Reproduction of Polynomials by Radial Basis Functions

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Abstract

For radial basis function interpolation of scattered data in $\mathbb{R}^d$, the approximative reproduction of high-degree polynomials is studied. Results include uniform error bounds and convergence orders on compact sets.

§1. Introduction

We consider interpolation of real-valued functions f defined on a set $\Omega \subseteq \mathbb{R}^d$, $d \geq 1$. These functions are interpolated on a set $X := \{x_1, \ldots, x_{N_X}\}$ of $N_X \geq 1$ pairwise distinct points $x_1, \ldots, x_{N_X}$ in Ω. Interpolation is done by linear combinations of translates $\Phi(x - x_j)$ of a single continuous real-valued function Φ defined on $\mathbb{R}^d$. For various reasons it is sometimes necessary to add the space $\mathbb{P}_m^d$ of d–variate polynomials of order not exceeding m to the interpolating functions. Interpolation is uniquely possible under the requirement

$$\text{If } p \in P_m^d \text{ satisfies } p(x_i) = 0 \text{ for all } x_i \in X \text{ then } p = 0, \tag{1}$$

and if Φ is conditionally positive definite of order m (see e.g. [8]):

Definition 1. *A function $\Phi : \mathbb{R}^d \to \mathbb{R}$ with $\Phi(-x) = \Phi(x)$ is conditionally positive definite of order m on $\mathbb{R}^d$, if for all sets $X = \{x_1, \ldots, x_{N_X}\} \subset \mathbb{R}^d$ with N_X distinct points and all vectors $\alpha := (\alpha_1, \ldots, \alpha_{N_X}) \in \mathbb{R}^{N_X}$ with*

$$\sum_{j=1}^{N_X} \alpha_j p(x_j) = 0 \quad \textit{for all } p \in \mathbb{P}_m^d \tag{2}$$

the quadratic form $\sum_{j,k=1}^{N_X} \alpha_j \alpha_k \Phi(x_j - x_k)$ attains nonnegative values and vanishes only if $\alpha = 0$.

We list a few examples where $\Phi(x) := \phi(\|x\|_2)$ is truly radial:

Multiquadrics $\phi(r) = (c^2 + r^2)^{\beta/2}$ for $\beta \in \mathbb{R}_{>-d} \setminus 2\mathbb{Z}$ and $2m > \beta$,
Thin-plate splines $\phi(r) = r^\beta$ for $\beta \in \mathbb{R}_{>0} \setminus 2\mathbb{Z}$ and $2m > \beta$,
Thin-plate splines $\phi(r) = (-1)^{\beta/2+1} r^\beta \log r$ for $\beta \in 2\mathbb{N}$, $2m > \beta$,

Sobolew splines $\phi(r) = \frac{2\pi^{d/2}}{\Gamma(k)} K_{k-d/2}(r)(r/2)^{k-d/2}$ for $k > d/2$ and $m \geq 0$, using the Macdonalds (or modified spherical Bessel) function K_ν,
Gaussians $\phi(r) = e^{-cr^2}$ for $c > 0$ and $m \geq 0$.

There has been some discussion concerning the relative merits of these radial basis functions. Gaussians and other integrable radial basis functions were said to have “a severe disadvantage”, because they are not exact on constant functions [1, p. 93]. The other choices, especially multiquadrics, were said to be “far superior”.

On the other hand, Gaussians have an even better convergence behavior than multiquadrics, when used on scattered data (Madych/Nelson [6]) for c fixed. Thus it is questionable whether the advantage of a method must be necessarily tied to its polynomial reproduction properties. The link between convergence orders and polynomial reproduction properties is clearly visible in theories on grids that make use of Strang and Fix conditions (see the review by W. Light [3]), but it is not at all evident for interpolation of scattered data on irregular domains. Exact reproduction may well be replaced by high-order approximation without any loss in theory and numerical practice.

Numerical results indicate that radial basis function interpolation behaves very well indeed on data from polynomials, provided that the centers are dense enough in and around the domain where the interpolant is evaluated. To add further support to this statement, this paper investigates the polynomial reproduction properties of radial basis function interpolation in the scattered data case.

§2. Spaces for Radial Basis Functions

Each conditionally positive definite function Φ allows two constructions of an inner-product space of functions. Both constructions are based on ideas of Madych and Nelson [4, 5], but we adopt the terminology of [8] here and omit details.

