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CONSTRUCTIVE APPROXIMATION

Multivariate Interpolation by Polynomials and Radial Basis Functions

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Abstract. In many cases, multivariate interpolation by smooth radial basis functions converges toward polynomial interpolants, when the basis functions are scaled to become flat. In particular, examples show and this paper proves that interpolation by scaled Gaussians converges toward the de Boor/Ron "least" polynomial interpolant. To arrive at this result, a few new tools are necessary. The link between radial basis functions and multivariate polynomials is provided by "radial polynomials" $\|x-y\|_2^{2\ell}$ that already occur in the seminal paper by C. A. Micchelli of 1986. We study the polynomial spaces spanned by linear combinations of shifts of radial polynomials and introduce the notion of a *discrete moment basis* to define a new well-posed multivariate polynomial interpolation process which is of minimal degree and also "least" and "degree-reducing" in the sense of de Boor and Ron. With these tools at hand, we generalize the de Boor/Ron interpolation process and show that it occurs as the limit of interpolation by Gaussian radial basis functions. As a byproduct, we get a stable method for preconditioning the matrices arising with interpolation by smooth radial basis functions.

1. Introduction

Let $\varphi : [0,\infty) \to \mathbf{R}$ be a radial basis function that can be written as

$$\varphi(r) = f(r^2) \quad \text{with a smooth function} \quad f : \mathbf{R} \to \mathbf{R},$$

and in particular we have in mind the Gaussians and inverse multiquadrics, i.e.,

$$\varphi(r) = \exp(-r^2) \qquad \text{and} \qquad \varphi(r) = (1+r^2)^{\beta/2}, \qquad \beta < 0.$$

We scale φ in such a way that the functions become flat, i.e., we define

$$\varphi_c(r) := \varphi(cr) = f(c^2r^2), \qquad c, r \geq 0, \tag{1}$$

and since we want to consider small c, we assume that f is analytic around zero.

We fix a set $X = \{x_1, \ldots, x_N\} \subset \mathbf{R}^d$ of scattered centers for interpolation, and consider the behavior of the Lagrange interpolation basis for $c \to 0$. The basis is obtainable as

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the solution $(u_1^c(x), \dots, u_M^c(x)) \in \mathbf{R}^M$ of the system

$$(2) \qquad \sum_{j=1}^{M} \varphi_c(\|x_j - x_k\|_2) u_j^c(x) = \varphi_c(\|x - x_k\|_2) \qquad \text{for all } 1 \le k \le M.$$

By a surprising observation of Driscoll and Fornberg [6] and Danzeglocke [5] there are many cases where the limits of the Lagrange basis functions $u_j^c(x)$ for $c \to 0$ exist and are multivariate polynomials in x. Our first goal is to prove this fact under certain assumptions on φ and X. From a recent paper by Fornberg, Wright, and Larsson [8] it is known that convergence may depend critically on the geometry of X and certain properties of φ. We study these connections and the final polynomial interpolant to some extent, but a complete characterization is still missing.

Our investigation of the limit process poses some interesting questions about multivariate polynomials and geometric properties of scattered data sets. In particular, we have to study "radial" polynomials of the form $\|x - y\|_2^{2\ell}$ because the matrix entries in (2) have series expansions

$$\varphi_c(\|x_j - x_k\|_2) = f(c\|x_j - x_k\|_2^2) = \sum_{\ell=0}^{\infty} \frac{f^{(\ell)}(0)}{\ell!} c^\ell \|x_j - x_k\|_2^{2\ell},$$

while the right-hand side contains

$$\varphi_c(\|x - x_k\|_2) = f(c\|x - x_k\|_2^2) = \sum_{\ell=0}^{\infty} \frac{f^{(\ell)}(0)}{\ell!} c^\ell \|x - x_k\|_2^{2\ell}.$$

Thus this paper requires a somewhat nonstandard approach to multivariate interpolation, namely via linear combinations of "radial polynomials." In particular, we define two different classes of multivariate polynomial interpolation schemes that can be formulated without taking recourse to limits of radial basis functions. Examples show that the various methods are actually different. For their analysis, some useful theoretical notions are introduced, i.e., "discrete moment conditions" and "discrete moment bases." To establish the link from interpolation by dilated Gaussians to the de Boor/Ron "least" polynomial interpolation [2], [3], [4], we generalize the latter and, in particular, introduce a scaling and relate the theory to reproducing kernel Hilbert spaces. Using the new notion of a "discrete moment basis" we finally prove that the interpolant of de Boor and Ron is the limit of radial basis function interpolation using the Gaussian kernel, as the kernel is dilated to become flat. Finally, we prove that properly scaled discrete moment bases can be used for preconditioning the systems arising in radial basis function interpolation.

2. Limits of Radial Basis Functions

Because we shall be working with determinants, we fix the numbering of the points in X now, i.e., we replace the notation $X = \{x_1, \dots, x_N\} \subset \mathbf{R}^d$ by $X = (x_1, \dots, x_M) \in (\mathbf{R}^d)^M$. For a second ordered set $Y = (y_1, \dots, y_M) \in (\mathbf{R}^d)^M$ with the same number M of points we define the matrix

$$A_{c,X,Y} := (\varphi_c(\|x_j - y_k\|_2))_{1 \le j,k \le M} = (f(c^2\|x_j - y_k\|_2^2))_{1 \le j,k \le M}.$$

Note that $A_{c,X,X}$ is symmetric and has a determinant that is independent of the order of the points in X. If φ is positive definite, the matrices $A_{c,X,X}$ are positive definite and hence have a positive determinant for all $c > 0$.

Since f is analytic around the origin, the matrices $A_{c,X,Y}$ have a determinant with a convergent series expansion

$$\det A_{c,X,Y} =: \sum_{k=0}^{\infty} c^{2k} p_k(X, Y) \tag{3}$$

for small c, where the functions $p_k(X, Y)$ are polynomials in the points of X and Y. In particular, they are sums of powers of terms of the form $\|x_j - y_k\|_2^2$. They can be determined by symbolic computation, and we shall give an explicit formula in Section 3 and prove the upper bound $2k$ for their total degree in Lemma 5. Note that the polynomials $p_k(X, X)$ are independent of the ordering of the points forming the components of $X = (x_1, \ldots, x_M) \in (\mathbf{R}^d)^M$.

We define $X_j := X \backslash \{x_j\}$, where x_j is deleted and the order of the remaining points is kept. Furthermore, in the sets $X_j(x) := (X \backslash \{x_j\}) \cup \{x\}$, $1 \leq j \leq M$, the point x_j is replaced by x, keeping the order.

The general structure of Lagrange basis functions is described by a standard technique:

Lemma 1 ([8]). *The Lagrange basis functions $u_j^c(x)$, $1 \leq j \leq M$, for interpolation in $X = (x_1, \ldots, x_M) \in (R^d)^M$ by a dilated positive definite radial function φ_c have the form*

$$u_j^c(x) := \frac{\det A_{c,X,X_j(x)}}{\det A_{c,X,X}} = \frac{\sum_{k=0}^{\infty} c^{2k} p_k(X, X_j(x))}{\sum_{k=0}^{\infty} c^{2k} p_k(X, X)}, \qquad 1 \leq j \leq M. \tag{4}$$

Proof. The quotient of determinants is in the span of the functions $\varphi_c(\|x - x_j\|_2)$, $1 \leq j \leq M$, and it satisfies $u_j(x_k) = \delta_{jk}$, $1 \leq j, k \leq M$. Since interpolation is unique, we are done. ■

From (4) it is clear that the convergence behavior of the Lagrange basis function $u_j^c(x)$ for $c \to 0$ crucially depends on the smallest value of k such that the real numbers $p_k(X, X)$ or $p_k(X, X_j(x))$ are nonzero. Examples show that this number in turn depends on the geometry of X, getting large when the set "degenerates" from "general position."

Definition 1. For $X = (x_1, \ldots, x_M) \in (\mathbf{R}^d)^M$ we define

$$\begin{aligned} k_0(X) &:= \min_{p_k(X,X) \neq 0} k, \\ \kappa(d, M) &:= \min_{X \in (\mathbf{R}^d)^M} k_0(X), \\ \delta(X) &:= k_0(X) - \kappa(d, M) \geq 0. \end{aligned} \tag{5}$$

Then $\kappa(d, M)$ is the minimal $k \geq 0$ such that the multivariate polynomial $X \mapsto p_k(X, X)$ is nontrivial as a function on $(\mathbf{R}^d)^M$. An $X = (x_1, \ldots, x_M) \in (\mathbf{R}^d)^M$ is *in* *general position with respect to* φ or *nondegenerate* if $\delta(X) = 0$, and thus $\delta(X)$ can be called the *degeneration order* of X. All of these quantities depend on φ, while $k_0(X)$ and $\delta(X)$ depend on the geometry of X, but not on the numbering of the points. If φ is positive definite, we can conclude that $p_{k_0(X)}(X, X) > 0$ holds for all X. With this notion, formula (4) immediately yields

Theorem 1 ([8]). *If $x \in \mathbf{R}^d$ and $j \in \{1, \ldots, M\}$ are such that*

$$p_k(X, X_j(x)) = 0 \qquad \text{for all } k < k_0(X), \tag{6}$$

then the limit of $u_j^c(x)$ for $c \to 0$ is the value of the polynomial

$$\frac{p_{k_0(X)}(X, X_j(x))}{p_{k_0(X)}(X, X)}. \tag{7}$$

If (6) *fails, then the limit is infinite.* ∎

In paper [8] of Fornberg et al. there are cases where (6) fails for certain geometries, e.g., when φ is a multiquadric (inverse or not), when the set X consists of five points on a line in $\mathbf{R}^2$ and when the evaluation point x does not lie on that line. The observations in [8] have led to the conjecture that in the case of dilated Gaussians, convergence takes place for all point geometries without exception, and we prove this by a slightly stronger statement, identifying the limit with an interpolation technique that never fails.

