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REPORT

FAST EVALUATION OF RADIAL BASIS FUNCTIONS: METHODS FOR GENERALISED MULTIQUADRICS IN $\mathbb{R}^n$

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Fast evaluation of radial basis functions: Methods for generalised multiquadrics in $\mathbb{R}^n$.

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Abstract

A generalised multiquadric radial basis function is a function of the form $s(x) = \sum_{i=1}^{N} d_i \phi(|x - t_i|)$, where $\phi(r) = \left(r^2 + \tau^2\right)^{k/2}$, $x \in \mathbb{R}^n$, and $k \in \mathbb{Z}$ is odd. The direct evaluation of an N centre generalised multiquadric radial basis function at m points requires $\mathcal{O}(mN)$ flops, which is prohibitive when m and N are large. Similar considerations apparently rule out fitting an interpolating N centre generalised multiquadric to N data points by either direct or iterative solution of the associated system of linear equations in realistic problems.

In this paper we will develop far field expansions, recurrence relations for efficient formation of the expansions, error estimates, and translation formulas, for generalised multiquadric radial basis functions in n-variables. These pieces are combined in a hierarchical fast evaluator requiring only $\mathcal{O}((m+N)\log N|\log\epsilon|^{n+1})$ flops for evaluation of an N centre generalised multiquadric at m points. This flop count compares very favourably with the cost of the direct method. Moreover, used to compute matrix-vector products, the fast evaluator provides a basis for fast iterative fitting strategies.

1 Introduction

Multiquadrics are a popular choice of radial basis function for interpolating scattered data in one or more dimensions. Many applications are described in the literature including geodesy, image processing and natural resource modelling (see, for example, Hardy [10]). The beautiful properties of multiquadric and other radial basis functions, such as the poisedness of suitable interpolation problems, are detailed in Cheney and Light [7, Ch. 12–16, 36]. Unfortunately, the adoption of multiquadrics for real problems with large data sets

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has been hindered by a perceived large computational cost. Indeed, the direct evaluation of an N centre multiquadric radial basis function at m points requires $\mathcal{O}(mN)$ flops which is prohibitive when m and N are large. Similar considerations apparently rule out fitting an interpolating N centre multiquadric to N data points by either direct or iterative solution of the associated system of linear equations in realistic problems.

However the use of hierarchical methods, fast multipole methods, and other multiresolution schemes allow fast evaluation and fitting of radial basis functions. This paper develops far field expansions for generalised multiquadric radial basis functions in n-variables of the form required by these new methods. Schemes of a hierarchical type can then be built upon these expansions that require only $\mathcal{O}((m+N)\log N|\log\epsilon|^{n+1})$ flops for evaluation of an N centre generalised multiquadric to accuracy ϵ at m points. This compares very favourably with the cost of the direct method. Moreover, used to compute matrix-vector products, the fast evaluator can be combined with suitable iterative methods and preconditioning strategies to yield fast iterative algorithms for interpolatory or smoothing fits (see e.g. [2]).

The first fast multipole method was that of Greengard and Rokhlin [9]. Since then the method has been modified and extended to apply in many different contexts [3]. For reasons of space we are forced to omit discussion of many important aspects of hierarchical and fast multipole methods from this paper. In particular, we have omitted almost all discussion of the crucial algorithmic details which enable a fast evaluation scheme for use in $\mathbb{R}^n$ to be built upon suitable far field expansions, such as the expansion for generalised multiquadrics developed in this paper.

A much fuller account of hierarchical and fast multipole methods is given in the survey paper [3]. The reader new to these methods is referred to that paper, and in particular to the tutorial section concerning hierarchical and fast multipole schemes in one dimension. Indeed the model problem of that section is fast evaluation of an ordinary multiquadric in $\mathbb{R}^1$. However, the treatment there concentrates exclusively on algorithmic aspects and suppresses the mathematical analysis of expansions and error bounds. Previous papers concerning fast multipole and related methods for fast evaluation of radial basis functions include [5, 4, 6].