The *algebraic* approach introduces a space F_Φ by direct reference to the conditional positive definiteness of Φ of order m. Functions of the form

$$f_\alpha(x) = \sum_{j=1}^{N} \alpha_j \Phi(x - x_j), \tag{3}$$

with (2) are in F_Φ and have a norm $\|f_\alpha\|_\Phi^2 = \sum_{j,k=1}^{N} \alpha_j \alpha_k \Phi(x_j - x_k)$. The *Fourier transform* approach makes use of the fact that all of the radial basis functions given in the introduction have a generalized Fourier transform in the sense of tempered distributions, and the latter coincides with a positive and continuous function φ on $\mathbb{R}^d \setminus \{0\}$ in the sense of Jones [2]. In this paper we assume the function φ to be continuous and positive on $\mathbb{R}^d \setminus \{0\}$, and to satisfy the conditions

$$\begin{aligned} |\varphi(\omega)| &\geq C \cdot \|\omega\|^{-d-s_0} &&, \omega \in U, \\ |\varphi(\omega)| &\geq c \cdot e^{-\gamma\|\omega\|^2} &&, \omega \notin U, \\ |\varphi(\omega)| &\leq c \cdot \|\omega\|^{-d-s_\infty} &&, \omega \notin U. \end{aligned} \tag{4}$$

on a neighborhood $U = K_R(0) = \{x \mid \|x\|_2 < R,\ x \neq 0\}$ of the origin in $\mathbb{R}^d \setminus \{0\}$. Examples are compiled conveniently in [1] and [8], and we add $\varphi(\omega) = (1 + \|\omega\|_2^2)^{-k}$ for Sobolew radial basis functions of order k. This function, for instance, satisfies (4) for $s_0 = -d$, $s_\infty = 2k - d$, and an arbitrary $\gamma > 0$ related to the radius R of the ball U.

The Fourier transform approach introduces the scalar product

$$(f, g)_\varphi := (2\pi)^{-d} \int_{\mathbb{R}^d} \frac{\hat{f}(\omega)\overline{\hat{g}(\omega)}}{\varphi(\omega)}\, d\omega$$

and the space

$$\mathcal{F}_\varphi := \{f : \mathbb{R}^d \to \mathbb{R} \mid \hat{f} \in L_1(\mathbb{R}^d),\ \|f\|_\varphi < \infty\}, \tag{5}$$

that occurs in [9] and dates back to a similar but different space defined by Madych and Nelson [5], using a nonstandard theory of generalized functions. Functions of the form (3) with (2) for some $m > s_0/2$ are also in $\mathcal{F}_\varphi$ and have a norm

$$\|f_\alpha\|_\varphi^2 = (2\pi)^{-d} \int_{\mathbb{R}_d} \frac{|\hat{f}_\alpha(\omega)|^2}{\varphi(\omega)}\, d\omega = \|f_\alpha\|_\Phi^2.$$

We finally note that the Fourier transform approach adds $\mathbb{P}_q^d$ to $\mathcal{F}_\varphi$ to perform interpolation, where $q > s_0/2$ holds for the smallest possible s_0 in (4). Reasons for this will become apparent later.

§3. Approximation of Polynomials

We shall now approximate polynomials by functions in the space $\mathcal{F}_\varphi$ of (5). First we represent the delta functional δ by the sequence of good functions $\gamma_k(\omega) = \left(\frac{k}{\pi}\right)^{d/2} e^{-k\|\omega\|^2}$ in the sense of Jones [2]. Then the generalized derivative $\mathcal{D}^\alpha\delta$ for a multi-index α is represented by the sequence $D^\alpha\gamma_k$, and the generalized Fourier transform of this sequence represents the polynomial $\widehat{\mathcal{D}^\alpha\delta}(x) = (+ix)^\alpha$. We now fix z and consider the test function $f_{k,\alpha,z}(x) := (i(x+z))^\alpha\hat{\gamma}_k(x+z) = \widehat{D^\alpha\gamma_k}(x+z)$ that satisfies $\delta(f_{k,\alpha,z}) = f_{k,\alpha,z}(0) = (iz)^\alpha\hat{\gamma}_k(z) = (iz)^\alpha e^{-\|z\|^2/4k}$ and converge to $(iz)^\alpha$ for $k \to \infty$, proving that the δ functional is bounded on these functions when $k \to \infty$. We shall make use of this fact later. The functions $f_{k,\alpha,z}(x)$ converge uniformly to the polynomial $(i(x+z))^\alpha$ on compact sets $\Omega \subset \mathbb{R}^d$, if k tends to infinity. This is due to

$$\hat{\gamma}_k(u) = e^{-\|u\|^2/4k} = 1 - \frac{\|u\|^2}{4k} + \frac{\|u\|^4}{16k^2} \pm \cdots \geq 1 - \frac{\|u\|^2}{4k}$$

