## A NEW CLASS OF OSCILLATORY RADIAL BASIS FUNCTIONS

BENGT FORNBERG \*, ELISABETH LARSSON <sup>†</sup>, AND GRADY WRIGHT <sup>‡</sup>

**Abstract.** Radial basis functions (RBFs) form a primary tool for multivariate interpolation, and they are also receiving increased attention for solving PDEs on irregular domains. Traditionally, only non-oscillatory radial functions have been considered. We find here that a certain class of oscillatory radial functions (including Gaussians as a special case) leads to non-singular interpolants with intriguing features especially as they are scaled to become increasingly flat. This flat limit is important in that it generalizes traditional spectral methods to completely general node layouts. Interpolants based on the new radial functions appear immune to many or possibly all cases of divergence that in this limit can arise with other standard types of radial functions (such as multiquadrics and inverse multiquadratics).

Key words. Radial basis functions, RBF, multivariate interpolation, Bessel functions.

**1. Introduction.** A radial basis function (RBF) interpolant of multivariate data  $(\underline{x}_k, y_k), \ k = 1, \ldots, n$  takes the form

$$s(\underline{x}) = \sum_{k=1}^{n} \lambda_k \ \phi(\|\underline{x} - \underline{x}_k\|) \ . \tag{1.1}$$

Here  $\|\cdot\|$  denotes the standard Euclidean vector norm,  $\phi(r)$  is some radial function, and an underline denotes that quantity to be a vector. The coefficients  $\lambda_k$  are determined in such a way that  $s(\underline{x}_k) = y_k$ , k = 1, ..., n, i.e. as the solution to the linear system

$$\begin{bmatrix} A \end{bmatrix} \begin{bmatrix} \lambda_1 \\ \vdots \\ \lambda_n \end{bmatrix} = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix}$$
(1.2)

where the entries of the matrix A are  $A_{i,j} = \phi(\|\underline{x}_i - \underline{x}_j\|), i = 1, ..., n, , j = 1, ..., n.$ 

Numerous choices for  $\phi(r)$  have been used in the past. Table 1 shows a few cases for which existence and uniqueness of the interpolants  $s(\underline{x})$  have been discussed in the literature; see for ex. [2], [3], [14], and [15]. For many of the radial functions in Table 1, existence and uniqueness are ensured for arbitrary point distributions. However, there are some that require the form of (1.1) to be augmented by some low-order polynomial terms.

In the infinitely smooth cases, we have included a shape parameter  $\varepsilon$  in such a way that  $\varepsilon \to 0$  corresponds to the basis functions becoming flat (as discussed extensively in for example [4], [7], [8], [11], [12]). The primary interest in this limit lies in the fact that it reproduces all the classical pseudospectral (PS) methods [6], such as Fourier, Chebyshev, and Legendre, whenever the data point locations are

<sup>\*</sup>University of Colorado, Department of Applied Mathematics, 526 UCB, Boulder, CO 80309, USA (fornberg@colorado.edu). The work was supported by NSF grants DMS-9810751 (VIGRE) and DMS-0309803.

<sup>&</sup>lt;sup>†</sup>Uppsala University, Department of Information Technology, Scientific Computing, Box 337, SE-751 05 Uppsala, Sweden (bette@it.uu.se). The work was supported by a grant from The Swedish Research Council.

<sup>&</sup>lt;sup>‡</sup>University of Utah, Department of Mathematics, 155 South 1400 East, JWB 233, Salt Lake City, UT 84112-0090, USA (wright@math.utah.edu). The work was supported by NSF VIGRE grant DMS-0091675.

Type of basis function	$\phi(r)$				
Piecewise smooth RBFs					
Generalized Duchon spline (GDS)	$r^{2k}\log r, \ k \in \mathbb{N}$				
	$r^{2\nu}, \ \nu > 0 \text{ and } \nu \notin \mathbb{N}$				
Wendland	$(1-r)_{+}^{k}p(r), p \text{ a polynomial}, k \in \mathbb{N}$				
Matérn	$\frac{2^{1-\nu}}{\Gamma(\nu)}r^{\nu}K_{\nu}(r), \ \nu > 0$				
Infinitely smooth RBFs					
Gaussian (GA)	$e^{-(\varepsilon r)^2}$				
Generalized multiquadric (GMQ)	$(1+(\varepsilon r)^2)^{\nu/2}, \ \nu \neq 0 \text{ and } \nu \notin 2\mathbb{N}$				
• Multiquadric (MQ)	$(1+(\varepsilon r)^2)^{1/2}$				
• Inverse multiquadric (IMQ)	$(1+(\varepsilon r)^2)^{-1/2}$				
• Inverse quadratic (IQ)	$(1+(\varepsilon r)^2)^{-1}$				
TABLE 1.1					

Some commonly used radial basis functions. Note: in all cases,  $\varepsilon > 0$ .

distributed in a corresponding manner. The interpolant (1.1) can therefore be seen as a major generalization of the PS approach, allowing scattered points in arbitrary numbers of dimensions, a much wider functional choice, and a free shape parameter  $\varepsilon$  that can be optimized.