The generic fast multipole method requires results of the following nature for the basic function Φ being used:

- The existence of a rapidly converging far field expansion, centred at 0, for the shifted basic function $\Phi(x-t)$. The existence of such an expansion implies that, for all x sufficiently far from 0, the spline $s(x) = \sum_{i=1}^{N} d_i \Phi(x-t_i)$ may be approximated to the desired accuracy by a short series. When N is large it will be much faster to use the series rather than to evaluate $s(x)$ directly.

- Error bounds that determine how many terms are required in each expansion to achieve a specified accuracy.

- Efficient recurrence relations for computing the coefficients of the expansions.

- Uniqueness results that justify indirect translation of expansions.

- Formulae for efficiently converting a far field expansion to a rapidly convergent local expansion.

This paper provides appropriate results of these types for generalised multiquadric radial basis functions in $\mathbb{R}^n$. That is for functions of the form

$$s(x) = \sum_{i=1}^{N} d_i \Phi(x - t_i; k, \tau), \tag{1.1}$$

where

$$\Phi(x) = \Phi(x; k, \tau) = \left(x^2 + \tau^2\right)^{k/2}, \tag{1.2}$$

k is an odd integer, $\tau \geq 0$ and $x \in \mathbb{R}^n$. Note we will usually use the notation $\Phi(x)$ which hides the dependence of Φ on k and τ. The derived series and the analysis also apply when τ varies, that is the multiquadric parameter τ changes with the centre t_i.

The paper is laid out as follows. First Sections 2 and 3 derive far field expansions of the following form

$$\Phi(x - t; k, \tau) = \sum_{\ell=0}^{\infty} P_\ell^{(k)}(|t|^2 + \tau^2, -2\langle t, v\rangle, |x|^2)/|x|^{2\ell-k} \tag{1.3}$$

where the $P_\ell^{(k)}$ are the polynomials

$$P_\ell(a, b, c) = P_\ell^{(k)}(a, b, c) = \sum_{j=\lfloor \frac{\ell+1}{2} \rfloor}^{\ell} \binom{k/2}{j} \binom{j}{\ell - j} b^{2j-\ell}(ac)^{\ell-j}, \qquad \ell \geq 0, \tag{1.4}$$

and $P_\ell^{(k)}$ is the zero function for ℓ negative. Section 3 also gives error bounds on approximations formed by truncating the series. Section 4 proves the uniqueness of the expansions. Section 5 discusses recurrence relations for the efficient direct calculation of the far field coefficients. It shows that the terms of the first $p + k + 1$ homogeneous orders in the series for an m centre cluster can be calculated in $\mathcal{O}(mn(p+k)^n)$ flops. Section 6 sets up some machinery which is used in Section 7 to establish methods for indirectly translating far field expansions. Section 8 shows how to efficiently convert a far field expansion into a local polynomial approximation. The paper concludes with some numerical results showing that multiquadric radial basis functions can indeed be evaluated using this approach at a cost that grows as $\mathcal{O}(N \log N)$ in the number N of centres.

A brief note about notation. We will use lower case ϕ for the basic function as a function of one variable and upper case Φ for the function of n variables, i.e., $\Phi = \phi(|\cdot|)$. It is common for the constant in the multiquadric basic function to be represented by c. However, we will use τ for this purpose, i.e., the ordinary multiquadric basic function will be $\phi(r) = \sqrt{r^2 + \tau^2}$. In the far field expansions, x is the *evaluation point* and u is the *centre of expansion*, although often we may take $u = 0$. This centre of expansion should not be confused with the *centres* $\{t_i\}$ which are the centres of the radially symmetric components in the RBF. In applications these centres will often be the nodes of interpolation or point sources of some potential field.

2 A Generating Function

In this section we develop some important properties of the functions

$$f_k(z) = (\sqrt{az^2+bz+c})^k, \qquad k \in \mathbb{Z} \text{ is odd.} \tag{2.1}$$

These functions will turn out to be the generating functions for the polynomials $P_\ell^{(k)}$ that occur in the far and near field expansions of the generalised multiquadric function.