for all $u \in \mathbb{R}^d$. More precisely, for each α and each compact set $\Omega \subset \mathbb{R}^d$ there is a constant c_0, independent of $k \in \mathbb{N}$ and $x \in \Omega$, such that

$$|(ix)^\alpha - f_{k,\alpha,0}(x)| \leq \frac{\|x\|^2}{4k} \tag{6}$$

holds for all $x \in \Omega$ and all $k \in \mathbb{N}$. In what follows, we shall use the symbols $c, c_0, c_1, \ldots$ to denote generic constants which may differ by certain factors, and we just state the variables that the constants do *not* depend on. Such "constants" may, however, depend on other variables that occur in the context, and these are mainly α, Φ, and Ω.

Now we assert that all the functions $f_{k,\alpha,z}(x)$ are in the spaces $\mathcal{F}_\varphi$ for all radial basis functions that satisfy the basic assumptions (4).

Lemma. *Let the given radial basis function satisfy (4). Then there are positive constants c_1 and c_2, independent of k and z, such that*

$$|f_{k,\alpha,z}|_\varphi^2 = \int \frac{|\widehat{f_{k,\alpha,z}}(\omega)|^2}{\varphi(\omega)}\, d\omega \le c_1 \cdot k^{|\alpha|-s_0/2} \tag{7}$$

holds for all $z \in \mathbb{R}^d$ and all $k \ge c_2$.

Proof: By elementary calculations,

$$\begin{aligned}\widehat{f_{k,\alpha,z}}(\omega) &= (2\pi)^d e^{i\langle z,\omega\rangle} D^\alpha \gamma_k(\omega)\\ &= (2\pi)^d e^{i\langle z,\omega\rangle} \left(\frac{k}{\pi}\right)^{d/2} D^\alpha e^{-k\|\omega\|^2}\end{aligned}$$

and we have to check these derivatives for $k \to \infty$. Using Hermite polynomials $H_n(x)$ defined here as $H_n(x) = (-1)^n e^{x^2/2} D^n e^{-x^2/2}$, we first treat the univariate case by

$$\frac{d^n}{dx^n}\, e^{-x^2/2} = (-1)^n H_n(x) e^{-x^2/2} = (\sqrt{2k})^{-n} \frac{d^n}{d\omega^n}\, e^{-k\omega^2}$$

with $x = \omega\sqrt{2k}$, giving

$$D^n e^{-k\omega^2} = (\sqrt{2k})^n (-1)^n H_n(\omega\sqrt{2k}) e^{-k\omega^2}.$$

The multivariate case is a product of univariate cases, because

$$\begin{aligned}D^\alpha e^{-k\|\omega\|^2} &= \prod_{j=1}^d \frac{\partial^{\alpha_j}}{\partial\omega_j^{\alpha_j}}\, e^{-k\omega_j^2}\\ &= \prod_{j=1}^d (\sqrt{2k})^{\alpha_j} (-1)^{\alpha_j} H_{\alpha_j}(\omega_j\sqrt{2k}) e^{-k\omega_j^2}\\ &= (-\sqrt{2k})^{|\alpha|} e^{-k\|\omega\|^2} H_\alpha(\omega\sqrt{2k}),\end{aligned}$$

where we defined a multivariate Hermite polynomial $H_\alpha(z) = \prod_{j=1}^d H_{\alpha_j}(z_j)$ for $z \in \mathbb{R}^d$, $\alpha \in \mathbb{Z}_{\ge 0}^d$. Using (4), the integral of (7) on U is bounded by

$$k^{d+|\alpha|} \int_U \|\omega\|^{d+s_0} \cdot e^{-2k\|\omega\|^2} \cdot |H_\alpha(\omega\sqrt{2k})|^2 d\omega$$

up to constants which are independent of k and z. By transformation $u = \omega\sqrt{2k}$ we get the bound

$$k^{d+|\alpha|}k^{-d-s_0/2}\int_{\|u\|\le R\sqrt{2k}}\|u\|^{d+s_0}e^{-\|u\|^2}|H_\alpha(u)|^2du \le c\cdot k^{|\alpha|-s_0/2}.$$