Theorem 2. *Interpolation with shifted Gaussians always converges to the de Boor/Ron polynomial interpolant when the Gaussians are dilated.*

The proof needs a rather special technique, and thus we postpone it to the penultimate section, proceeding now with our investigation of convergence in general. Unfortunately, condition (6) contains an unsymmetric term, and we want to replace it by

$$k_0(X_j(x)) \geq k_0(X), \ \text{ i.e., } \delta(X_j(x)) \geq \delta(X), \ \text{ i.e., } p_k(X_j(x), X_j(x)) = 0 \ \text{ for all } k < k_0(X). \tag{8}$$

Then we can extend the results by Fornberg et al. in [6], [8].

Theorem 3. *If the degeneration order $\delta(X)$ of X is not larger than the degeneration order $\delta(X_j(x))$ of $X_j(x)$, then the polynomial limit of the Lagrange basis function $u_j^c(x)$ for $c \to 0$ exists. In particular, convergence takes place when X is in general position with respect to φ.*

The proof needs some specific results about positive definite radial basis functions and their "native" Hilbert spaces. Details can be found in [14] or [15], but we try to be as explicit as possible here. For $X = \{x_1, \ldots, x_N\} \subset \mathbf{R}^d$, a linear combination

$$s(x) := \sum_{j=1}^{M} \alpha_j \varphi_c(\|x - x_j\|_2)$$

of shifts of a scaled positive definite radial basis function φ_c has the norm

$$\|s\|_{\varphi_c}^2 := \sum_{j=1}^{M}\sum_{k=1}^{M}\alpha_j\alpha_k\varphi_c(\|x_j - x_k\|_2)$$

in a "native" Hilbert space associated to φ_c that arises as the completion of the span of all such functions. If s interpolates values $f(x_k)$ on X, this norm takes the form

$$\|s\|_{\varphi_c}^2 = \sum_{k=1}^{M}\alpha_k f(x_k),$$

because the coefficients solve the system

$$\sum_{j=1}^{M}\alpha_j\varphi_c(\|x_j - x_k\|_2) = f(x_k), \qquad 1 \le k \le M.$$

We now apply this to a Lagrange basis function.

Lemma 2.

$$\|u_j^c\|_{\varphi_c}^2 = \frac{\det A_{c,X_j,X_j}}{\det A_{c,X,X}} \tag{9}$$

for $1 \le j \le M, c > 0$.

Proof. If α_j is the coefficient of $\varphi_c(\|x - x_j\|_2)$ in the representation of u_j^c, we have

$$\|u_j^c\|_{\varphi_c}^2 = \alpha_j$$

by the above argument. Then (9) follows from Cramer's rule applied to the interpolation problem with Kronecker data δ_{jk}, $1 \le k \le M$, solved by u_j^c. ■

For a fixed $X = \{x_1, \dots, x_N\} \subset \mathbf{R}^d$ and a fixed point $x \in \mathbf{R}^d$ one can define the functional

$$f \mapsto f(x) - \sum_{j=1}^{M} u_j^c(x) f(x_j)$$

that takes the pointwise error of interpolation by translates of φ_c. Its Hilbert space norm turns out to be an explicitly available function $P_X(x)$ called the "power function" with the representations

(10)

$$\begin{aligned} P_X^2(x) &= \varphi_c(0) - 2\sum_{j=1}^{M} u_j^c(x)\varphi_c(\|x - x_j\|_2) + \sum_{j=1}^{M}\sum_{k=1}^{M} u_j^c(x)u_k^c(x)\varphi_c(\|x_j - x_k\|_2) \\ &= \varphi_c(0) - \sum_{j=1}^{M} u_j^c(x)\varphi_c(\|x - x_j\|_2). \end{aligned}$$

The second form is somewhat nonstandard. It follows from the first by the Lagrange interpolation property, and details can be retrieved from [14, p. 92, (4.3.14)].

Lemma 3. *The power function has the representation*

$$P_X^2(x) = \frac{\det A_{c,X\cup\{x\},X\cup\{x\}}}{\det A_{c,X,X}}.$$

Proof. By expansion of the numerator, using (4), and the representation (10). ∎

Since $P_X(x)$ is the Hilbert norm of the pointwise error functional at x, there is an error bound of the form

$$\left| f(x) - \sum_{j=1}^{M} u_j^c(x) f(x_j) \right| \leq P_X(x) \|f\|_{\varphi_c}$$

for all functions f in the native Hilbert space for φ_c. Since zero is the interpolant to u_j^c on $X_j = X\backslash\{x_j\}$, we can specialize this to $f = u_j^c$ on X_j to get

Lemma 4.

$$(11) \qquad |u_j^c(x)| \leq P_{X_j}(x) \|u_j^c\|_{\varphi_c}$$

for all $x \in \mathbf{R}^d$, *all* $c > 0$, *and all* j, $1 \leq j \leq M$.

To finish the proof of Theorem 3, we assert boundedness of $u_j^c(x)$ for $c \to 0$ and then use Theorem 1. The above results yield

$$P_{X_j}^2(x_j) = \frac{\det A_{c,X,X}}{\det A_{c,X_j,X_j}}, \qquad \|u_j^c\|_{\varphi_c}^2 = \frac{1}{P_{X_j}^2(x_j)},$$

and

$$|u_j^c(x)| \leq P_{X_j}(x) \|u_j^c\|_{\varphi_c} \leq \frac{P_{X_j}(x)}{P_{X_j}(x_j)}.$$

With the representation of the power function via determinants we get

$$(12) \qquad (u_j^c(x))^2 \leq \frac{P_{X_j}^2(x)}{P_{X_j}^2(x_j)} = \frac{\det A_{c,X_j(x),X_j(x)}}{\det A_{c,X,X}}.$$

The numerator and denominator of the right-hand side contain sets of M points each. If we assume (8), we arrive at

$$(u_j^c(x))^2 \leq \frac{\sum_{k=k_0(X_j(x))}^{\infty} c^k p_k(X_j(x), X_j(x))}{\sum_{k=k_0(X)}^{\infty} c^k p_k(X, X)} < \infty$$

which concludes the proof of Theorem 3. ∎

Remark. The first part of (12) is an interesting bound on Lagrange basis functions in radial basis function interpolation. If the set X is formed recursively by adding to X the point x_{M+1} where $P_X(x)$ is maximal (this adds the data location where the worst-case error occurs), one gets a sequence of Lagrange basis functions that is strictly bounded by 1 in absolute value. The implications on Lebesgue constants and stability of the interpolation process should be clear, but cannot be pursued here.

3. Basic Polynomial Determinants

To derive a formula for the polynomials p_k in (3) and to prove upper bounds for their degree we need the expansion

$$f(z) = \sum_{k=0}^{\infty} f_k z^k \tag{13}$$

of f around the origin. If φ is positive definite, we know by the standard Bernstein–Widder representation (see [16] for a short summary) that all $(-1)^k f_k$ are positive. Furthermore, we use the standard formula for determinants

$$\det(b_{ij})_{1\le i,j\le M} = \sum_{\pi\in\mathcal{S}_M} (-1)^{\pi} \prod_{j=1}^{M} b_{j\pi(j)},$$

where π varies over all permutations in the symmetric group $\mathcal{S}_M$ and $(-1)^{\pi}$ is the number of inversions in π. Then

$$\begin{aligned}
\det A_{c,X,Y} &= \sum_{\pi\in\mathcal{S}_M} (-1)^{\pi} \prod_{j=1}^{M} f(c^2\|x_j - y_{\pi(j)}\|_2^2) \\
&= \sum_{\pi\in\mathcal{S}_M} (-1)^{\pi} \prod_{j=1}^{M} \sum_{m=0}^{\infty} f_m c^{2m} \|x_j - y_{\pi(j)}\|_2^{2m} \\
&= \sum_{\pi\in\mathcal{S}_M} (-1)^{\pi} \sum_{\rho_1=0}^{\infty} \sum_{\rho_2=0}^{\infty} \cdots \sum_{\rho_M=0}^{\infty} \prod_{j=1}^{M} (f_{\rho_j} c^{2\rho_j} \|x_j - y_{\pi(j)}\|_2^{2\rho_j}) \\
&= \sum_{\pi\in\mathcal{S}_M} (-1)^{\pi} \sum_{\rho\in\mathbf{N}_0^M} f_\rho c^{2|\rho|} \prod_{j=1}^{M} \|x_j - y_{\pi(j)}\|_2^{2\rho_j} \\
&= \sum_{\rho\in\mathbf{N}_0^M} f_\rho c^{2|\rho|} \sum_{\pi\in\mathcal{S}_M} (-1)^{\pi} \prod_{j=1}^{M} \|x_j - y_{\pi(j)}\|_2^{2\rho_j} \\
&= \sum_{k=0}^{\infty} c^{2k} \sum_{\substack{\rho\in\mathbf{N}_0^M \\ |\rho|=k}} f_\rho d_\rho(X,Y),
\end{aligned}$$

with multi-index notation

$$\begin{aligned}
f_\rho &:= \prod_{j=1}^{M} f_{\rho_j}, \\
d_\rho(X,Y) &:= \det(\|x_i - y_j\|_2^{2\rho_i})_{1\le i,j\le M}, \\
p_k(X,Y) &= \sum_{\substack{\rho\in\mathbf{N}_0^M \\ |\rho|=k}} f_\rho d_\rho(X,Y).
\end{aligned}$$

