsuitable, it turns out that the former case will be of particular interest in connecting RBF with pseudospectral (PS) methods.

3. Flat basis functions. It was discovered in [3] that RBF interpolants in 1-D, in the limit of $\varepsilon \rightarrow 0$, approach polynomial interpolants, with generalizations to more dimensions investigated in [9]. From this follows the connection between RBF and PS methods noted earlier. In many tests, it has been seen that ε not quite equal to zero could give better results still than $\varepsilon = 0$ (e.g. [11] and Figure 5.1 below),

| Type of radial function | | |
|--------------------------|-------------------|--|
| Piecewise smooth | | |
| MN | monomial | $ r ^{2m+1}$ |
| TPS | thin plate spline | $ r ^{2m} \ln r $ |
| Infinitely smooth | | |
| MQ | multiquadric | $\frac{\sqrt{1 + (\varepsilon r)^2}}{1}$ |
| IQ | inverse quadratic | $\frac{1}{1 + (\varepsilon r)^2}$ |
| IMQ | inverse MQ | $\frac{1}{\sqrt{1 + (\varepsilon r)^2}}$ |
| GA | Gaussian | $e^{-(\varepsilon r)^2}$ |

TABLE 2.1

Definition and Fourier transforms for some cases of radial functions

with explanations provided in [10] and [12]. Direct calculation of RBF interpolants through (2.4) and (2.3) lead to extreme ill-conditioning when $\varepsilon \rightarrow 0$. All the elements of the A -matrix (the coefficient matrix in (2.4)) then approach one. For example in 2-D, with 41 scattered nodes, the determinant of the A -matrix will go to zero like $O(\varepsilon^{416})$. High precision arithmetic can be used to overcome some of the ill-conditioning, but the cost for this will increase without bound in the $\varepsilon \rightarrow 0$ limit. It was for a long time thought that this numerical ill-conditioning was unavoidable in low- ε RBF calculations (cf. the ‘uncertainty principle’ [2] Section 5.3.4, originally stated in [16]). The Contour-Padé method [8] clearly showed that this is not so. Direct use of (2.4), (2.3) merely amounts to an ill-conditioned numerical implementation of a genuinely well-conditioned problem. A second stable algorithm for the $\varepsilon \rightarrow 0$ case, the RBF-QR method, is now under development [7].

4. The Gibbs phenomenon. What is known as the Gibbs phenomenon was first observed in the context of truncated Fourier expansions, but other versions of it arise also for interpolation methods. It is shown in [5] that RBF interpolants feature a remarkable richness in the possibilities that can arise already in the case of equispaced nodes on an infinite grid in 1-D. In Figure 4.1 a, we see for TPS a transition from two-sided to one-sided oscillations near $x = 5$, and in part b a similar transition in case of IQ, located at a point which drifts out to infinity when $\varepsilon \rightarrow 0$. In part c, we see that no such transition ever occurs in the case of GA RBFs. The theory underlying these different versions is explained in [5], which in turn draws heavily on the analysis of *RBF locality* in [6]. This topic is in itself of great potential significance for devising fast iterative solution methods for (2.4).

5. The Runge phenomenon (RP). Figure 5.1 illustrates how the error when $\varepsilon \rightarrow 0$ at first decreases and then, when the polynomial interpolant is approached (with its well-known RP), again increases. Another connection between RP and RBFs is illustrated in Figure 5.2. In part a, there is no RP visible, but the equispaced RBF approximation lacks sufficient resolution near the center where the data features a very sharp gradient. In part b, we have inserted two extra nodes in the critical area and, in part c, still two more points are inserted. The most striking result of this local refinement is a severe RP. In contrast to this, Figure 5.3 shows that one can obtain excellent accuracy if one uses good choices for node point locations *and* for ε_i -values (different at the different nodes $x_i \in [-1, 1]$). Although the multivariate