On the complement of U and for $2k > \gamma$ we can use the bound $|H_n(x)| \le c(n)\cdot|x|^n$ for Hermite polynomials $H_n(x)$ for large arguments, and we find

$$\begin{aligned} & k^{2|\alpha|}k^d\int_R^\infty r^{d-1}e^{\gamma r^2}r^{2|\alpha|}e^{-2kr^2}dr \\ \le\, & c\cdot\frac{k^{2|\alpha|}k^d}{(2k-\gamma)^{(d+2|\alpha|)/2}}\int_{R\sqrt{2k-\gamma}}^\infty s^{d-1+2|\alpha|}e^{-s^2}ds \end{aligned}$$

which vanishes exponentially for $k\to\infty$. Thus we finally have (7) with constants that depend only on α, Ω, d, φ, and R, but not on z or k. ■

The above argument proves that for $s_0 > 0$ the delta functional is not continuous on $\mathcal{F}_\varphi$, because one can pick any α with $0 \le |\alpha| < s_0/2$ to get

$$\lim_{k\to\infty}\frac{|\delta(f_{k,\alpha,z})|}{\|f_{k,\alpha,z}\|_\varphi} = \infty$$

for all $z \in \mathbb{R}^d\setminus\{0\}$. More generally,

Theorem 1. *A functional of the form*

$$\epsilon_x f = f(x) - \sum_{j=1}^N u_j(x)f(x_j) \tag{8}$$

is bounded on $\mathcal{F}_\varphi$, iff it vanishes on all polynomials of degree less than $s_0/2$.

Proof: The functional is continuous if it vanishes on P_q^d (see [5], [9]). To prove the converse, assume ϵ_x to be bounded on $\mathcal{F}_\varphi$. Then

$$\lim_{k\to\infty}|\epsilon_x f_{k,\alpha,z}| \le c(x)\cdot\lim_{k\to\infty}\|f_{k,\alpha,z}\|_\varphi = 0$$

for all $|\alpha| < s_0/2$ and all z. On the other hand, by the mollification and (6),

$$\lim_{k\to\infty}\epsilon_x f_{k,\alpha,z} = (i(x+z))^\alpha - \sum_j u_j(x)(i(x_j+z))^\alpha$$

for all $|\alpha| < s_0/2$ and all z. But this means that ϵ_x must vanish on all polynomials of degree $< s_0/2$ if it should be continuous on $\mathcal{F}_\varphi$. ■

Theorem 1 throws some light on the admissible values of q. It is possible to define the space $\mathcal{F}_\varphi$ of (5) with values of q that do not satisfy $q > s_0/2$, but this inequality is required to let the usual radial basis function interpolants be contained in $\mathcal{F}_\varphi$. At the same time $q > s_0/2$ ensures that functionals of the form (8) are continuous on $\mathcal{F}_\varphi$ if they are exact on P_q^d, and Theorem 1 proves a partial result for the converse assertion, making reproduction of low-degree polynomials a *necessary* condition for boundedness of the error functional. The consequence is that one cannot use values of q that do not satisfy $q > s_0/2$ without throwing the interpolants out of $\mathcal{F}_\varphi$ or making the error functional discontinuous on this space.

Due to Theorem 1, there are two situations:

1. For $s_0 \notin 2\mathbb{N}$, continuity of the error functional is equivalent to exactness on $\boldsymbol{P}_q^d$ for the smallest $q > s_0/2$. This value of q yields the smallest possible error bound.
2. For $s_0 = 2k \in 2\mathbb{N}$ the necessary and sufficient conditions differ. Exactness on $\boldsymbol{P}_q^d$ for any $q > k$ is sufficient for continuity, and exactness on P_q^d for all $q \le k$ is necessary. This gap occurs for thin–plate splines $\phi(r) = r^{2k} \log r$.

Furthermore the proof of Theorem 1 now implies that interpolants from multiquadrics $\Phi(\|x\|) = \sqrt{c^2 + \|x\|^2}$ without addition of constant polynomials will not lead to a bounded error functional on the space $\mathcal{F}_\varphi$.

On the space $\mathcal{F}_\varphi$ defined for thin-plate splines $\Phi(x) = \|x\|^3$, interpolation by multiquadrics will have an unbounded error, if linear polynomials are not added to the multiquadrics.

However, there can possibly exist larger and more interesting spaces than $\mathcal{F}_\varphi$ that still contain the interpolants and may lead to error estimates in weaker norms. These spaces could possibly allow smaller values of q, but they are still to be found.