To see a bound on the degree, consider $|\rho| = k$ and conclude that

$$d_\rho(X, Y) := \det(\|x_i - y_j\|_2^{2\rho_i})_{1\le i,j\le M} = \sum_{\pi\in\mathcal{S}_M} (-1)^\pi \prod_{j=1}^{M} \|x_j - y_{\pi(j)}\|_2^{2\rho_j}$$

has total degree at most $2|\rho| = 2k$. Altogether we have

Lemma 5. *The polynomials $p_k(X, Y)$ have maximal degree $2k$ as polynomials in X and Y.* ■

Examples show that this bound is sharp in general, but is attained mainly in one-dimensional cases. Lemma 10 will provide smaller bounds for higher-dimensional sets, but it requires more tools.

We can also deduce that $k_0(X)$ for $X \in (\mathbf{R}^d)^M$ increases with M due to the bound

$$M \le \binom{2k_0(X) + d}{d}$$

which follows from

Lemma 6. *If $p_k(X, Y)$ is nonzero for some specific sets X, Y with $M = \#X = \#Y$, then $M \le \binom{2k+d}{d}$. In other words, if $M > \binom{2k+d}{d}$, then $p_k(X, Y) = 0$ for all $X, Y \in (\mathbf{R}^d)^M$.*

Proof. If some $d_\rho(X, Y)$ is nonzero for $X, Y \in (\mathbf{R}^d)^M$, there are M linearly independent d-variate polynomials of degree at most $2|\rho| = 2k$. This proves the first assertion, because the latter polynomials form a space of dimension $\binom{2k+d}{d}$. The second assertion is the contrapositive of the first. ■

Example 1. Let us look at some special cases that we prepared with MAPLE. We reproduce the results in [8], but we have a somewhat different background and notation. The one-dimensional case with $M = 2$ has in general $p_0(X, X) = 0$, $p_1(X, X) = -2f(0)f'(0)(x_2 - x_1)^2$. Thus $\kappa(1, 2) = 1$ and there is no degeneration except coalescence. The bound in Lemma 5 turns out to be sharp here. The case $M = 3$ leads to $\kappa(1, 3) = 3$ with

$$p_3(X, X) = -2f'(0)(3f(0)f''(0) - f'(0)^2)(x_1 - x_2)^2(x_1 - x_3)^2(x_2 - x_3)^2.$$

Geometrically, there is no degeneration except coalescence. The factor $3f(0)f''(0) - f'(0)^2$ could possibly lead to some discussion, but for positive definite φ it must be positive because we know that $f(0), -f'(0), f''(0)$, and $p_3(X, X)$ are positive. We further find $\kappa(1, 4) = 6$ with

$$\begin{aligned} p_6(X, X) = & -\tfrac{4}{3}(3f''(0)^2 - 5f'(0)f'''(0))(3f(0)f''(0) - f'(0)^2) \\ & \times (x_1 - x_2)^2(x_1 - x_3)^2(x_1 - x_4)^2(x_2 - x_3)^2(x_2 - x_4)^2(x_3 - x_4)^2. \end{aligned}$$

The general situation seems to be $\kappa(1, M) = M(M-1)/2$ with $p_{\kappa(1,M)}$ being (up to a factor) the polynomial that consists of a product of all $(x_j - x_k)^2$ for $1 \le j < k \le M$, which is of degree $2\kappa(1, M) = M(M-1)$. Thus the maximal degree in Lemma 5 is actually attained again. Note that the one-dimensional situation also carries over to the case when X and $X_j(x)$ lie on the same line in R^d.

Now let us look at two-dimensional situations. The simplest nontrivial two-dimensional case is for $M = 2$ when the evaluation is not on the line connecting the points of X. But from the one-dimensional case we can infer

$$\kappa(2, 2) = 1 = k_0(X) = k_0(X_j(x))$$

and do not run into problems, because we have Theorem 3. In particular, we find

$$p_1(X, X) = -2f(0)f'(0)((x_1^1 - x_2^1)^2 + (x_1^2 - x_2^2)^2).$$

Now we look at $M = 3$ in two dimensions. The general expansion yields $\kappa(2, 3) = 2$ with

$$p_2(X, X) = 4f(0)f'(0)^2(\det B_X)^2$$

and B_X being the standard 3×3 matrix for calculation of barycentric coordinates based on X. Its determinant vanishes iff the points in X are collinear. Thus nondegeneracy of three-point sets with respect to positive definite radial basis functions is equivalent to the standard notion of the general position of three points in $\mathbf{R}^2$. To look for higher-order degeneration, we consider three collinear points now, and since everything is invariant under shifts and orthogonal transformations, we can assume that the data lie on the x-axis. This boils down to the one-dimensional case, and we get $p_3(X, X) > 0$ with no further possibility of degeneration. But now we have to look into the first critical case, i.e., when X is collinear but $X_j(x)$ is not. This means that we evaluate the interpolant off the line defined by X. Theorem 3 does not help here. If we explicitly go back to (6), we still get convergence if we prove that $p_2(X, X_j(x)) = 0$ for all collinear point sets X and all $x \in \mathbf{R}^2$. Fortunately, MAPLE calculates

$$p_2(X, X_j(x)) = 4f(0)f'(0)^2(\det B_X)(\det B_{X_j(x)})$$

and thus there are no convergence problems. However, the ratio of the terms $p_3(X, X_j(x))$ and $p_3(X, X)$ now depends on φ.

Now we go for $M = 4$ in two dimensions and first find $\kappa(2, 4) = 4$ from MAPLE, but it cannot factor the polynomial $p_4(X, X)$ properly or write it as a sum of squares. Taking special cases of three points not on a line, the polynomial $p_4(X, X)$ seems to be always positive except for coalescence. In particular, contrary to expectations, it does not vanish for four noncollinear points on a circle or a conic. Taking cases of three points on a line, the polynomial $p_4(X, X)$ vanishes iff the fourth point also lies on that line. Thus there is some experience supporting the conjecture that nondegeneracy of four points in two dimensions with respect to positive definite functions just means that the points are not on a line. But if they are on a line, we find $k_0(X) = 6$ due to the one-dimensional case, and thus $p_5(X, X)$ also vanishes. This is confirmed by MAPLE, and we now check the case where the points of X are on a line but those of $X_j(x)$ are not. It turns out that then (6) holds for $k_0(X) = 6$, and the case does not show divergence.

The $M = 5$ situation in $\mathbf{R}^2$ has $\kappa(2, 5) = 6$. The geometric interpretation of points in general position with respect to φ is unknown, because the zero set of $p_6(X, X)$ is hard to determine in general. If four points are fixed at the corners of the square $[0, 1]^2$, and if the polynomial $\frac{2}{3} p_6(X, X)$ is evaluated for inverse multiquadrics with $\beta = -1$ as a function of the remaining point $x_5 = (\xi, \eta) \in \mathbf{R}^2$, we get the nonnegative polynomial

$$3\xi^2(1-\xi)^2 + 3\eta^2(1-\eta)^2 + (\xi(1-\xi) + \eta(1-\eta))^2$$

which vanishes only at the corners of the square. Thus it can be ruled out that degeneracy systematically occurs when four or five points are on a circle or three points are on a line. However, it turns out that $p_6(X, X)$ always vanishes if four points are on a line. If calculated for four points on a line, the next coefficient $p_7(X, X)$ vanishes either if the fifth point also lies on the line, or for $\beta = 0, 2, 3, 7$, or for coalescence. The final degeneration case thus occurs when all five points are on a line, and from one dimension we then expect $k_0(X) = 10$.