The RBF literature has so far been strongly focused on radial functions  $\phi(r)$  that are non-oscillatory. We are not aware of any compelling reason for why this needs to be the case. Although we will show that  $\phi(r)$  oscillatory implies that the interpolation problem can become singular in a sufficiently high dimension, we will also show that this does not cause problems when the dimension is fixed. The present study focuses on the radial functions

$$\phi_d(r) = \frac{J_{\frac{d}{2}-1}(\varepsilon r)}{(\varepsilon r)^{\frac{d}{2}-1}}, d = 1, 2, \dots,$$
(1.3)

where  $J_{\alpha}(r)$  denotes the *J* Bessel function of order  $\alpha$ . For odd values of *d*,  $\phi_d(r)$  can be alternatively expressed by means of regular trigonometric functions:

$$\phi_1(r) = \sqrt{\frac{2}{\pi}} \cos(\varepsilon r)$$
  

$$\phi_3(r) = \sqrt{\frac{2}{\pi}} \frac{\sin(\varepsilon r)}{\varepsilon r}$$
  

$$\phi_5(r) = \sqrt{\frac{2}{\pi}} \frac{\sin(\varepsilon r) - \varepsilon r \cos(\varepsilon r)}{(\varepsilon r)^3}$$
  
:

We will later find it useful to note that these  $\phi_d(r)$  – functions can also be expressed in terms of the hypergeometric  ${}_0F_1$  function:

$$\phi_d(r) = 2^{\frac{2}{d}-1} \Gamma\left(\frac{d}{2}\right) \psi_d(r)$$



FIG. 1.1. Comparison between  $2^{\delta} \delta! \frac{J_{\delta}(2\sqrt{\delta}r)}{(2\sqrt{\delta}r)^{\delta}}$  for d = 3, 5, 10 (i.e.  $\delta = \frac{1}{2}, \frac{3}{2}, 4$ ) and the  $d \to \infty$  limit  $e^{-r^2}$ .

where

$$\psi_d(r) = {}_0F_1(\frac{d}{2}, -\frac{1}{4}(\varepsilon r)^2).$$
(1.4)

From the relation

$$\lim_{\delta \to \infty} 2^{\delta} \delta! \, \frac{J_{\delta}(2\sqrt{\delta}r)}{(2\sqrt{\delta}r)^{\delta}} = e^{-r^2} \,, \tag{1.5}$$

it follows that if we write  $\delta$  in place of d/2 - 1 and choose  $\varepsilon = 2\sqrt{\delta}$ , then  $\phi_d(r)$  in the limit as  $d \to \infty$  (i.e. with  $\delta$  and  $\varepsilon$  also tending to infinity) will recover the Gaussian (GA). This is illustrated in Figure 1.1 for d = 3, 5, and 10.

For these radial functions  $\phi_d(r)$ , we will prove non-singularity for arbitrarily scattered data in up to d dimensions (when d > 1). However, numerous other types of radial functions share this property. What makes the present class of Bessel-type basis functions outstanding relates to the flat basis function limit as  $\varepsilon \to 0$ . As a consequence of the limit (when it exists) taking the form of an interpolating polynomial, it connects pseudospectral (PS) methods [6] with RBF interpolants [8]. It was conjectured in [8] and shown in [16] that GA (in contrast to, say, MQ, IMQ, and IQ) will never diverge in this limit, no matter how the data points are located. The results in this study raise the question whether the present class of Bessel-type radial functions might represent the most general class possible of radial functions with this highly desirable feature.

The radial functions  $\phi_d(r)$  have previously been considered in [17] (where (1.5) and the positive semi-definiteness of the  $\phi_d(r)$ -functions were noted), and in an example in [9] (in the different context of frequency optimization). They were also noted very briefly in [8] as appearing immune to a certain type of  $\varepsilon \to 0$  divergence – the main topic of this present study. 2. Some observations regarding oscillatory radial functions. Expansions in different types of basis functions are ubiquitous in computational mathematics. It is often desirable that such functions are orthogonal to each other with regard to some type of scalar product. A sequence of such basis functions then needs to be increasingly oscillatory, as is the case for example with Fourier and Chebyshev functions. It can be shown that no such fixed set of basis functions can feature guaranteed non-singularity in more than 1-D when the data points are scattered [13]. The RBF approach circumvents this problem by making the basis functions dependent on the data point locations. It uses different translates of one single radially symmetric function, centered at each data point in turn. Numerous generalizations of this approach are possible (such as using different basis functions at the different data point locations, or not requiring that the basis functions be radially symmetric).

The first question we raise here is why it has become customary to consider only non-oscillatory radial functions (with a partial exception being GDS  $\phi(r) = r^{2k} \log r$ which changes sign at r = 1). One reason might be the requirements in the primary theorem that guarantees non-singularity for quite a wide class of RBF interpolants [3], [15]:

THEOREM 2.1. If  $\Phi(r) = \phi(\sqrt{r})$  is completely monotone but not constant on  $[0,\infty)$ , then for any points  $\underline{x}_k$  in  $\mathbb{R}^d$ , the matrix A in (1.2) is positive definite.

The requirement for  $\phi(\sqrt{r})$  to be completely monotone is far more restrictive than  $\phi(r)$  merely being non-oscillatory:

DEFINITION 2.2. A function  $\Phi(r)$  is completely monotone on  $[0, \infty)$ , if (i)  $\Phi(r) \in C[0, \infty)$ (ii)  $\Phi(r) \in C^{\infty}(0, \infty)$ (iii)  $(-1)^k \frac{d^k}{dr^k} \Phi(r) \ge 0$  for r > 0 and k = 0, 1, 2, ...

An additional result that might discourage the use of oscillatory radial functions is the following:

THEOREM 2.3. If  $\phi(r) \in C[0,\infty)$  with  $\phi(0) > 0$  and  $\phi(\rho) < 0$  for some  $\rho > 0$ , then there is an upper limit on the dimension d for which the interpolation problem is non-singular for all point distributions.

*Proof.* Consider the point distributions shown in Figure 2.1. The first row in the A-matrix will have the d + 1 entries

$$\left[\phi(0), \ \phi(\rho), \ \phi(\rho), \ \phi(\rho), \dots, \ \phi(\rho)\right].$$

For d sufficiently large, the sum of all the elements will be negative. By replacing  $\rho$  with some  $\hat{\rho} < \rho$  we can make the sum exactly zero. Then the sum of all the other rows of A will also be zero. Hence,  $[1, 1, 1, \ldots, 1]^T$  is an eigenvector with eigenvalue zero, i.e. A is singular.  $\Box$ 

However, as we will see below, the particular class of radial functions  $\phi_d(r)$  given by (1.3) offers non-singularity for arbitrarily scattered data in up to d dimensions.