To fully explore the expansions of f_k we will need to use Gauss's hypergeometric function.

LEMMA 2.1: The *hypergeometric function*,

$$F(a,b;c;z) = F(b,a;c;z) := \frac{\Gamma(c)}{\Gamma(a)\Gamma(b)} \sum_{n=0}^{\infty} \frac{\Gamma(a+n)\Gamma(b+n)}{\Gamma(c+n)} \frac{z^n}{n!},$$

satisfies

$$F(a,b;c;z) = (1-z)^{c-a-b} F(c-a, c-b; c; z), \tag{2.2a}$$

$$\frac{d}{dz} F(a,b;c;z) = \frac{ab}{c} F(a+1, b+1; c+1; z). \tag{2.2b}$$

Furthermore, if a or b is equal to $-m$, m a non-negative integer, then $F(a,b;c;z)$ reduces to a polynomial of degree m in z.

Proof. See [1, Ch. 15]. ∎

LEMMA 2.2: Let $m, p \in \mathbb{N}_0$ and $|h| < 1$. Then

$$\sum_{n=p}^{\infty} \binom{n+m}{m} h^n = \frac{h^p}{(1-h)^{m+1}} \frac{(p+m)!}{p!\, m!} F(-m, p; p+1; h).$$

Proof.

$$\begin{aligned}
\sum_{n=p}^{\infty} \binom{n+m}{m} h^n &= \frac{(p+m)!}{p!\, m!} \frac{p!}{(p+m)!} h^p \sum_{n=0}^{\infty} \frac{(n+p+m)! n!}{(n+p)!} \frac{h^n}{n!} \\
&= \frac{(p+m)!}{p!\, m!} h^p F(m+p+1, 1; p+1; h) \\
&= \frac{(p+m)!}{p!\, m!} h^p (1-h)^{-(m+1)} F(-m, p; p+1; h),
\end{aligned}$$

where the last equality follows from (2.2a). ∎

We now present the major result of this section which gives a series expansion for f_k and a bound for the error in approximating f_k by a truncation of this series.

LEMMA 2.3: Let $k \in \mathbb{Z}$ be odd and let $a, b, c \in \mathbb{R}$, with $a, c > 0$ and $b^2 \leq 4ac$. Then for all $z \in \mathbb{C}$ such that $|z| < \sqrt{c/a}$,

$$f_k(z) = (\sqrt{az^2 + bz + c})^k = c^{k/2} \sum_{\ell=0}^{\infty} \left(\frac{z}{c}\right)^{\ell} P_{\ell}^{(k)}(a, b, c) \tag{2.3}$$

where the $P_{\ell}^{(k)}$ are the polynomials defined in Equation (1.4). Moreover, for all z such that $|z| < \sqrt{c/a}$ and $\nu \in \mathbb{N}$,

$$\left| (az^2 + bz + c)^{k/2} - c^{k/2} \sum_{\ell=0}^{\nu} \left(\frac{z}{c}\right)^{\ell} P_{\ell}^{(k)}(a, b, c) \right|$$
$$\leq \begin{cases} 2^k c^{k/2} \left(\dfrac{|z|}{\sqrt{c/a}}\right)^{\nu+1} \dfrac{\sqrt{c/a}}{\sqrt{c/a} - |z|}, & \text{if } k > 0 \\[2ex] \dbinom{\nu - k}{\nu + 1} c^{k/2} \left(\dfrac{|z|}{\sqrt{c/a}}\right)^{\nu+1} \left(\dfrac{\sqrt{c/a}}{\sqrt{c/a} - |z|}\right)^{-k} \\ \qquad \times F\left(k+1, \nu+1; \nu+2; \dfrac{z}{\sqrt{c/a}}\right), & \text{if } k < 0. \end{cases}$$