§4. Approximative Polynomial Reproduction

We use results concerning the approximation order of radial basis function interpolants [4, 5, 8]. For a given radial basis function Φ with a generalized Fourier transform coinciding with φ on $\mathbb{R}^d \setminus \{0\}$ satisfying (4), a given compact set $\Omega \subset \mathbb{R}^d$ and a given constant $\rho > 0$ there are positive constants c_3 and c_4 such that for all finite sets $X = \{x_1, \dots, x_{N_X}\} \subset \mathbb{R}^d$ of centers and all points $x \in \Omega$ with

$$h_{X,\rho}(x) := \sup_{\|y-x\|_2 \le \rho} \min_{1 \le j \le N_X} \|y - x_j\|_2 \le c_3 \tag{9}$$

the interpolation error of x is bounded by $c_4 \cdot \|f\|_\varphi h_{X,\rho}^{s_\infty/2}(x)$, where s_∞ is determined by φ at infinity via (4). Here, the constants c_3 and c_4 are independent of x, X, and $h_{X,\rho}(x)$. With this (7) yields

$$|f_{k,\alpha,z}(x) - \sum_j u_j^*(x) f_{k,\alpha,z}(x_j)|^2 \le c \cdot k^{|\alpha| - s_0/2} \cdot h_{X,\rho}^{s_\infty}(x) \tag{10}$$

for all $z \in \mathbb{R}^d$, where $u_j^*(x)$ are optimal for Φ, and where c is independent of k, z, X, and x. This estimate interests us for $|\alpha| \ge s_0/2$, in order to prove something about the behaviour of optimal interpolation processes on high–degree polynomials. Defining $s_{X,k,\alpha}(x) := \sum_{j=1}^{N_X} u_j^*(x) f_{k,\alpha,0}(x_j)$ as a quasi-interpolant that is an interpolant to a mollification of the polynomial $(ix)^\alpha$, we get

$$|f_{k,\alpha,0}(x) - s_{X,k,\alpha}(x)|^2 \le c_5 k^{|\alpha|-s_0/2} \cdot h_{X,\rho}^{s_\infty}(x)$$

and add (6) to yield

$$|x^\alpha - (-i)^{|\alpha|} s_{X,k,\alpha}(x)| \le \frac{c_6}{k} + c_7 k^{|\alpha|/2-s_0/4} h_{X,\rho}^{s_\infty/2}(x)$$

with constants that are independent of k, X, and $h_{X,\rho}(X)$.

This bounds the approximation error of a polynomial in the space of radial basis function interpolants. Special approximations of the monomial x^α are obtained here via interpolation of the test functions $f_{k,\alpha,0}$ that uniformly converge to x^α on compact sets at the rate $\mathcal{O}(k^{-1})$ for $k \to \infty$. The error depends on the centers X and their local density $h_{X,\rho}(x)$ at x, of course, but also on the free parameter k that controls the mollification.

We now tie k to $h_{X,\rho}(x)$ by making the two terms in the error bound approximately equal, and we are interested in the convergence rate of the error for centers X with densities $h_{X,\rho}(x)$ tending to zero. This is done by choosing $k \approx h_{X,\rho}(x)^{-s_\infty/(2+|\alpha|-s_0/2)}$ which tends to infinity for $h_{X,\rho}(x)$ tending to zero, whenever the inequalities $|\alpha| > s_0/2 - 2$, $s_\infty > 0$ hold. Under these conditions, we finally have

$$|x^\alpha - (-i)^{|\alpha|} s_{X,k,\alpha}(x)| \le c_7 (h_{X,\rho}(x))^{s_\infty/(2+|\alpha|-s_0/2)} \tag{11}$$

for all sets X of centers and all points $x \in \Omega$ satisfying (9), and with a constant c_7 that is independent of x, X, and $h_{X,\rho}(x)$. From (11) we can read off a number of statements:

Theorem 2. *In the space $\mathcal{F}_\varphi$ generated by any of the usual radial basis functions Φ, polynomials are dense with respect to uniform convergence on compact sets. Polynomials of degree less than $s_0/2$ must necessarily be exactly reproduced to make error functionals of the form (8) continuous on $\mathcal{F}_\varphi$. Polynomials of degree $n \ge s_0/2$ can be approximated on compact sets by interpolants of certain mollifications of themselves with a guaranteed uniform convergence rate that depends on the radial basis function and on the local density $h_{X,\rho}$ of the set X of centers. For $h_{X,\rho}(x) \to 0$ the convergence order in terms of $h_{X,\rho}$ is $s_\infty/(2+n-s_0/2)$ with the following special implications:*

1. *For multiquadrics, inverse multiquadrics, and Gaussians with fixed parameters c, the convergence order is arbitrarily large.*
2. *For thin-plate splines with parameter β, the order is at least $\beta/(2+n-\beta/2)$.*
3. *For splines in Sobolew spaces of order k, the approximation order is at least $k/(2+n-k/2)$.*

Proof: *For the last three statements we simply use the appropriate values of s_0 and s_∞.* ■

§5. References

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