3. Some basic features of the Bessel-based radial functions  $\phi_d(r)$ . The functions  $\phi_d(r)$ , as given in (1.3), arise as eigenfunctions to Laplace's operator in d dimensions. Assuming symmetry around the origin, the Laplace eigenvalue problem

$$\Delta \phi + \varepsilon^2 \phi = 0 \tag{3.1}$$



FIG. 2.1. Distributions of d + 1 points in d dimensions such that all points have a distance  $\rho$  between each other.

transforms to

$$\phi''(r) + \frac{d-1}{r}\phi'(r) + \varepsilon^2\phi(r) = 0,$$

for which the solutions that are bounded at the origin become (1.3). An immediate consequence of (3.1) is that the RBF interpolant  $s(\underline{x})$  based on  $\phi_d(r)$  in d dimensions will itself satisfy (3.1), i.e.

$$\Delta s + \varepsilon^2 s = 0. \tag{3.2}$$

This result puts a tremendous restraint on  $s(\underline{x})$ . For example,  $s(\underline{x})$  can never feature a local maximum (at which  $\Delta s(\underline{x}) \leq 0$ ) unless  $s(\underline{x})$  at that point is non-negative. However, if  $\phi_d(r)$  is used in less than d space dimensions, no similar problem appears to be present.

THEOREM 3.1. The radial functions given by (1.3) will give nonsingular interpolation in up to d dimensions when  $d \ge 2$ .

*Proof.* Let n denote the number of data points. We first note that when n = 1, the theorem is trivially true, so we focus on the case of  $n \ge 2$ . Second, we note that if the result for  $\phi_d(r)$  holds in d dimensions, it automatically holds also in less than d dimensions (since that is a sub-case of the former). Also, we can simplify the notation by setting  $\varepsilon = 1$ . The second equality in the equation below is a standard one, related to Hankel transforms:

$$\phi_d(\|\underline{x}\|) = \frac{J_{\frac{d}{2}-1}(\|\underline{x}\|)}{\|\underline{x}\|^{\frac{d}{2}-1}} = \frac{1}{(2\pi)^{\frac{d}{2}}} \int_{\|\underline{\omega}\|=1} e^{i\,\underline{x}\cdot\underline{\omega}}\,d\underline{\omega}$$
(3.3)

(see for example [2, p. 53]; it also arises as a special case of a general formula for  $\int_{\|\underline{\omega}\|=1} f(\underline{x} \cdot \underline{\omega}) \ d\underline{\omega}$  [10, pp. 8-9]). Here  $\underline{x}, \underline{\omega} \in \mathbb{R}^d$  and  $\int_{\|\underline{\omega}\|=1}$  represents the surface integral over the unit sphere in  $\mathbb{R}^d$ . For d = 1 ( $\underline{x} = x$ ), the right hand side of (3.3) should be interpreted as  $\frac{1}{\sqrt{2\pi}} (e^{ix} + e^{-ix})$ .

To show first that A is positive semi-definite (a result that was previously noted in [17]; see also [18]), we follow an argument originally given in [1]. Let  $\underline{\alpha} = [\alpha_1, \ldots, \alpha_n]^T$  be any column vector and A be the matrix in (1.2). Then

$$\begin{bmatrix} \underline{\alpha}^T \end{bmatrix} \begin{bmatrix} A \end{bmatrix} \begin{bmatrix} \underline{\alpha} \end{bmatrix} = \sum_{j=1}^n \sum_{k=1}^n \alpha_j \alpha_k \phi_d \left( \left\| \underline{x}_j - \underline{x}_k \right\| \right) = 5$$

$$\frac{1}{(2\pi)^{\frac{d}{2}}} \sum_{j=1}^{n} \sum_{k=1}^{n} \alpha_{j} \alpha_{k} \int_{\|\underline{\omega}\|=1} e^{i (\underline{x}_{j} - \underline{x}_{k}) \cdot \underline{\omega}} d\underline{\omega} =$$

$$\frac{1}{(2\pi)^{\frac{d}{2}}} \int_{\|\underline{\omega}\|=1} \sum_{j=1}^{n} \sum_{k=1}^{n} \alpha_{j} \alpha_{k} e^{i (\underline{x}_{j} - \underline{x}_{k}) \cdot \underline{\omega}} d\underline{\omega} =$$

$$\frac{1}{(2\pi)^{\frac{d}{2}}} \int_{\|\underline{\omega}\|=1} \left| \sum_{j=1}^{n} \alpha_{j} e^{i \underline{x}_{j} \cdot \underline{\omega}} \right|^{2} d\underline{\omega} \ge 0$$

The finishing step is to show that A is not just positive semi-definite, but indeed positive definite. For this, we need to show that  $f(\underline{\omega}) = \sum_{m=1}^{n} \alpha_m e^{i \underline{\omega} \cdot \underline{x}_m} \equiv 0$  on the surface of the unit ball  $\|\underline{\omega}\| = 1$  implies that all  $\alpha_m = 0$ . Since the surface of the unit ball in  $R^d$  has measure zero in that space, the desired result cannot be concluded from Lemma 6 in [3, p.91]. We therefore provide a proof for d = 2 (and higher). However, before doing so, we note why the result will not hold when d = 1:

d = 1 (The theorem is not valid):  $\|\underline{\omega}\| = 1$  includes only two values,  $\omega = -1$  and  $\omega = 1$ . For n > 2, the two equations  $\sum_{m=1}^{n} \alpha_m e^{-ix_m} = 0$  and  $\sum_{m=1}^{n} \alpha_m e^{ix_m} = 0$  clearly possess non-trivial solutions for  $\alpha_m$ , being just two homogeneous equations in n unknowns. For n = 2, the existence of non-trivial solutions depends on the values of  $x_1$  and  $x_2$ . For example, with  $x_1 = \pi$  and  $x_2 = 0$ , any  $\alpha_1 = \alpha_2 \in \mathbb{C}$  is a solution.