Proof. Let $\sqrt{\cdot}$ denote the principal branch of the complex square root. Then f_k is analytic whenever $q(z) = az^2 + bz + c$ is away from the branch cut. That is whenever $q(z)$ is not a non-positive real. Completing the square,

$$q(z) = a\left\{\left(z + \frac{b}{2a}\right)^2 + \frac{4ac - b^2}{4a^2}\right\},$$

and since $b^2 \leq 4ac$, it is easily seen that f_k is analytic away from

$$\left\{z = -\frac{b}{2a} + \mathrm{i}y : y \in \mathbb{R} \text{ and } |y| \geq \sqrt{\frac{4ac - b^2}{4a^2}}\right\}.$$

Hence f_k is analytic on the disc

$$D = D_\epsilon = \left\{z \in \mathbb{C} : |z| \leq \rho = (1 - \epsilon)\sqrt{c/a}\right\}, \qquad 0 < \epsilon < 1.$$

For all sufficiently small $|z|$, two applications of the Binomial Theorem and some reordering gives

$$f_k(z) = c^{k/2} \left(1 + \frac{bz + az^2}{c}\right)^{k/2}$$

$$
\begin{aligned}
&= c^{k/2} \sum_{j=0}^{\infty} \binom{k/2}{j} \left(\frac{bz + az^2}{c} \right)^j \\
&= c^{k/2} \sum_{j=0}^{\infty} \binom{k/2}{j} \sum_{q=0}^{j} \binom{j}{q} \frac{(bz)^{j-q} (az^2)^q}{c^j} \\
&= c^{k/2} \sum_{\ell=0}^{\infty} \sum_{j=\lfloor \frac{\ell+1}{2} \rfloor}^{\ell} \binom{k/2}{j} \binom{j}{\ell - j} \frac{(bz)^{2j-\ell} (az^2)^{\ell-j}}{c^j} \\
&= c^{k/2} \sum_{\ell=0}^{\infty} \left(\frac{z}{c} \right)^{\ell} \sum_{j=\lfloor \frac{\ell+1}{2} \rfloor}^{\ell} \binom{k/2}{j} \binom{j}{\ell - j} b^{2j-\ell} (ac)^{\ell-j} \\
&= c^{k/2} \sum_{\ell=0}^{\infty} \left(\frac{z}{c} \right)^{\ell} P_{\ell}^{(k)}(a, b, c).
\end{aligned}
$$

This relation extends to all of D by the uniqueness of the Maclaurin series of f_k, proving the first part of the Lemma.

We will prove the second part separately for $k > 0$ and $k < 0$. For $k > 0$ we will apply a well known bound for the error in Taylor polynomial approximation given in Lemma 2.4 below. Fix z with $|z| < \sqrt{c/a}$ and choose ϵ with $0 < \epsilon < 1$ so small that $z \in D_\epsilon$. We apply the bound with $C = \partial D_\epsilon$. Firstly, note that

$$
q(z) = a(z - \xi_+)(z - \xi_-), \qquad \xi_{\pm} = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a},
$$

and that both roots of q are outside D. Since $f_k(z) = q(z)^{k/2}$,

$$
\max_{w \in C} |f_k(w)| = \left(\max_{w \in C} |q(w)| \right)^{k/2}.
$$

For $u \in \partial D$,

$$
|w - \xi_{\pm}| \le |w| + |\xi_{\pm}| = \rho + \sqrt{c/a} < 2\sqrt{c/a},
$$

and thus

$$
\max_{w \in \partial D} |q(w)| = |a| \max_{w \in \partial D} \{ |w - \xi_+| |w - \xi_-| \} \le |a| (2\sqrt{c/a})^2 = 4|c|.
$$

Now applying Lemma 2.4,

$$
\begin{aligned}
&\left| (az^2 + bz + c)^{k/2} - c^{k/2} \sum_{\ell=0}^{\nu} \left(\frac{z}{c} \right)^{\ell} P_{\ell}^{(k)}(a, b, c) \right| \\
&\qquad \le \max_{w \in \partial D} |f_k(w)| \left(\frac{|z|}{\rho} \right)^{\nu+1} \frac{1}{1 - |z|/\rho} \\
&\qquad \le (4c)^{k/2} \left(\frac{|z|}{(1-\epsilon)\sqrt{c/a}} \right)^{\nu+1} \frac{(1-\epsilon)\sqrt{c/a}}{(1-\epsilon)\sqrt{c/a} - |z|}.
\end{aligned}
$$

Taking the limit as ϵ goes to zero from above gives the result for $k > 0$.