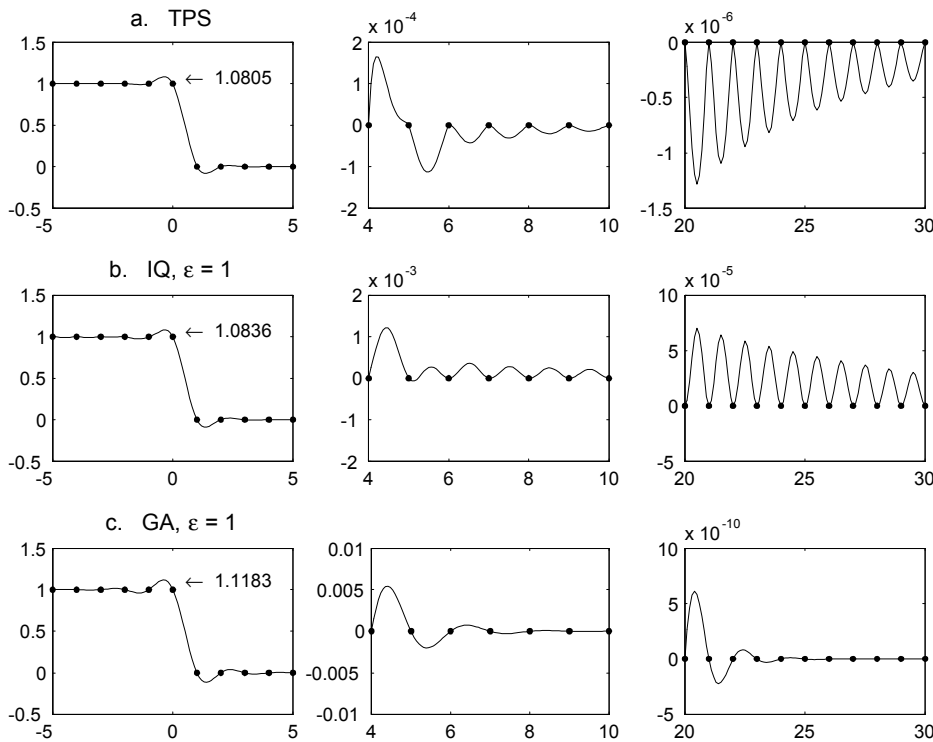


FIG. 4.1. The Gibbs oscillations both at a jump in the data, and further out from it, in the cases of (a) TPS, (b) IQ, $\varepsilon = 1$, and (c) GA, $\varepsilon = 1$.

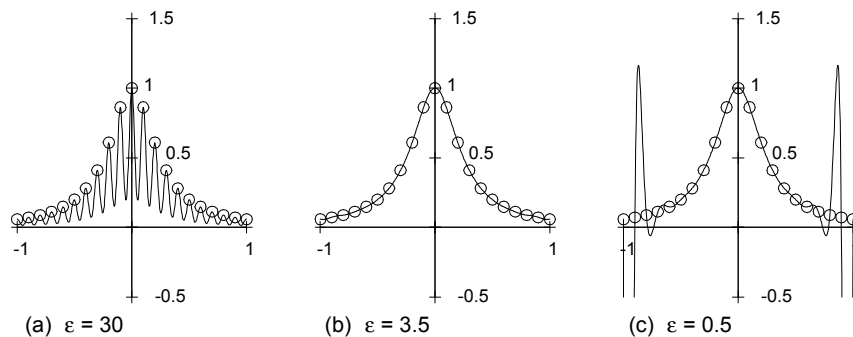


FIG. 5.1. GA interpolants of $f(x) = \frac{1}{1+16x^2}$ for a wide range of ε -values: $\varepsilon = 30$, 3.5 , and 0.5 respectively.

optimizer used in obtaining Figure 5.3 (based on Matlab's Genetic Algorithm toolbox) appears to have found only a local optimum (in contrast to the global one, for which the oscillations in the error most likely would all be of the same amplitude), the error level that is reached is nevertheless spectacular in comparison with what can be achieved with, say, polynomial interpolation at the Chebyshev nodes (corresponding to a typical non-periodic PS method). As Figure 5.4 shows, $n = 170$ nodes are needed to match the max norm accuracy of $2.5 \cdot 10^{-5}$ that RBF can achieve using

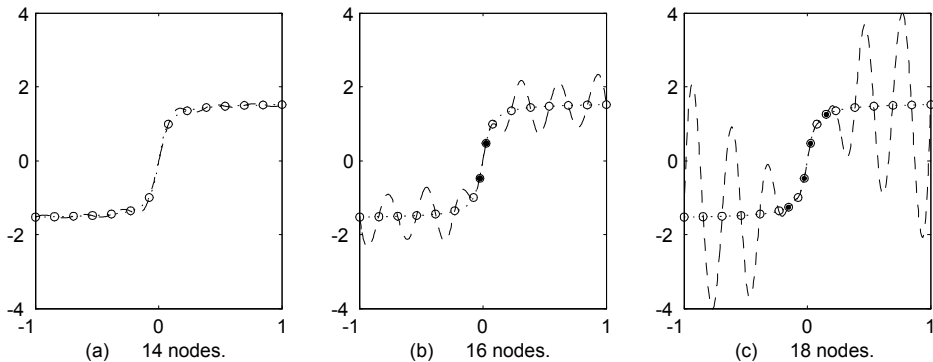


FIG. 5.2. MQ RBF $\varepsilon = 2$ interpolants (dashed curves) of $f(x) = \arctan(20x)$ (dotted curves) over $[-1, 1]$ (a) 14 equispaced points, (b) two extra points inserted near the center, and (c) still two more points inserted near the center.