d = 2: Now there are infinitely many points  $\underline{\omega}$  satisfying  $\|\underline{\omega}\| = 1$ , but still only nunknowns—so we would not expect any non-trivial solutions. More precisely: With  $\underline{\omega} = [\cos \theta, \sin \theta]$ , we can write  $f(\underline{\omega})$  as  $f(\theta) = \sum_{m=1}^{n} \alpha_m e^{i\|\underline{x}_m\| \cos(\theta - \beta_m)}$  where  $\beta_m$  is the argument of  $\underline{x}_m$ . This is an *entire* function of  $\theta$ . Thus, since we have assumed  $f(\theta) \equiv 0$  when  $\theta$  is real (corresponding to  $\|\underline{\omega}\| = 1$ ), the same holds also for all complex values of  $\theta$ . Let k be such that  $\|\underline{x}_k\| \geq \|\underline{x}_m\|$ ,  $m = 1, \ldots, n$  and choose  $\theta = \beta_k + \frac{\pi}{2} + i\xi$ , where  $\xi$  is real and  $\xi > 0$ . With the assumption that the node points are distinct, the term multiplying the coefficient  $\alpha_k$  in the sum will then grow faster than the term multiplying any other coefficient as  $\xi$  increases. Since  $\xi$  can be arbitrarily large, we must have  $\alpha_k = 0$ . The argument can then repeated for all remaining coefficients. Hence, the only way  $f(\underline{\omega}) \equiv 0$  for  $\|\underline{\omega}\| = 1$  is if  $\alpha_m = 0$  for  $m = 1, \ldots, n$ .

d = 3 (and higher): The space  $\|\underline{\omega}\| = 1$  is even larger (a sphere, or higher). The argument for the d = 2 case carries over virtually unchanged.  $\Box$ 

## 4. Properties of the $\phi_d(r)$ interpolants in the limit of $\varepsilon \to 0$ .

**4.1. Taylor expansion of**  $\phi_d(r)$ . The Taylor expansion of  $\phi_d(r)$  contains only even powers of  $\varepsilon r$ :

$$\phi_d(r) = a_0 + a_1(\varepsilon r)^2 + a_2(\varepsilon r)^4 + a_3(\varepsilon r)^6 + \dots$$
(4.1)

where the coefficients are functions of d. Since an RBF interpolant is unaffected if the radial function is multiplied by a constant factor, we instead use  $\psi_d(r)$  (1.4) so that  $a_0 = 1$ . With the appropriate normalization of the series expansion of  $J_{d/2-1}(\varepsilon r)$ , the coefficients in (4.1) then become

$$a_k = \frac{(-1)^k}{2^k k!} \frac{1}{\prod_{i=0}^{k-1} (d+2i)}, \quad k = 1, 2, \dots ,$$
(4.2)

 $a_{0} = 1$   $a_{1} = -\frac{1}{2d}$   $a_{2} = \frac{1}{8 d(d+2)}$   $a_{3} = -\frac{1}{48 d(d+2)(d+4)}$   $a_{4} = \frac{1}{384 d(d+2)(d+4)(d+4)}$ :

**4.2. Interpolation when the data is located in 1-D.** The situation when all the data points  $x_j$ , as well as the interpolation point x, are located in 1-D was analyzed in [4]. It was shown that the interpolant s(x) converges to Lagrange's interpolation polynomial when  $\varepsilon \to 0$  on condition that all of the determinants  $G_{0,k}$  and  $G_{1,k}$ ,  $k = 0, 1, 2, \ldots$  are non-zero, where

$$G_{0,k} = \begin{vmatrix} \begin{pmatrix} 0 \\ 0 \end{pmatrix} a_0 & \begin{pmatrix} 2 \\ 2 \end{pmatrix} a_1 & \cdots & \begin{pmatrix} 2k \\ 2k \end{pmatrix} a_k \\ \begin{pmatrix} 2 \\ 0 \end{pmatrix} a_1 & \begin{pmatrix} 4 \\ 2 \end{pmatrix} a_2 & \cdots & \begin{pmatrix} 2k+2 \\ 2k \end{pmatrix} a_{k+1} \\ \vdots & \vdots & \vdots \\ \begin{pmatrix} 2k \\ 0 \end{pmatrix} a_k & \begin{pmatrix} 2k+2 \\ 2 \end{pmatrix} a_{k+1} & \cdots & \begin{pmatrix} 4k \\ 2k \end{pmatrix} a_{2k} \end{vmatrix}$$
(4.3)

and

$$G_{1,k} = (-1)^{k+1} \begin{vmatrix} \binom{2}{1}a_1 & \binom{4}{3}a_2 & \cdots & \binom{2k+2}{2k+1}a_{k+1} \\ \binom{4}{1}a_2 & \binom{6}{3}a_3 & \cdots & \binom{2k+4}{2k+1}a_{k+2} \\ \vdots & \vdots & \vdots \\ \binom{2k+2}{1}a_{k+1} & \binom{2k+4}{3}a_{k+2} & \cdots & \binom{4k+2}{2k+1}a_{2k+1} \end{vmatrix}.$$
(4.4)

In the present case, with Taylor coefficients given by (4.2), the determinants can be evaluated in closed form:

$$G_{0,k} = \prod_{j=0}^{k-1} \frac{(d+2j-1)^{k-j}}{(2j+2)! \ (d+2j)^{k+1} \ (d+2k+2j)^{k-j}},$$

and

$$G_{1,k} = G_{0,k} \prod_{j=0}^{k} \frac{1}{(2j+1) (d+2k+2j)}$$

These determinants are all zero when d = 1 and k > 0, but never zero for  $d = 2, 3, \ldots$ . The singular behavior for d = 1 should be expected, since  $\phi_1(r) = \cos(r)$  (when normalized so that  $a_0 = 1$ ). In 1-D, any three translates of this function are linearly dependent, and these functions can therefore not serve as a basis for interpolation. However, the result shows that, when using  $\phi_d(r)$  with  $d \ge 2$ , the  $\varepsilon \to 0$  limit will always become the Lagrange interpolation polynomial (i.e. the interpolation polynomial of lowest possible degree).