For the case $k < 0$, write the polynomial q in the form

$$\begin{aligned} q(z) =& az^2 + bz + c = c\left\{1 + \frac{b}{\sqrt{ac}}\left(\frac{z}{\sqrt{c/a}}\right) + \left(\frac{z}{\sqrt{c/a}}\right)^2\right\} \\ =& c(1 - 2x\xi + \xi^2), \end{aligned}$$

where

$$x = -\frac{1}{2}\frac{b}{\sqrt{ac}} \qquad \text{and} \qquad \xi = \frac{z}{\sqrt{c/a}}.$$

Now recall [11, (4.7.23)] that $\left(1 - 2x\xi + \xi^2\right)^{-\lambda}$ is the generating function for the *Gegenbauer (or ultraspherical) polynomials* $C_\ell^{(\lambda)}(x)$, i.e.,

$$\sum_{\ell=0}^{\infty} C_\ell^{(\lambda)}(x)\xi^\ell = (1 - 2x\xi + \xi^2)^{-\lambda}.$$

Letting $\lambda = -k/2$, we see that

$$f_k(z) = c^{k/2}\sum_{\ell=0}^{\infty} C_\ell^{(\lambda)}(x)\xi^n,$$

and thus equating coefficients

$$\left(\frac{z}{c}\right)^\ell P_\ell^{(k)}(a, b, c) = C_\ell^{(\lambda)}(x)\xi^n, \qquad \ell \in \mathbb{N}_0. \tag{2.4}$$

For $-1 \le x \le 1$,

$$\left|C_n^{(\lambda)}(x)\right| \le \binom{n + 2\lambda - 1}{n}, \qquad \lambda > 0,$$

[1, 22.14.2]. By the statement of the lemma, $b^2 \le 4ac$ and $|z| < \sqrt{c/a}$. This means that $-1 \le x \le 1$ and $|\xi| < 1$ and thus

$$\begin{aligned} \left|f_k(z) - c^{k/2}\sum_{\ell=0}^{\nu}\left(\frac{z}{c}\right)^\ell P_\ell^{(k)}(a, b, c)\right| &= \left|f_k(z) - c^{k/2}\sum_{\ell=0}^{\nu} C_\ell^{(-k/2)}(x)\xi^\ell\right| \\ &\le c^{k/2}\sum_{\ell=\nu+1}^{\infty}\binom{\ell - k - 1}{\ell}|\xi|^\ell \end{aligned} \tag{2.5}$$

By Lemma 2.2,

$$\sum_{\ell=\nu+1}^{\infty}\binom{\ell - k - 1}{\ell}|\xi|^\ell = \binom{\nu - k}{\nu + 1}\frac{|\xi|^{\nu+1}}{(1 - |\xi|)^{-k}} F\left(k + 1, \nu + 1; \nu + 2; |\xi|\right).$$

Using this in (2.5) we have

$$\left| f_k(z) - c^{k/2} \sum_{\ell=0}^{\nu} \left(\frac{z}{c}\right)^{\ell} P_\ell^{(k)}(a,b,c) \right|$$
$$\leq c^{k/2} \binom{\nu-k}{\nu+1} \left(\frac{|z|}{\sqrt{c/a}}\right)^{\nu+1} \left(\frac{\sqrt{c/a}}{\sqrt{c/a}-|z|}\right)^{-k}$$
$$\times F\left(k+1, \nu+1; \nu+2; \frac{z}{\sqrt{c/a}}\right).$$

∎

In the proof of Lemma 2.3 above we have made use of the following well known bound for the error in a truncated Taylor series expansion [8, pp. 127–128].