Let us examine the divergence case described by Fornberg et al. in [8]. It occurs when X consists of five points on a line, while evaluation takes place off that line. The one-dimensional case teaches us that we should get $k_0(X) = 10$ for five collinear points, and MAPLE verifies this, at least for the fixed five collinear equidistant points on $[0, 1] \times \{0\}$. However, we also find that

$$\begin{aligned} p_9(X, X_1(x)) \;=\; & \frac{-9}{8388608}\eta^2(5f'(0)f'''(0) - 3f''(0)^2) \\ & \times (f(0)f''(0)f'''(0) + f'(0)f''(0)^2 - 2f'(0)^2 f'''(0)) \end{aligned}$$

for points $x = (\xi, \eta) \in \mathbf{R}^2$. If we put in multiquadrics, i.e., $f(t) = (1+t)^{\beta/2}$, we get the same result as in [8], which reads

$$p_9(X, X_1(x)) = \frac{-9}{268435456}\eta^2\beta^4(\beta-7)(\beta-2)^2$$

in our notation, proving that divergence occurs for multiquadrics except for the strange case $\beta = 7$. Another curiosity is that for multiquadrics the value $p_{10}(X, X)$ vanishes for the conditionally positive definite cases $\beta = 7$ and $\beta = 11.790$. As expected, this polynomial is positive for the positive definite cases, e.g., for negative β.

Checking the case where exactly four points of X are on a line, we find that (6) holds for $k_0(X) = 7$, and thus there is no convergence problem.

4. A Related Class of Polynomial Interpolation Methods

We can ignore the limit process $c \to 0$ completely if we boldly take (7) to define

$$u_j(x) := \frac{p_{k_0(X)}(X, X_j(x))}{p_{k_0(X)}(X, X)} \tag{14}$$

for all $1 \le j \le M$ and all $x \in \mathbf{R}^d$. The denominator will always be positive if we start with a positive definite function, and the discussion at the beginning of Section 3 shows that the polynomials $p_k(X, Y)$ will always vanish if either X or Y have two or more coalescing points. Thus we get Lagrange interpolation polynomials for any kind of geometry. The result will be dependent on the function f and its Taylor expansion, and thus there is a full scale of polynomial interpolation methods which is available without any limit process. However, it is clear from (7) that polynomial limits of radial basis function interpolants, if they exist, will usually have the above form. Paper [7] (added in the refereeing process) by Fornberg and Wright provides a numerical technique and examples for the multiquadric case. It provides an interesting and completely different technique, using FFT on the expansion of the interpolant with respect to c in the complex plane. It will be interesting to study how the polynomial interpolation method of de Boor and Ron [2], [3], [4] relates to this. However, it uses a different truncation strategy.

Example 2. Let us check how the above technique overcomes the five-point degeneration case in Example 1. If we take the five equidistant points on $[0, 1] \times \{0\}$ and classical multiquadrics, the Lagrange basis function u_0 corresponding to the origin becomes

$$u_0(\xi, \eta) = \tfrac{1}{3}(\xi - 1)(4\xi - 3)(2\xi - 1)(4\xi - 1) + \tfrac{8}{21}\xi\eta^2(18\xi - 25),$$

and the second term is missing if we take the Gaussian. For $f(t) = \log(1 + t)$ the additional term is

$$\frac{-2}{3339}\eta^2(5195 + 15240\xi - 11424\xi^2 + 1008\eta^2).$$

There is dependence on f, but no degeneration. We simply ignore p_9 and focus on the quotient of values of p_{10}.

5. Point Sets, Polynomials, and Moments

Our results so far require knowledge and numerical availability of $k_0(X)$ and $p_{k_0(X)}(X, X_j(x))$. Section 3 gives a first idea for the evaluation of these quantities, but it still uses the limit process. It suggests that one looks at polynomials of the form $\|x - y\|_2^{2\ell}$, and we shall use this section to make a fresh start into multivariate polynomials and point sets. The relation to the earlier sections will turn up later.

Let $\mathbb{P}_m^d$ be the space of all d-variate real-valued polynomials of order m (i.e., of degree $< m$), and let $X = \{x_1, \dots, x_M\}$ be a fixed set of M points in $\mathbf{R}^d$. With the dimension $Q = \binom{m + d - 1}{d}$ and a basis $p_1, \dots, p_Q$ of $\mathbb{P}_m^d$ we can form the $Q \times M$ matrices P_m and the $M \times M$ matrices A_ℓ with

$$(15) \quad P_m := (p_i(x_j))_{1 \le i \le Q,\ 1 \le j \le M}, \qquad A_\ell = ((-1)^\ell \|x_j - x_k\|_2^{2\ell})_{1 \le j,k \le M}, \quad \ell \ge 0,$$

to provide a very useful notion that is closely related to multivariate divided differences (see, e.g., de Boor [1], Sauer and Xu [13], Kunkle [9], and Rabut [11]).

Definition 2. A vector $\alpha \in \mathbf{R}^M$ satisfies *discrete moment conditions of order* m *with respect to* X if $P_m\alpha = 0$ or

$$\sum_{j=1}^{M} \alpha_j p(x_j) = 0 \qquad \text{for all } p \in \mathbb{P}_m^d$$

holds. These vectors form a linear subspace $MC_m(X) := \ker P_m$ of $\mathbf{R}^M$ for $M = \#X$.

Note that the definition involves all polynomials of order m, while the following involves radial polynomials of the form $\|x - x_j\|^{2\ell}$ for $0 \le \ell < m$.

Theorem 4 (Remark 3.1 in Micchelli [10]). *A vector $\alpha \in \mathbf{R}^M$ satisfies discrete moment conditions of order m with respect to X iff*

$$\alpha^T A_\ell \alpha = 0 \tag{16}$$

holds for all $0 \le \ell < m$.

Note that the condition $A_\ell \alpha = 0$ would be more restrictive. It will come up later. The proof of Theorem 4 uses Micchelli's lemma from [10], which we restate here because we make frequent use of its proof technique later.

Lemma 7 (Micchelli [10]). *If $\alpha \in \mathbf{R}^M$ satisfies discrete moment conditions of order m, then the numbers $\alpha^T A_\ell \alpha$ vanish for all $\ell < m$ and $\alpha^T A_m \alpha$ is nonnegative. The latter quantity vanishes iff α satisfies discrete moment conditions of order $m+1$.*

Proof. Let us take a vector $\alpha \in \mathbf{R}^M$ satisfying discrete moment conditions of order m, and pick any $\ell \le m$ to form

$$\begin{aligned}(-1)^\ell \alpha^T A_\ell \alpha &= \sum_{j=1}^M \sum_{k=1}^M \alpha_j \alpha_k (\|x_j - x_k\|_2^2)^\ell \\ &= \sum_{j=1}^M \sum_{k=1}^M \alpha_j \alpha_k \sum_{\ell_1+\ell_2+\ell_3=\ell} \frac{\ell!}{\ell_1!\,\ell_2!\,\ell_3!} \|x_j\|_2^{2\ell_1} (-2(x_j, x_k))^{\ell_2} \|x_k\|_2^{2\ell_3} \\ &= \sum_{j=1}^M \sum_{k=1}^M \alpha_j \alpha_k \sum_{\substack{\ell_1+\ell_2+\ell_3=\ell \\ \ell_2+2\ell_3 \ge m \\ \ell_2+2\ell_1 \ge m}} \frac{\ell!}{\ell_1!\,\ell_2!\,\ell_3!} \|x_j\|_2^{2\ell_1} (-2(x_j, x_k))^{\ell_2} \|x_k\|_2^{2\ell_3}.\end{aligned}$$

This value vanishes for $\ell < m$, and this also proves one direction of the second statement if we formulate it for $m-1$. For $\ell = m$ the two inequalities can only hold if $\ell_1 = \ell_3$. Thus $(-1)^\ell = (-1)^{\ell_2}$, and we can write in multi-index notation

$$\begin{aligned}\alpha^T A_\ell \alpha &= \sum_{j=1}^M \sum_{k=1}^M \alpha_j \alpha_k (-1)^\ell \|x_j - x_k\|_2^{2\ell} \\ &= \sum_{\substack{\ell_2=0 \\ \ell-\ell_2=:2\ell_1 \in 2\mathbf{Z}}}^{\ell} 2^{\ell_2} \frac{\ell!}{\ell_1!\,\ell_2!\,\ell_1!} \sum_{j=1}^M \sum_{k=1}^M \alpha_j \alpha_k \|x_j\|^{\ell-\ell_2} \|x_k\|^{\ell-\ell_2} (x_j, x_k)_2^{\ell_2} \\ &= \sum_{\substack{\ell_2=0 \\ \ell-\ell_2=:2\ell_1 \in 2\mathbf{Z}}}^{\ell} 2^{\ell_2} \frac{\ell!}{\ell_1!\,\ell_2!\,\ell_1!} \sum_{j=1}^M \sum_{k=1}^M \alpha_j \alpha_k \|x_j\|^{\ell-\ell_2} \|x_k\|^{\ell-\ell_2} \sum_{\substack{i \in \mathbf{N}_0^d \\ |i|=\ell_2}} \binom{\ell_2}{i} x_j^i x_k^i\end{aligned}$$

$$= \sum_{\substack{\ell_2=0 \\ \ell-\ell_2=:2\ell_1\in 2\mathbf{Z}}}^{\ell} 2^{\ell_2} \frac{\ell!}{\ell_1!\,\ell_2!\,\ell_1!} \sum_{\substack{i\in\mathbf{N}_0^d \\ |i|=\ell_2}} \binom{\ell_2}{i} \sum_{j=1}^M \sum_{k=1}^M \alpha_j \alpha_k \|x_j\|^{\ell-\ell_2} \|x_k\|^{\ell-\ell_2} x_j^i x_k^i$$

$$= \sum_{\substack{\ell_2=0 \\ \ell-\ell_2=:2\ell_1\in 2\mathbf{Z}}}^{\ell} 2^{\ell_2} \frac{\ell!}{\ell_1!\,\ell_2!\,\ell_1!} \sum_{\substack{i\in\mathbf{N}_0^d \\ |i|=\ell_2}} \binom{\ell_2}{i} \left(\sum_{j=1}^M \alpha_j \|x_j\|^{\ell-\ell_2} x_j^i \right)^2 \geq 0.$$