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i.e.

**4.3. Interpolation when the data is located in** *m***-D.** In *m* dimensions, there are similar conditions for the RBF interpolant to converge to a unique lowest-degree interpolating polynomial as  $\varepsilon \to 0$ . The following two conditions need to be fulfilled:

- (i) The point set is unisolvent, i.e. there is a unique polynomial of lowest possible degree that interpolates the given data.
- (ii) The determinants  $G_{i,k}$  are non-zero for i = 0, ..., m and k = 0, 1, ...

A thorough discussion of the condition (i) and what it means when it fails, together with the general definitions of  $G_{i,k}$ , are given in [12]. For the oscillatory RBFs considered here, we can again give the determinants in closed form as

$$G_{0,k} = \prod_{j=0}^{k-1} \frac{(d-m+2j)^{p_m(k-j-1)}}{\left[(2j+1)(2j+2)\right]^{mp_m(k-j-1)}} (d+2j)^{p_m(k)} (d+2k+2j)^{p_m(k)-p_m(j)}}$$

and

$$G_{i+1,k} = G_{i,k} \prod_{j=0}^{k} \frac{1}{(2j+1)^{p_{m-1}(k-j)} (d+2k+2j+2i)^{p_{m-1}(j)}} ,$$

where

$$p_m(k) = \binom{m+k}{k}.$$

Note that the expressions given for interpolation in 1-D are just special cases of the general expressions above. The determinants are all zero for k > 0 when d = m. They are also zero for k > j, when d = m - 2j,  $j = 0, \ldots, \lfloor \frac{m-1}{2} \rfloor$ . However, the determinants are never zero for d > m. Accordingly, when  $\phi_d(r)$  with d > m are used as basis functions, the RBF interpolant  $s(\underline{x})$  always converges to the lowest degree interpolating polynomial as  $\varepsilon \to 0$ , provided this is uniquely determined by the data.

4.4. Convergence/divergence when points are located along a straight line, but evaluated off the line. There are several reasons for being interested in this case. It was first noted in [8] that

- The cases of points along a straight line provide the simplest known examples of divergence in the  $\varepsilon \to 0$  limit,
- Divergence can arise for some radial functions in cases where polynomial unisolvency fails. The most extreme such case is the one with all points along a line (a 1-D subset of a higher-dimensional space). Divergence has never been observed for any point distributions, unless also this special case produces divergence,
- The straight line situation permits some exact analysis.

We proved in [8] that GA will never diverge when all points lie along a line and the interpolant is evaluated off the line. The proof that the same holds for all the  $\phi_d(r)$  functions for  $d \ge 2$  is easiest in the case of d = 2, and we consider that case first:

LEMMA 4.1. If the polynomial q(x, y) is not identically zero, and  $p(x, y) = y^n q(x, y)$  satisfies Laplace's equation  $\Delta p = 0$ , then n = 0 or n = 1.

*Proof.* Assume that n is the highest power of y that can be factored out of p(x, y). Substituting  $p = y^n q$  into  $\Delta p = 0$  and dividing by  $y^{n-2}$  gives

$$y^{2}q_{xx} + n(n-1) q + 2n y q_{y} + y^{2}q_{yy} = 0.$$
(4.5)

Unless n = 0 or n = 1, this shows that  $q(x, 0) \equiv 0$ , contradicting the initial assumption in this proof.  $\Box$ 

THEOREM 4.2. When all the data is located along a straight line, interpolants based on the  $\phi_d(r)$  radial functions (for  $d \ge 2$ ) will not diverge at any location off that line when  $\varepsilon \to 0$ .

*Proof.* We again assume first that d = 2 and that the data is located along the x-axis. Knowing from [8] that the RBF interpolant is expandable in powers of  $\varepsilon^2$  with coefficients that are polynomials in  $\underline{x} = (x, y)$ , we have

$$s(\underline{x},\varepsilon) = \frac{1}{\varepsilon^{2m}} p_{-2m}(x,y) + \frac{1}{\varepsilon^{2m-2}} p_{-2m+2}(x,y) + \dots + p_0(x,y) + \varepsilon^2 p_2(x,y) + \dots$$
(4.6)

We assume that  $p_{-2m}(x, y)$ , with m > 0, is not identically zero, and we will show that this leads to a contradiction. Substituting (4.6) into (3.2) and equating powers of  $\varepsilon^2$  gives rise to a sequence of equations

$$\Delta p_{-2m}(x,y) = 0 \Delta p_{-2m+2}(x,y) = -p_{-2m}(x,y) .$$
(4.7)

Knowing from Section 4.2 that we get convergence along the line y = 0 (to Lagrange's interpolating polynomial),  $p_{-2m}(x, y)$  must be identically zero when y = 0. Since  $s(\underline{x}, \varepsilon)$  and therefore also  $p_{-2m}(x, y)$  are even functions of y, it holds that

$$p_{-2m}(x,y) = y^2 q(x,y)$$
(4.8)

where q(x, y) is a polynomial in x and y. From the Lemma above follows now that  $p_{-2m}(x, y) \equiv 0$ , and the proof for the d = 2-case is finished.

The argument above generalizes to d > 2. With  $\underline{x} = (x, x_2, x_3, \dots, x_d)$ , radial symmetry assumed in all but the first variable, and with  $r^2 = x_2^2 + \ldots + x_d^2$ , equation (4.5) generalizes to

$$r^{2}q_{xx} + n(n+d-3)q + (2n+d-2) r q_{r} + r^{2}q_{rr} = 0,$$

and only n = 0 becomes permissible. The rest follows as above.