LEMMA 2.4: Let $C = \{w \in \mathbb{C} : |w| = \rho\}$. If f is analytic inside and on C then for $|z| < \rho$,

$$|f(z) - (T_\nu f)(z)| \leq \max_{w \in C} |f(w)| \left(\frac{|z|}{\rho}\right)^{\nu+1} \frac{1}{1-|z|/\rho},$$

where $T_\nu f$ is the Maclaurin polynomial of f of degree ν.

In the case $k = -1$, the polynomial $F(k+1, \nu+1; \nu+2; z/\sqrt{c/a})$ that appears in the error bound of Lemma 2.3 is constant and has value 1. For all other negative values of k consider the function $F(k+1, p+1; p+2; \cdot)$ where $p \in \mathbb{N}_0$. Rephrasing Lemma 2.2 as

$$F(k+1, p; p+1; z) = \frac{p!\,(-k-1)!}{(p-k-1)!} \frac{(1-z)^{-k}}{z^p} \sum_{n=p}^{\infty} \binom{n-k-1}{-k-1} z^n,$$

it is easily seen that $F(k+1, p+1; p+2; \cdot)$ is non-negative on $[0, 1)$. Using (2.2b) to differentiate F, we see that for $z \in [0, 1)$

$$\frac{d}{dz} F(k+1, p; p+1; z) = \frac{(k+1)p}{p+1} F(k+2, p+1; p+2; z) \leq 0,$$

since $k < -1$. Since $F(\cdot, \cdot; \cdot; 0) = 1$, it follows that

$$F(k+1, \nu+1; \nu+2; z/\sqrt{c/a}) \leq 1, \qquad k \in \mathbb{Z}_-, \quad |z| \leq \sqrt{c/a}. \tag{2.6}$$

As was observed in the proof of Lemma 2.3 and particularly in Equation (2.4), for $k < 0$ the polynomials $P_\ell^{(k)}$ are closely related to the Gegenbauer polynomials $C_\ell^{(\lambda)}$ with $\lambda = -k/2$. However, many properties of the Gegenbauer polynomials are derived using their orthogonality with respect to the weight function $w(x) = (1-x^2)^{\lambda-1/2}$. This function is not integrable over the interval $[-1, 1]$ when $\lambda \leq -1/2$, and thus we are unable to exploit properties of the Gegenbauer polynomials derived from orthogonality when $k \geq 1$. The following lemma can be identified as a well known recurrence for the Gegenbauer polynomials with parameter $\lambda = -k/2 > -1/2$. Our proof here is based on the characterisation (2.3) and hence holds for all odd integers k.

LEMMA 2.5: Let $k \in \mathbb{Z}$ be odd. Then the polynomials $P_\ell^{(k)}$ defined in (1.4), satisfy the following recurrence relation for all $a, b, c \in \mathbb{R}$, and $\ell \in \mathbb{N}$:

$$(\ell+1)P_{\ell+1}^{(k)}(a,b,c) = \left(\frac{k}{2} - \ell\right) bP_\ell^{(k)}(a,b,c) + \big(k - (\ell-1)\big)acP_{\ell-1}^{(k)}(a,b,c). \tag{2.7}$$

Proof. We will first prove the identity under the additional assumptions $a, c > 0$, and $b^2 \leq 4ac$. Making these assumptions and differentiating the right hand side of (2.3) term by term gives

$$f_k'(z) = c^{(k-2)/2} \sum_{\ell=0}^{\infty} \left(\frac{z}{c}\right)^\ell (\ell+1)P_{\ell+1}^{(k)}(a,b,c), \tag{2.8}$$

the term by term differentiation being valid for $|z| < \sqrt{c/a}$.