If this vanishes, all expressions

$$\sum_{j=1}^M \alpha_j \|x_j\|^{\ell-\ell_2} x_j^i$$

with $0 \leq \ell_2 \leq \ell$, $\ell - \ell_2 \in 2\mathbf{Z}$, $i \in \mathbf{N}_0^d$, $|i| = \ell_2$ must vanish, and this implies that α satisfies discrete moment conditions of order $\ell + 1 = m + 1$. ■

It is now easy to prove Theorem 4. If α satisfies discrete moment conditions up to order m, Micchelli's lemma proves that (16) holds. For the converse, assume that (16) is true for some $\alpha \in \mathbf{R}^M$ and proceed by induction. There is nothing to prove for order zero, and if we assume that we have the assertion up to order $m-1 \geq 0$, then we use it to conclude that α satisfies discrete moment conditions of order $m-1$ because it satisfies (16) up to $\ell = m - 1$. Then we apply Micchelli's lemma again on the level $m - 1$, and since we have $\alpha^T A_{m-1} \alpha = 0$, we conclude that α satisfies discrete moment conditions of order m. ■

Discrete moment conditions are useful for degree reduction of linear combinations of high-degree radial polynomials:

Lemma 8. *If a vector $\alpha \in \mathbf{R}^M$ satisfies discrete moment conditions of order m, then for all $2\ell \geq m$ the polynomials*

$$\sum_{k=1}^M \alpha_k \|x - x_k\|_2^{2\ell}$$

have degree at most $2\ell - m$.

Proof. Assume that $\alpha \in \mathbf{R}^M$ satisfies discrete moment conditions of order m. We look at

$$\begin{aligned} \sum_{k=1}^M \alpha_k \|x - x_k\|_2^{2\ell} &= \sum_{k=1}^M \alpha_k \sum_{\ell_1+\ell_2+\ell_3=\ell} \|x\|_2^{2\ell_1} (-2(x, x_k))^{\ell_2} \|x_k\|_2^{2\ell_3} \\ &= \sum_{k=1}^M \alpha_k \sum_{\substack{\ell_1+\ell_2+\ell_3=\ell \\ \ell_2+2\ell_3\geq m}} \frac{\ell!}{\ell_1!\,\ell_2!\,\ell_1!} \|x\|_2^{2\ell_1} (-2(x, x_k))^{\ell_2} \|x_k\|_2^{2\ell_3}, \end{aligned}$$

and this is of degree at most $2\ell_1 + \ell_2 = 2\ell - 2\ell_3 - \ell_2 \leq 2\ell - m$. ■

Now we use that the discrete moment spaces for a finite point set $X = \{x_1, \ldots, x_M\} \subset \mathbf{R}^d$ form a decreasing sequence

$$\cdots \subseteq MC_{m+1}(X) \subseteq MC_m(X) \subseteq \cdots \subseteq MC_0(X) = R^M. \tag{17}$$

This sequence must stop with some zero space at least at order M, because we can always separate M points by polynomials of degree $M-1$, using properly placed hyperplanes.

Definition 3. For any finite point set $X = \{x_1, \ldots, x_M\} \subset \mathbf{R}^d$ there is a unique minimal natural number $\mu = \mu(X)$ such that $MC_\mu(X) = \{0\}$. We call $\mu(X)$ the *discrete moment order* of X.

With this notion, the sequence (17) can be written as

$$MC_\mu(X) = \{0\} \neq MC_{\mu-1}(X) \subseteq \cdots \subseteq MC_0(X) = R^M. \tag{18}$$

There is a fundamental observation linked to the discrete moment order.

Theorem 5. *Any well-defined linear polynomial interpolation process based on a set X must work with polynomials of order at least $\mu(X)$.*

Proof. If the interpolation works with polynomials of order m, the matrix P_m must be of full rank M. But since $MC_{\mu-1} = \ker P_{\mu-1}$ is not trivial, we have $m \geq \mu$. ■

Definition 4. A polynomial interpolation process for a point set X is of *minimal order* if it works with polynomials of order at most $\mu(X)$.

This notion is considerably weaker than "minimal-degree interpolation" as studied by Sauer [12] and the notions of "least" interpolation and the "degree-reducing" property of de Boor and Ron [2], [3], [4].

Remark. Below we shall see a couple of minimal-order polynomial interpolation processes on X, including the one by de Boor and Ron.

We now go back to where we started from, and relate $\mu(X)$ to the quantity $k_0(X)$ defined in (5).

Lemma 9. *For all sets X and Y of M points in $\mathbf{R}^d$ we have*

$$p_k(X, Y) = 0 \qquad \textit{for all } k \textit{ with} \quad 2k < \mu(Y) - 1,$$

and $2k_0(X) \geq \mu(X) - 1$.

Proof. Take a vector $\rho \in \mathbf{Z}_0^M$ and form the matrix

$$(\|x_i - y_j\|_2^{2\rho_i})_{1 \leq i, j \leq M}.$$

We multiply by a nonzero vector $\alpha \in MC_m$ for $m < \mu := \mu(Y)$ and get

$$\begin{aligned}\sum_{j=1}^{M} \alpha_j \|x_i - y_j\|_2^{2\rho_i} &= \sum_{j=1}^{M} \alpha_j \sum_{\ell_1+\ell_2+\ell_3=\rho_i} \frac{\rho_i}{\ell_1!\,\ell_2!\,\ell_3!} \|x_i\|^{2\ell_1} (-2(x_i^T y_j))^{\ell_2} \|y_j\|_2^{2\ell_3} \\ &= \sum_{\ell_1=0}^{\rho_i} \|x_i\|^{2\ell_1} \sum_{\substack{\ell_2+\ell_3=\rho_i-\ell_1 \\ \ell_2+2\ell_3 \geq m}} \frac{\rho_i}{\ell_1!\,\ell_2!\,\ell_3!} \sum_{j=1}^{M} \alpha_j (-2(x_i^T y_j))^{\ell_2} \|y_j\|_2^{2\ell_3}\end{aligned}$$

for all i, $1 \leq i \leq M$. Since $\ell_2 + 2\ell_3 \geq m$ means $2\rho_i - m \geq 2\ell_1 + \ell_2$, this vanishes for those i where $2\rho_i < m$. Thus the matrix is singular if $2\rho_i < m$ for all i or if $2\|\rho\|_\infty < m$. Since the polynomials $p_k(X, Y)$ are superpositions of determinants of such matrices with $2\|\rho\|_1 = 2k \geq 2\|\rho\|_\infty$, all polynomials $p_k(X, Y)$ are zero for $2k < m$. The special case $X = Y$ and the definition of $k_0(X)$ imply the second statement. ■

Lemma 10. *The Lagrange basis polynomials of* (7) *are of degree at most* $2k_0(X) - \mu(X) + 1$.

Proof. We look at the above argument, but swap the meaning of X and Y there, replacing X by $X_j(x)$ and Y by X. The determinants vanish unless $2\|\rho\|_\infty \geq \mu(X) - 1$, and the remaining terms are of degree at most

$$\begin{aligned}2\ell_1 + \ell_2 &= 2\rho_i - \ell_2 - 2\ell_3 \leq 2\rho_i - (\mu(X) - 1) \\ &\leq 2\|\rho\|_\infty - \mu(X) + 1 \leq 2\|\rho\|_1 - \mu(X) + 1 \leq 2k - \mu(X) + 1\end{aligned}$$

for $k = k_0(X) = \|\rho\|_1$. ■

We note that there is a lot of leeway between the result of Lemma 10 and the actually observed degrees of the $p_{k_0(X)}(X, X_j(x))$. The latter seem to be bounded above by $\mu(X) - 1$ instead of $2k_0(X) - (\mu(X) - 1)$.

Theorem 6. *If all expansion coefficients f_k of f are nonzero, then*

$$k_0(X) = \sum_{j=1}^{\mu(X)-1} j(\dim MC_j - \dim MC_{j+1}) \geq \mu(X) - 1. \tag{19}$$

Proof. Let $\mu = \mu(X)$, $m := \mu - 1$, and take a nonzero vector $\alpha \in MC_m$ to evaluate the quadratic form

$$\begin{aligned}\alpha^T A_{c,X,X} \alpha &= \sum_{s=0}^{\infty} c^{2s} f_s \alpha^T A_s \alpha \\ &= \sum_{s=m}^{\infty} c^{2s} f_s \alpha^T A_s \alpha \\ &= c^{2m} f_m \alpha^T A_m \alpha + \sum_{s=m+1}^{\infty} c^{2s} f_s \alpha^T A_s \alpha.\end{aligned}$$

By Courant's minimum-maximum principle, this implies that $A_{c,X,X}$ has at least $\dim MC_m$ eigenvalues which decay at least as fast as c^{2m} to zero for $c \to 0$.