One key tool for analytically exploring this  $\varepsilon \to 0$  limit is the following theorem, previously given in [8]:

THEOREM 4.3. For cardinal data  $y_k = \begin{cases} 1 & \text{if } k = 1 \\ 0 & \text{otherwise} \end{cases}$ , the RBF interpolant of the form (1.1) becomes

$$s(\underline{x}) = \frac{\det \begin{bmatrix} \phi(\|\underline{x} - \underline{x}_1\|) & \phi(\|\underline{x} - \underline{x}_2\|) & \cdots & \phi(\|\underline{x} - \underline{x}_n\|) \\ \phi(\|\underline{x}_2 - \underline{x}_1\|) & \phi(\|\underline{x}_2 - \underline{x}_2\|) & \cdots & \phi(\|\underline{x}_2 - \underline{x}_k\|) \\ \vdots & \vdots & \ddots & \vdots \\ \phi(\|\underline{x}_n - \underline{x}_1\|) & \phi(\|\underline{x}_n - \underline{x}_2\|) & \cdots & \phi(\|\underline{x}_n - \underline{x}_n\|) \end{bmatrix}}{\det \begin{bmatrix} \phi(\|\underline{x}_1 - \underline{x}_1\|) & \phi(\|\underline{x}_1 - \underline{x}_2\|) & \cdots & \phi(\|\underline{x}_1 - \underline{x}_n\|) \\ \phi(\|\underline{x}_2 - \underline{x}_1\|) & \phi(\|\underline{x}_2 - \underline{x}_2\|) & \cdots & \phi(\|\underline{x}_2 - \underline{x}_k\|) \\ \vdots & \vdots & \ddots & \vdots \\ \phi(\|\underline{x}_n - \underline{x}_1\|) & \phi(\|\underline{x}_n - \underline{x}_2\|) & \cdots & \phi(\|\underline{x}_n - \underline{x}_n\|) \end{bmatrix}}.$$
(4.9)

It turns out that placing up to four points along a line (say, the x-axis) will not cause divergence at any evaluation point off the line. For five points, evaluating at a location (x, y) off the x-axis (for example by means of substituting the Taylor expansions (4.1) for a general radial function  $\phi(r)$  into (4.9)) gives

$$s(x,y) = \frac{4 y^2}{(x_1 - x_2)(x_1 - x_3)(x_1 - x_4)(x_1 - x_5)} \cdot (4.10)$$
  
$$\cdot \frac{(a_1 a_2^2 - 3a_1^2 a_3 + 3a_0 a_2 a_3)}{(6a_2^3 + 225a_0 a_3^2 + 70a_1^2 a_4 - 30a_1 a_2 a_3 - 420a_0 a_2 a_4)} \frac{1}{\varepsilon^2} + O(1)$$

Assuming we are dealing with a radial function  $\phi(r)$  such that the determinants in (4.3) and (4.4) are non-zero, the requirements  $2a_2^2 - 5a_1a_3 \neq 0$  (needed for a cancellation while deriving (4.10)) and  $6a_2^3 + 225a_0a_3^2 + 70a_1^2a_4 - 30a_1a_2a_3 - 420a_0a_2a_4 \neq 0$  (to avoid a divide by zero in (4.10)) follow from  $G_{1,1} \neq 0$  and  $G_{0,2} \neq 0$ , respectively. We can conclude that divergence will occur for s(x, y) unless

$$a_1 a_2^2 - 3a_1^2 a_3 + 3a_0 a_2 a_3 = 0. (4.11)$$

With *Mathematica*, we have been able to push the same analysis up to 8 points along a line. For each case, we need the previously obtained conditions, and again that certain additional  $G_{i,k}$ -determinants (4.3) and (4.4) are non-zero. The requirements that enter for different numbers of points turn out to be

5 points	$a_1a_2^2 - 2 \cdot \frac{3}{2}a_1^2a_3 + \frac{3}{1}a_0a_2a_3$	$_{3} = 0$
6 points	$a_2a_3^2 - 2 \cdot \frac{4}{3}a_2^2a_4 + \frac{4}{2}a_1a_3a_4$	$_{4} = 0$
7 points	$a_3a_4^2 - 2 \cdot \frac{5}{4}a_3^2a_5 + \frac{5}{3}a_2a_4a_5$	5 = 0
8 points	$a_4a_5^2 - 2 \cdot \frac{6}{5}a_4^2a_6 + \frac{6}{4}a_3a_5a_6$	$_{3} = 0$

Unfortunately, at present, the algebra becomes too extensive for us to generate additional conditions, corresponding to still higher numbers of data points. However, it does not seem far-fetched to hypothesize that the pattern above will continue indefinitely, i.e.

• Precisely one additional condition (beyond the previous ones) will enter each time we include an additional point, and

• When including point n + 2,  $n = 3, 4, 5, \ldots$ , the new requirement will be

$$a_{n-2}a_{n-1}^2 - 2 \cdot \frac{n}{n-1}a_{n-2}^2a_n + \frac{n}{n-2}a_{n-3}a_{n-1}a_n = 0$$
(4.12)

Of the smooth radial functions in Table 1, MQ, IMQ, and IQ violate already the condition for 5 points. Hence, interpolants based on these will diverge in the  $\varepsilon \to 0$  limit. In contrast, GA and the  $\phi_d(r)$  functions (for all  $\varepsilon$  and d) satisfy (4.12) for all values of  $n = 3, 4, 5, \ldots$ . This is in complete agreement with our result just above that the  $\phi_d(r)$  functions will not cause divergence for any number of points along a line.

It is of interest to ask which is the most general class of radial functions for which the Taylor coefficients obey (4.12) - i.e. the interpolants do not diverge in the  $\varepsilon \to 0$  limit.

THEOREM 4.4. On assumption that (4.12) holds, the corresponding radial function  $\phi(r)$  can only differ from the class  $\phi_d(r)$  by some trivial scaling.