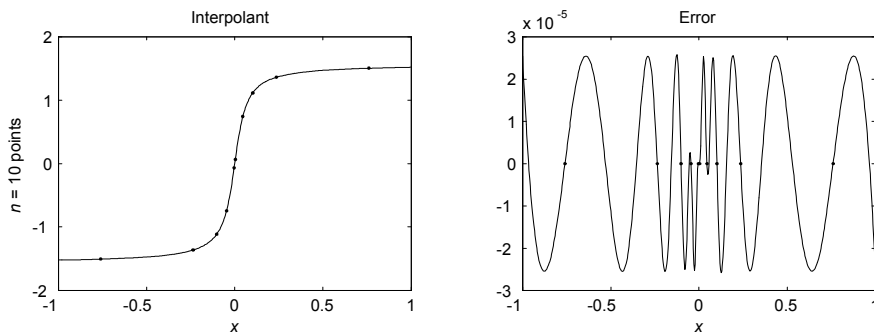


FIG. 5.3. 10-point interpolation of the same function as in Figure 5.2 when both node locations and spatially variable ε were chosen to minimize the interpolation error. (a) Node locations and interpolant, (b) Error across $[-1, 1]$.

only $n = 10$ interpolation nodes. Once the opportunities offered by spatially variable shape parameters can be fully utilized - research in progress - we anticipate that RBF methods will surpass PS methods not only in geometric flexibility, but also in their ability to incorporate node refinements to enhance local accuracy wherever this is needed.

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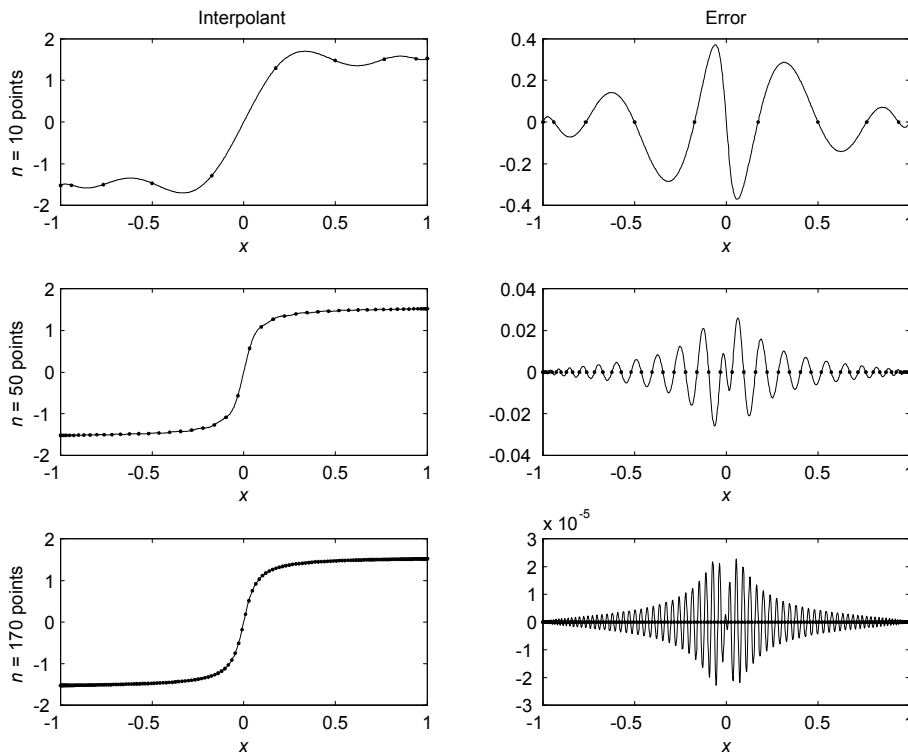


FIG. 5.4. 10-point, 50-point and 170-point Chebyshev interpolants for $\arctan(20x)$ over $[-1,1]$; display of the interpolants and their errors.

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