But there are no eigenvalues that decay faster than that. To see this, take, for each $c > 0$, a normalized nonzero eigenvector α_c such that the smallest eigenvalue

$$\alpha_c^T A_{c,X,X}\alpha_c = \sum_{s=0}^{\infty} c^{2s} f_s \alpha_c^T A_s \alpha_c =: \lambda_c$$

decays like c^{2m} or faster. The coefficients $\alpha_c^T A_s \alpha_c$ can increase with s only like $(\mathrm{diam}(X))^{2s}$, and thus we have a stable limit of the analytic function λ_c of c with respect to $c \to 0$. Now we pick a sequence of c's that converges to zero such that α_c converges to some nonzero normalized vector α. Since the decay is assumed to be like c^{2m} or faster, we see that necessarily $\alpha \in MC_m$. Because of $\alpha \notin MC_\mu = \{0\}$ and since we assume $f_m \neq 0$ the function λ_c of c cannot decay faster than c^{2m} for $c \to 0$. Going back to Courant's minimum-maximum principle, we now know that $A_{c,X,X}$ has precisely $\dim MC_m$ eigenvalues that decay exactly like c^{2m} to zero for $c \to 0$.

We can now repeat this argument on the subspace of MC_{m-1} that is orthogonal to MC_m. For each nonzero vector of this space, the quadratic form decays like $c^{2(m-1)}$, and there are $\dim MC_{m-1} - \dim MC_m$ linear independent vectors with this property. Now we look for arbitrary vectors α_c that are orthogonal to the already determined $\dim MC_m$ eigenvectors of $A_{c,X,X}$ with eigenvalues of decay c^{2m}, and we assume that they provide eigenvalues with fastest possible decay. This decay cannot be of type c^{2m} or faster due to the assumed orthogonality, which allows passing to the limit. It must thus be of exact decay $c^{2(m-1)}$. Induction now establishes the fact that for each j, $0 \le j \le m$, there are $\dim MC_j - \dim MC_{j+1}$ eigenvalues of $A_{c,X,X}$ with exact decay like c^{2j} for $\to 0$. Thus the determinant decays exactly like the product of these, and this proves our assertion. ∎

Note that the above discussion fails to prove that the limiting polynomial interpolation process coming from a smooth radial basis function is of minimal order in the case of nonvanishing expansion coefficients. Numerical results by Driscoll and Fornberg [6] show that nonminimal degrees actually occur if expansion coefficients vanish.

Though $k_0(X)$ will exceed $\mu(X)$, for instance in one-dimensional situations, there is plenty of cancellation in the polynomials $p_{k_0(X)}(X, X_j(x))$ that we have not accounted for, so far. On the other hand, we have not found any example with nonvanishing expansion coefficients where the polynomial limit of a radial basis function interpolation is not of minimal order.

There is another interesting relation of μ to the spaces spanned by radial polynomials:

Lemma 11. *Define the M-vectors*

$$F_\ell(x) := ((-1)^\ell \|x - x_k\|_2^{2\ell})_{1\le k\le M}.$$

Then the $M \times M(s+1)$ matrix with columns $F_\ell(x_j)$, $1 \le j \le M$, $0 \le \ell \le s$, has full rank M if $s + 1 \ge \mu$, and μ is the smallest possible number with this property.

Proof. Assume that the matrix does not have full rank M for a fixed s. Then there is a nonzero vector $\alpha \in \mathbf{R}^M$ such that

$$\alpha^T A_\ell = 0 \qquad \text{for all } 0 \le \ell \le s,$$

and by Theorem 4 this implies discrete moment conditions of order $s+1$. Thus $s+1 \le \mu - 1$. ■

This teaches us that when aiming at interpolation by radial polynomials of the form $\|x - x_k\|_2^{2\ell}$ one has to go up to $\ell = \mu - 1$ to get anywhere. But in view of Theorem 5, which states a minimal order $\mu(X)$ instead of $2\mu(X) - 1$ in Lemma 11, we have to find order-reducing linear combinations of radial polynomials which make up a minimal-order basis of an M-dimensional subspace of polynomials. The following notion does this and will be very helpful for the rest of the paper.

Definition 5. A *discrete moment basis of R^M with respect to X* is a basis

$$\alpha^1, \dots, \alpha^M \quad \text{such that} \quad \alpha^j \in MC_{t_j} \backslash MC_{t_j+1}$$

for the decomposition sequence (18) and $t_1 = 0 \le \cdots \le t_M = \mu - 1$.

Remark. A discrete moment basis $\alpha^1, \dots, \alpha^M$ of $\mathbf{R}^M$ can be chosen to be orthonormal, when starting with α_M, spanning the spaces $MC_{\mu-1} \subseteq \cdots \subseteq M_0 = R^M$ one after the other. But there are other normalizations that make sense, in particular the one that uses conjugation via A_ℓ on $MC_\ell \backslash MC_{\ell+1}$, because this matrix is positive definite there due to Micchelli's lemma. There is a theoretical and numerical connection of discrete moment bases to properly pivoted LU factorizations of Vandermonde-type matrices of values of polynomials (see also the papers [3], [4] of de Boor and Ron and [13] of Sauer and Xu), but we shall neither go into detail nor require the reader to figure this out before we proceed.

We now consider the polynomials

$$v_j(x) := \sum_{i=1}^{M} \alpha_i^j \|x - x_i\|^{2t_j}, \qquad 1 \le j \le M, \tag{20}$$

which are of degree at most $t_j \le \mu$ due to Lemma 8 and the definition of the discrete moment basis. They are low-degree linear combinations of radial polynomials, and their definition depends crucially on the geometry of X.

Lemma 12. *The $M \times M$ matrix with entries $v_j(x_k)$ is nonsingular.*

Proof. We multiply this matrix with the nonsingular $M \times M$ matrix containing the discrete moment basis $\alpha^1, \dots, \alpha^M$ and get a matrix with entries

$$\gamma_{jm} = \sum_{i=1}^{M} \sum_{k=1}^{M} \alpha_i^j \alpha_k^m \|x_i - x_k\|^{2t_j}$$

for $1 \le j, m \le M$. Consider $m > j$ and use $t_m \ge t_j$ to see that $\gamma_{jm} = 0$ as soon as $t_m > t_j$, because the entries can be written as values of a polynomial of degree $2t_j - t_j - t_m < 0$. Thus the matrix is block triangular, and the diagonal blocks consist of entries $\alpha_i^j \alpha_k^m \|x_i - x_k\|^{2t}$ with $t = t_j = t_m$. But these symmetric submatrices must be definite due to Lemma 7 and our construction of a discrete moment basis. We even could have chosen the basis such that the diagonal blocks are unit matrices, if we had used conjugation with respect to A_t. ■

Theorem 7. *A polynomial interpolation of minimal order on X is possible using the functions v_j of Lemma* 12. *These are of order at most $\mu = \mu(X)$, and thus*

$$\binom{\mu(X)+d}{d} \le M \le \binom{\mu(X)+d-1}{d} \le \binom{k_0(X)+d}{d}.$$

Example 3. Let us look at the special case with $M = 4$, $d = 2$, and points

$$x_1 := (0,0)^T, \qquad x_2 := (1,0)^T, \qquad x_3 := (0,1)^T, \qquad x_4 := (\tfrac{1}{2}, 1)^T.$$

The discrete moment conditions on vectors $\alpha \in \mathbf{R}^4$ are

$$\sum_{j=1}^{4} \alpha_j \;=\; 0 \qquad \text{for all } \alpha \in MC_1,$$

$$\sum_{j=1}^{4} \alpha_j \;=\; 0, \qquad \alpha_2 + \alpha_4/2 = 0, \qquad \alpha_3 + \alpha_4 = 0 \qquad \text{for all } \alpha \in MC_2.$$

Furthermore, we find $MC_3 = \{0\}$, $MC_2 = \text{span}\{\alpha^4 := (1,-1,-2,2)^T\}$, $MC_0 = \mathbf{R}^4$, and $MC_1 \setminus MC_2 = \text{span}\{\alpha^2 := (1,-1,0,0)^T, \alpha^3 := (1,0,-1,0)^T\}$, such that a discrete moment basis of $\mathbf{R}^4$ can be formed by $\alpha^1 := (1,0,0,0)^T$ with α^2, α^3, and α^4 together with $t_0 = 0 < t_1 = t_2 = 1 < t_3 = 2 = \mu - 1$. From Theorem 6 we conclude that $k_0(X) = 1 \cdot 2 + 2 \cdot 1 = 4$. MAPLE confirms this, and the Lagrange basis of the form (14) comes out to be quadratic for all f that one could start with, but the result depends on f. For example, the Lagrange basis function for the origin is

$$1 - \tfrac{2}{9}x^2 + \tfrac{8}{9}xy - \tfrac{7}{9}x - y \qquad \text{for } f(t) = e^{-t}, \qquad \varphi = \text{Gaussian},$$

$$\tfrac{1}{37}(37 + 32xy - 35y - 10x^2 - 2y^2 - 27x) \text{ for } f(t) = 1/(1+t),\ \varphi = \text{inverse multiquadric}.$$

The Gaussian case coincides with the de Boor/Ron solution from Section 6 of [3]. The method based on (20) yields the basis function

$$\tfrac{1}{19}(19 - 13x - 17y - 6x^2 - 2y^2 + 16xy).$$

Thus we have different methods, but we note that the de Boor/Ron interpolation method coincides with the limit of interpolation with shifted and scaled Gaussians.