*Proof.* Equation (4.12) can be written as

$$a_n = \frac{a_{n-2}a_{n-1}^2}{n\left(\frac{2}{n-1}a_{n-2}^2 - \frac{1}{n-2}a_{n-3}a_{n-1}\right)}, \quad n = 3, 4, 5, \dots$$
 (4.13)

This is a non-linear recursion relation that determines  $a_n$ , n = 3, 4, 5, ... from  $a_0, a_1$ , and  $a_2$ . Since any solution sequence can be multiplied by an arbitrary constant, we can set  $a_0 = 1$ . Then choosing  $a_1 = \beta$  and  $a_2 = \gamma \beta^2$  lead to the closed form solution

$$a_n = \frac{2^{n-1} \beta^n \gamma^{n-1}}{n \prod_{k=1}^{n-1} (k - 2(k-1)\gamma)} \quad (n \ge 1),$$

as is easily verified by induction. Thus

$$\phi(r) = \sum_{n=0}^{\infty} a_n r^{2n} = \ _0 F_1 \left[ \frac{2\gamma}{1-2\gamma}, \frac{2\gamma}{1-2\gamma} r^2 \right].$$

Apart from a trivial change of variables, this agrees with (1.4), and thus also with (1.3). With  $\beta = -\varepsilon^2$  and taking the limit  $\gamma \to \frac{1}{2}$ , this evaluates to  $e^{-(\varepsilon r)^2}$ , again recovering the GA radial function as a special case  $\Box$ 

Some of the results above are illustrated in the following example:

EXAMPLE 4.5. Let the data be cardinal (first value one and the remaining values zero), and the point locations be  $x_k = k-1, k = 1, ..., n$ . Evaluate the RBF interpolant off the x-axis at (0,1). This produces the values (to leading order) as shown in Table 4.1. The computation was carried up to n = 10, with the same general pattern continuing, i.e.

- For the 'general case', represented here by MQ, IMQ, and IQ, the divergence rate increases with n; as  $O\left(1/\varepsilon^{2\left[\frac{n-3}{2}\right]}\right)$  where  $[\cdot]$  denotes the integer part,
- For GA, the limit is in all cases = 1 (as follows from results in [8] and [16]),
- For each  $\phi_d(r)$  function, there is always convergence to some constant.

n	1	2	3	4	5	6	7	8
MQ	1	1	$\frac{5}{4}$	$\frac{5}{4}$	$\frac{1}{168\varepsilon^2}$	$\frac{3}{616\varepsilon^2}$	$\frac{1}{13770\varepsilon^4}$	$\frac{1337}{24180120\varepsilon^4}$
IMQ	1	1	$\frac{9}{8}$	$\frac{37}{32}$	$\frac{1}{168\varepsilon^2}$	$\frac{333}{176648\epsilon^2}$	$\frac{5}{304296\varepsilon^4}$	$\frac{208631}{12790879496\varepsilon^4}$
IQ	1	1	$\frac{11}{10}$	$\frac{17}{15}$	$\frac{1}{894\varepsilon^2}$	$\frac{43}{32482\varepsilon^2}$	$\frac{11}{1207125\epsilon^4}$	$\frac{73298}{7256028375\varepsilon^4}$
GA	1	1	1	1	1	1	1	1
$\phi_2(r)$	1	1	$\frac{1}{2}$	0	$-\frac{5}{12}$	$-\frac{3}{4}$	$-\frac{73}{72}$	$-\frac{11}{9}$
$\phi_3(r)$	1	1	$\frac{3}{4}$	$\frac{1}{2}$	$\frac{55}{192}$	$\frac{7}{64}$	$-\frac{427}{11520}$	$-\frac{457}{2880}$
$\phi_4(r)$	1	1	$\frac{5}{6}$	$\frac{2}{3}$	$\frac{47}{90}$	$\frac{2}{5}$	$\frac{1121}{3780}$	$\frac{197}{945}$
TABLE 4.1								

Values of RBF interpolants at location (0,1) in Example 4.5, to leading order.

## 4.5. Two additional examples regarding more general point distributions.

EXAMPLE 4.6. Place n points along a parabola instead of along a straight line. It transpires that for this example we won't get divergence (for any smooth radial function) when  $n \leq 7$ . For n = 8, divergence (when evaluating off the parabola) will occur unless (4.11) holds.

This raises the question if possibly different non-unisolvent point distributions might impose the same conditions as (4.12) for non-divergence—just that more points are needed before the conditions come into play. If this were the case, non-divergence in the special case of all points along a line would suffice to establish the same for general point distributions.

Another point distribution case which gives general insight is the following:

EXAMPLE 4.7. Instead of scattering the points in 1-D and evaluating the interpolant in 2-D, scatter the points randomly in d dimensions, and then evaluate the interpolant in the d+1 dimension (i.e. scatter the points randomly on a d-dimensional hyperplane, and evaluate the interpolant at a point off the hyperplane). In the d = 1case, divergence for any radial function can arise first with  $n_1 = 5$  points. This divergence comes from the fact that the Taylor expansions of the numerator and denominator in (4.9) then become  $O(\varepsilon^{18})$  and  $O(\varepsilon^{20})$  respectively, i.e. a difference in exponents by two. Computations (using the Contour-Padé algorithm [7]) for  $d \leq 8$  suggest that this  $O(\frac{1}{\varepsilon^2})$  divergence generalizes to  $n_d = 1 + \binom{d+3}{3} = 1 + \frac{1}{6}(d+1)(d+2)(d+3)$  points. The GA and  $\phi_k(r)$  functions were exceptional in this example. Divergence was never observed for GA or for  $\phi_k(r)$  as long as the dimension d < k. When d = k, we were able to computationally find (for  $k \leq 8$ ) a point distribution that led to  $O(\frac{1}{2})$  divergence when the interpolant was evaluated at a point in the d+1 dimension. Table 4.2 lists the minimum number of points  $n_d$  that produced this type of divergence, as well as the leading power of  $\varepsilon$  in the numerator and denominator in (4.9). Interestingly, we found that no divergence resulted when d > k. The computations suggest that  $\phi_k(r)$ will lead  $O(\frac{1}{\epsilon^2})$  divergence when d = k, the evaluation point is in d + 1 dimensions, and  $n_d = d(d+1)/2$ . This is consistent with the GA radial function being the limiting case of  $\phi_k(r)$  as  $k \to \infty$  and GA function never leading to divergence as shown in [16].

5. Conclusions. Many types of radial functions have been considered in the literature. Almost all attention has been given to non-oscillatory ones, in spite of

Radial	Min. number	Leading power $\varepsilon$	Leading power $\varepsilon$			
function $\phi_d(r)$	of points $n_d$	in numerator	in denominator			
d = 2	6	16	18			
d = 3	10	30	32			
d = 4	15	48	50			
d = 5	21	70	72			
d = 6	28	96	98			
d = 7	36	126	128			
d = 8	45	160	162			
TABLE 4.2						

Minimum number of points to produce  $O(\frac{1}{\varepsilon^2})$  divergence in  $\phi_d(r)$  radial functions when the points are distributed on a d-dimensional hyperplane and the corresponding interpolant is evaluated at a point off the hyperlane. Also displayed are the corresponding leading powers of  $\varepsilon$  in the numerator and denominator of (4.9)

the fact that basis functions in other contexts typically are highly oscillatory (such as Fourier and Chebyshev functions). We show here that one particular class of oscillatory radial functions, given by (1.3), not only possesses unconditional non-singularity (with respect to point distributions) for  $\varepsilon > 0$ , but also appears immune to divergence in the flat basis function limit  $\varepsilon \to 0$ . Among the standard choices of radial functions, such as MQ or IQ, only GA was previously known to have this property. When this  $\varepsilon \to 0$  limit exists, pseudospectral (PS) approximations can be seen as the flat basis function limit of RBF approximations. The present class of Bessel function based radial functions (including GA as a special case) thus appears to offer a particularly suitable starting point for exploring this relationship between PS and RBF methods (with the latter approach greatly generalizing the former to irregular point distributions in an arbitrary number of dimensions).

An important issue that warrants further investigation is how this new class of radial functions fits in with the standard analysis on RBF error bounds. In contrast to most radial functions, the present class is band limited. This feature in itself needs not detract from its approximation qualities, as is evidenced by polynomials. For these, the (generalized) Fourier transform is merely a combination (at the origin) of a delta function and its derivatives. Indeed, the present class of RBFs support a rich set of exact polynomial reproductions on infinite lattices, as is shown in [5].

## REFERENCES

- S. BOCHNER, Monotone functionen, stieltjes integrale und harmonische analyse, Math. Ann., 108 (1933), pp. 378–410.
- [2] M. D. BUHMANN, Radial Basis Functions: Theory and Implementations, 12. Cambridge Monographs on Applied and Computational Mathematics, Cambridge University Press, Cambridge, 2003.
- [3] E. W. CHENEY AND W. A. LIGHT, A Course in Approximation Theory, Brooks/Cole, New York, 2000.
- [4] T. A. DRISCOLL AND B. FORNBERG, Interpolation in the limit of increasingly flat radial basis functions, Comput. Math. Appl., 43 (2002), pp. 413–422.
- [5] N. FLYER, Exact polynomial reproduction for oscillatory radial basis functions on infinite lattices, Comput. Math. Appl., Submitted (2004).
- [6] B. FORNBERG, A Practical Guide to Pseudospectral Methods, Cambridge University Press, Cambridge, 1996.
- [7] B. FORNBERG AND G. WRIGHT, Stable computation of multiquadric interpolants for all values of the shape parameter, Comput. Math. Appl., 48 (2004), pp. 853–867.

- [8] B. FORNBERG, G. WRIGHT, AND E. LARSSON, Some observations regarding interpolants in the limit of flat radial basis functions, Comput. Math. Appl., 47 (2004), pp. 37–55.
- S. JAKOBSSON, Frequency optimization, radial basis functions and interpolation, Scientific Report FOI-R-0984-SE, Swedish Defence Research Agency, Division of Aeronautics, Stockholm, 2004.
- [10] F. JOHN, Plane Waves and Spherical Means, Interscience Publishers, New York, 1955. Reprinted by Dover Publications (2004).
- [11] E. LARSSON AND B. FORNBERG, A numerical study of some radial basis function based solution methods for elliptic PDEs, Comput. Math. Appl., 46 (2003), pp. 891–902.
- [12] —, Theoretical and computational aspects of multivariate interpolation with increasingly flat radial basis functions, Comput. Math. Appl., 49 (2005), pp. 103–130.
- [13] R. J. Y. MCLEOD AND M. L. BAART, Geometry and Interpolation of Curves and Surfaces, Cambridge University Press, Cambridge, 1998.
- [14] C. A. MICCHELLI, Interpolation of scattered data: distance matrices and conditionally positive definite functions, Constr. Approx., 2 (1986), pp. 11–22.
- [15] M. J. D. POWELL, The theory of radial basis function approximation in 1990, in Advances in Numerical Analysis, Vol. II: Wavelets, Subdivision Algorithms and Radial Functions, W. Light, ed., Oxford University Press, Oxford, UK, 1992, pp. 105–210.
- [16] R. SCHABACK, Multivariate interpolation by polynomials and radial basis functions, Constr. Approx., Submitted (2004).
- [17] I. J. SCHOENBERG, Metric spaces and completely monotone functions, Ann. Math., 39 (1938), pp. 811–841.
- [18] J. H. WELLS AND L. R. WILLIAMS, Embeddings and Extensions in Analysis, Ergenisse der Mathematik und ihrer Grenzgebiete, Band 84, Springer-Verlag, New York, 1975.