6. The Method of de Boor and Ron Revisited

The goal of this section is to prove Theorem 2. For this we require at least a scaled version of the de Boor/Ron technique, and we take the opportunity to rephrase with slightly increased generality.

For all $\beta \in \mathbf{Z}_0^d$ let w_β be a positive real number, and consider the inner product

$$(p, q)_w := \sum_{\beta \in \mathbf{Z}_0^d} \frac{1}{w_\beta} (D^\beta p)(0)(D^\beta q)(0)$$

on the space $\mathbb{P}_\infty^d$ of all d-variate polynomials. Such more general inner products have been considered before, e.g., by T. Sauer. The de Boor/Ron interpolant arises in the special case $w_\beta = \beta!$.

Now we want to link the theory to radial basis function techniques. If we assume

$$\sum_{\beta \in \mathbf{Z}_0^d} \frac{w_\beta}{\beta!^2} < \infty$$

and define the kernel

$$K_w(x, y) := \sum_{\beta \in \mathbf{Z}_0^d} w_\beta \frac{x^\beta}{\beta!} \frac{y^\beta}{\beta!}, \tag{21}$$

all polynomials $p \in \mathbb{P}_\infty^d$ are reproduced via

$$p(x) = (p, K_w(x, \cdot))_w \tag{22}$$

and this identity carries over to the Hilbert space completion

$$\mathcal{H}_w := \left\{ g \in \mathbf{C}^\infty(\mathbf{R}^d) : g(x) = \sum_{\beta \in \mathbf{Z}_0^d} (D^\beta g)(0) \frac{x^\beta}{\beta!}, \ \sum_{\beta \in \mathbf{Z}_0^d} \frac{1}{w_\beta} (D^\beta g)^2(0) < \infty \right\}$$

of the polynomials under the above inner product. The kernel K_w is positive definite on $[-1, 1]^d$, and larger domains can be treated by scaling. Since polynomials separate points, it is clear that for all finite sets $X = \{x_1, \ldots, x_N\} \subset [-1, 1]^d$ we have linear independence of the functions $K_w(\cdot, x_j)$, and interpolation in X by the span of these functions is uniquely possible.

So far, we used standard arguments of radial basis function theory. In the papers of de Boor and Ron, transition to a polynomial interpolation process is done via truncation, not via passing to the limit of a scaling. For all functions g from $\mathcal{H}_w$ the notation

$$g^{[k]}(x) := \sum_{\substack{\beta \in \mathbf{Z}_0^d \\ |\beta| = k}} (D^\beta g)(0) \frac{x^\beta}{\beta!}$$

is introduced, while $g\!\downarrow$ stands for the nonzero function $g^{[k]}$ with minimal k. For a finite set $X = \{x_1, \ldots, x_N\} \subset [-1, 1]^d$ the spaces

$$E_{w,X} := \operatorname{span}\{K_w(x, \cdot) \ : \ x \in X\}, \qquad P_{w,X} := \operatorname{span}\{g\!\downarrow \ : \ g \in E_{w,X}\},$$

are introduced, and $P_{w,X}$ is a space of polynomials.

Theorem 8. *Interpolation on X by functions in $P_{w,X}$ is uniquely possible.*

Proof. Assume that there is some nonzero $p \in P_{w,X}$ such that $p_{|X} = 0$. We take some nontrivial function g_p such that $p = g_p\downarrow$. Then (22) yields orthogonality $(p, g)_w = 0$ for all $g \in E_{w,X}$, and we have the contradiction

$$0 = (p, g_p)_w = (g_p\downarrow, g_p)_w = (g_p\downarrow, g_p\downarrow)_w.$$

So far, we have followed the proof of de Boor and Ron, but now we want to use a discrete moment basis $\alpha^1, \dots, \alpha^M$ to link the process with what we have done in previous sections. We define functions

$$v_r(y) := \sum_{j=1}^{M} \alpha_j^r K_w(x_j, y) = \sum_{|\beta| \ge t_r} w_\beta \frac{y^\beta}{\beta!} \sum_{j=1}^{M} \alpha_j^r \frac{x_j^\beta}{\beta!}, \quad g_r := v_r\downarrow, \quad 1 \le r \le M. \tag{23}$$

Due to the property of a discrete moment basis we see that not all of the quantities

$$c_{\beta,r} := \sum_{j=1}^{M} \alpha_j^r \frac{x_j^\beta}{\beta!}$$

for $|\beta| = t_r$ can vanish, because otherwise $\alpha^r \in MC_{t_r+1}$. Thus we have the homogeneous representation

$$g_r(y) = v_r\downarrow(y) = \sum_{|\beta| = t_r} w_\beta c_{\beta,r} \frac{y^\beta}{\beta!} \tag{24}$$

and $(g_r, g_s)_w = 0$ for $t_r \ne t_s$. The matrix formed by the $(g_r, g_s)_w$ is a positive semidefinite block-diagonal Gramian. To prove its definiteness, we can focus on a single diagonal block with $t = t_r = t_s$. Collecting the indices r with $t_r = t$ into a set I_t, we assert linear independence of the functions g_r for $r \in I_t$. For a vanishing linear combination

$$\begin{aligned} 0 &= \sum_{r \in I_t} \gamma_r g_r(y) \\ &= \sum_{r \in I_t} \gamma_r \sum_{|\beta| = t} w_\beta c_{\beta,r} \frac{y^\beta}{\beta!} \\ &= \sum_{|\beta| = t} \frac{y^\beta}{\beta!} w_\beta \sum_{r \in I_t} \gamma_r c_{\beta,r} \\ &= \sum_{|\beta| = t} \frac{y^\beta}{\beta!} w_\beta \sum_{r \in I_t} \gamma_r \sum_{j=1}^{M} \alpha_j^r \frac{x_j^\beta}{\beta!} \\ &= \sum_{|\beta| = t} \frac{y^\beta}{\beta!} w_\beta \sum_{j=1}^{M} \left(\sum_{r \in I_t} \gamma_r \alpha_j^r \right) \frac{x_j^\beta}{\beta!} \end{aligned}$$

we conclude that $\sum_{r \in I_t} \gamma_r \alpha^r$ is a vector in MC_{t+1}, and this can hold only if the coefficients are zero. Thus the space $P_{w,X}$ contains the M linearly independent homogeneous polynomials $g_1, \dots, g_M$ of increasing degrees $0 = t_1 \leq \cdots \leq t_M = \mu - 1$, and the theorem is proven. Due to Theorem 5, the order is minimal, as known from the de Boor/Ron papers. ■

We now proceed toward proving that the limit of interpolants by Gaussians is equal to the de Boor/Ron polynomial interpolant. We need something that links kernels of the form (21) to radial kernels.

Lemma 13. *If φ is a positive definite analytic radial basis function that can be written via an analytic function f satisfying* (1) *and* (13), *then*

$$f(x^T y) = \sum_{\beta \in \mathbf{Z}_0^d} \frac{f^{|\beta|}(0)}{\beta!} x^\beta y^\beta = \sum_{\beta \in \mathbf{Z}_0^d} f_{|\beta|} x^\beta y^\beta \tag{25}$$

for all $x, y \in \mathbf{R}^d$.

Proof. We use the Bernstein–Widder representation

$$f(r) = \int_0^\infty e^{-rt}\, d\mu(t), \qquad r \geq 0,$$

to get

$$(-1)^j f^{(j)}(0) = (-1)^j j!\, f_j = \int_0^\infty t^j\, d\mu(t) \in (0, \infty) \qquad \text{for all } j \geq 0,$$

and similarly, factoring the exponential in the integral,

$$D_x^\beta f(x^T y) = y^\beta \int_0^\infty (-1)^{|\beta|} t^{|\beta|} e^{-t x^T y}\, d\mu(t)$$

and

$$D_x^\beta f(x^T y)_{|x=0} = y^\beta f^{|\beta|}(0) = y^\beta \beta!\, f_{|\beta|}$$

where D_x^β takes derivatives of order β with respect to x. The assertion follows from putting the result into the power series expansion at zero. ■

At first sight, the above result is disappointing, because one cannot easily use (25) in (21), since the coefficients in (25) are alternating. However, a closer look reveals that the major part of the de Boor/Ron theory does not rely on the signs of the coefficients. It is the link to positive definite radial basis functions as reproducing kernels that does not work without further arguments. This has a positive consequence: the generalized de Boor/Ron approach as given at the start of this section will yield many new cases of positive definite nonradial interpolants with polynomial truncations that furnish polynomial interpolants of minimal order in the sense of this paper. On the downside, we cannot expect to find a direct link between interpolation by general positive definite radial basis functions and the generalized de Boor/Ron method.

But for Gaussians, we can add some more work, factoring

$$\exp(-c\|x_j - x_k\|_2^2) = \exp(-c\|x_j\|_2^2) \cdot \exp(2cx_j^T x_k) \cdot \exp(-c\|x_k\|_2^2).$$

We then rewrite the Lagrange system

$$\sum_{j=1}^{M} u_j^c(x) \exp(-c\|x_j - x_k\|_2^2) = \exp(-c\|x - x_k\|_2^2), \qquad 1 \le k \le M,$$

in the form

$$\begin{aligned}\sum_{j=1}^{M} z_j^c(x) \exp(2cx_j^T x_k) \;&=\; \sum_{j=1}^{M} u_j^c(x) \exp(-c(\|x_j\|^2 - \|x\|^2)) \exp(2cx_j^T x_k)\\ &=\; \exp(2cx^T x_k), \qquad 1 \le k \le M,\end{aligned}$$

with $z_j^c(x) := u_j^c(x) \exp(-c(\|x_j\|^2 - \|x\|^2))$, $1 \le j \le M$. Now we can use the technique of the previous lemma directly, putting in the expansions for the exponential and working with the kernel $K_c(x, y) := \exp(2cx^t y)$ in our presentation of the de Boor/Ron technique, with a slight abuse of notation. This implies that the functions $z_j^c(x)$ form a Lagrange basis for the span of the $K_c(x_j, x) = \exp(2cx_j^t x)$. Any interpolation by scaled Gaussians can be converted by the above transformation to and from an interpolation using the kernel K_c.

We now look at what happens if the de Boor/Ron truncation process is carried out on interpolants defined via K_c. The functions in (24) come out as

$$\begin{aligned} g_r^c(y) \;&=\; \sum_{|\beta|=t_r} w_\beta^c c_{\beta,r} \frac{y^\beta}{\beta!}\\ &=\; \sum_{|\beta|=t_r} \frac{(2c)^{|\beta|}}{\beta!} c_{\beta,r} \frac{y^\beta}{\beta!}\\ &=\; (2c)^{t_r} \sum_{|\beta|=t_r} \frac{1}{\beta!} c_{\beta,r} \frac{y^\beta}{\beta!}\\ &=\; (2c)^{t_r} g_r^{dBR}(y),\end{aligned}$$

i.e., they are just scalar multiples of the functions g_r^{dBR} of the de Boor/Ron process. Thus the polynomial space spanned by truncation of the K_c is independent of c and coincides with the de Boor/Ron polynomial interpolation space. Note that de Boor and Ron have already observed that $P_{w,X}$ is independent of scaling.

We have successfully moved from interpolation by Gaussian radial basis functions to interpolation by scaled exponentials, and we have seen that the truncation of the latter is the de Boor/Ron polynomial space. But we now have to investigate the limit of the interpolants spanned by the scaled exponentials $K_c(x_j, \cdot)$ for $c \to 0$ to see whether they converge toward the de Boor/Ron truncation.

We go back to (23) to define functions v_r^c as

$$v_r^c(y) \;:=\; \sum_{j=1}^{M} \alpha_j^r K_c(x_j, y)$$

$$= \sum_{|\beta|\geq t_r} \frac{(2c)^{t_r}}{\beta!} \frac{y^\beta}{\beta!} c_{\beta,r}$$

$$= \sum_{s\geq t_r} (2c)^s \sum_{|\beta|=s} \frac{1}{\beta!} \frac{y^\beta}{\beta!} c_{\beta,r},$$

hence

$$\lim_{c\to 0} \frac{v_r^c(y)}{(2c)^{t_r}} = g_r^{dBR}(y), \qquad 1 \leq r \leq M.$$

This means that the space spanned by the $K_c(x_j, \cdot)$ contains a basis that converges toward a basis of the de Boor/Ron polynomial space for $c \to \infty$. Consequently, the Lagrange basis for interpolation in the span of the $K_c(x_j, \cdot)$ converges toward a polynomial limit. This ends the proof of Theorem 2. ■

7. Preconditioning

The transition from the Gaussian system to the scaled basis $v_r^c(y)/(2c)^{t_r}$ should be useful as a preconditioning technique. In general, we show in this section how to use a discrete moment basis for preconditioning badly conditioned matrices arising from interpolation by general smooth radial basis functions. This is not yet intended for large-scale numerical use, but it yields full insight into what is going on for kernels whose flatness leads to ill-conditioning. It seems to be the first investigation in this direction.

We go back to the beginning of the paper and precondition the matrix $A_{c,X,X}$ arising in (2) by a scaled discrete moment basis

$$c^{-t_1/2}\alpha^1, \dots, c^{-t_M/2}\alpha^M \tag{26}$$

in the following way. If we put the discrete moment basis into an $M \times M$ matrix B_c and form the positive definite symmetric matrix $Z(c) := B_c A_{c,X,X} B_c^T$, the matrix entries will be

$$\begin{aligned} z_{rs}(c) &:= \sum_{j,k=1}^{M} \alpha_j^r c^{-t_r/2} \alpha_k^s c^{-t_s/2} \varphi_c(\|x_j - x_k\|_2), \qquad 1 \leq r, s \leq M, \\ &= \sum_{n=0}^{\infty} f_n c^{n-t_r/2-t_s/2} \sum_{j,k=1}^{M} \alpha_j^r \alpha_k^s \|x_j - x_k\|_2^{2n} \\ &= \sum_{\substack{n=0 \\ 2n\geq t_r+t_s}}^{\infty} f_n c^{n-t_r/2-t_s/2} \sum_{j,k=1}^{M} \alpha_j^r \alpha_k^s \|x_j - x_k\|_2^{2n} \end{aligned}$$

with well-defined limits

$$z_{rs}(0) = \begin{Bmatrix} f_{(t_r+t_s)/2} \sum_{j,k=1}^{M} \alpha_j^r \alpha_k^s \|x_j - x_k\|_2^{t_r+t_s}, & t_r + t_s \text{ even} \\ 0, & \text{else} \end{Bmatrix}$$

for $c \to 0$. The matrix $Z(0)$ is positive semidefinite by construction, and we assert

Theorem 9. *The matrix $Z(0)$ is positive definite if all expansion coefficients are nonzero.*

Proof. We use the proof technique of Theorem 6. The product of all eigenvalues of $A_{c,X,X}$ decays with exponent $k_0(X)$ as in (19), while the maximum eigenvalue stays bounded above independent of c. But our matrix transformation performs a multiplication of the spectral range by $c^{-k_0(X)}$, because $k_0(X) = \sum_{j=1}^{M} t_j$ is just another way to write (19). Thus the smallest eigenvalue of the product must stay away from zero when $c \to 0$. But since the matrix $Z(0)$ is well defined, the maximal eigenvalue of the product $Z(c)$ must be bounded, and $Z(0)$ altogether has a strictly positive spectrum. ■

Example 4. If we go back to the four points in $\mathbf{R}^2$ of Example 3 and scale the discrete moment basis as in (26) via

$$B_c := \begin{pmatrix} 1 & 0 & 0 & 0 \\ 1/\sqrt{c} & -1/\sqrt{c} & 0 & 0 \\ 1/\sqrt{c} & 0 & -1/\sqrt{c} & 0 \\ 1/c & -1/c & -2/c & 2/c \end{pmatrix},$$

MAPLE produces a limit matrix

$$Z(0) := \begin{pmatrix} 1 & 0 & 0 & \frac{1}{2} \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ \frac{1}{2} & 0 & 0 & \frac{19}{4} \end{pmatrix}$$

for Gaussians and

$$Z(0) := \begin{pmatrix} 1 & 0 & 0 & -\frac{1}{4} \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ -\frac{1}{4} & 0 & 0 & -\frac{19}{16} \end{pmatrix}$$

for (negative definite) inverse multiquadrics with $\beta = -1$. If we take four equidistant points on the line $[0, 1] \times \{0\}$, we find

$$Z(0) := \begin{pmatrix} 1 & 0 & -\frac{2}{9} & 0 \\ 0 & \frac{2}{9} & 0 & -\frac{4}{27} \\ -\frac{2}{9} & 0 & \frac{4}{27} & 0 \\ 0 & -\frac{4}{27} & 0 & \frac{40}{243} \end{pmatrix} \text{ for } B_c := \begin{pmatrix} 1 & 0 & 0 & 0 \\ 1/\sqrt{c} & -1/\sqrt{c} & 0 & 0 \\ 1/c & -2/c & 1/c & 0 \\ 1/c\sqrt{c} & -3/c\sqrt{c} & 3/c\sqrt{c} & -1/c\sqrt{c} \end{pmatrix}$$

in the case of Gaussians. The discrete moment basis now contains divided differences, and the zero structure is different from the previous case, because we have $t_j = j - 1$, $1 \le j \le 4$, here.

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