On the other hand differentiating the expression $f_k(z) = (\sqrt{az^2+bz+c})^k$ then expanding gives

$$\begin{aligned} f_k'(z) &= \frac{k}{2}(az^2+bz+c)^{(k-2)/2}(2az+b) \\ &= \frac{k}{2} f_{k-2}(z)(2az+b) \\ &= \frac{k}{2} c^{(k-2)/2} \sum_{\ell=0}^{\infty} \left(\frac{z}{c}\right)^\ell (2az+b) P_\ell^{(k-2)}(a,b,c) \\ &= c^{(k-2)/2} \left\{ \sum_{\ell=0}^{\infty} \left(\frac{z}{c}\right)^\ell \frac{k}{2} bP_\ell^{(k-2)}(a,b,c) + \sum_{\ell=1}^{\infty} \left(\frac{z}{c}\right)^\ell kacP_{\ell-1}^{(k-2)}(a,b,c) \right\}. \end{aligned} \tag{2.9}$$

Equating (2.8) and (2.9), then comparing coefficients gives

$$(\ell+1)P_{\ell+1}^{(k)}(a,b,c) = \frac{k}{2} bP_\ell^{(k-2)}(a,b,c) + kacP_{\ell-1}^{(k-2)}(a,b,c), \quad \ell \in \mathbb{N}. \tag{2.10}$$

Using the obvious recurrence on f_k and then expanding gives

$$\begin{aligned} f_k(z) &= (az^2+bz+c)f_{k-2}(z) \\ &= c^{k/2} \left\{ \sum_{\ell=2}^{\infty} \left(\frac{z}{c}\right)^\ell acP_{\ell-2}^{(k-2)}(a,b,c) + \sum_{\ell=1}^{\infty} \left(\frac{z}{c}\right)^\ell bP_{\ell-1}^{(k-2)}(a,b,c) \right. \\ &\qquad \left. + \sum_{\ell=0}^{\infty} \left(\frac{z}{c}\right)^\ell P_\ell^{(k-2)}(a,b,c) \right\}. \end{aligned} \tag{2.11}$$

Equating (2.3) and (2.11), then comparing coefficients gives

$$P_{\ell+1}^{(k)}(a,b,c) = P_{\ell+1}^{(k-2)}(a,b,c) + bP_\ell^{(k-2)}(a,b,c) + acP_{\ell-1}^{(k-2)}(a,b,c), \quad \ell \in \mathbb{N}. \tag{2.12}$$

To obtain (2.7), multiply (2.12) by (ℓ+1) and equate to (2.10). Solving for $P_{\ell+1}^{(k-2)}(a,b,c)$ and making the index change $(k-2) \mapsto k$ gives (2.7).

This completes the proof when $a, c > 0$ and $b^2 \leq 4ac$. This set in $\mathbb{R}^3$ contains a non-trivial open ball and polynomials in n variables are determined everywhere by their behaviour on any non-trivial open ball in $\mathbb{R}^n$. Hence (2.7) holds for all $a, b, c \in \mathbb{R}$ since the right and left hand sides of (2.7) are polynomial.

3 Multivariate Expansions.

Let $\Phi(x) = \left(x^2+\tau^2\right)^{k/2}$, where $\tau \geq 0$ and $k \in \mathbb{Z}$ is odd and where we have used the notational convenience $x^2 = \langle x, x\rangle = |x|^2$ for $x \in \mathbb{R}^n$. The following result gives a far field expansion for $\Phi(x-t)$ considered as a function of x, together with an error estimate for approximation with truncations of this expansion. The numerator polynomials $P_\ell^{(k)}(t^2+\tau^2, -2\langle t, x\rangle, x^2)$ that feature in the expansion are homogeneous of degree ℓ in x. Correspondingly, the ℓth term in the expansion is homogeneous of degree $k-\ell$ in x.

LEMMA 3.1: Let $k \in \mathbb{Z}$ be odd, $t \in \mathbb{R}^n$ and $\tau \geq 0$. For all $x \in \mathbb{R}^n$ with $|x| > \sqrt{t^2+\tau^2}$,

$$\Phi(x-t) = \left((x-t)^2+\tau^2\right)^{k/2} = \sum_{\ell=0}^{\infty} P_\ell^{(k)}(t^2+\tau^2, -2\langle t, x\rangle, x^2)/|x|^{2\ell-k}$$

where the polynomials $P_\ell^{(k)}$ are defined in Equation (1.4). Moreover, for all x such that $|x| > \sqrt{t^2+\tau^2}$, and for all $p \in \mathbb{N}$ such that $p+k > 0$,

$$\left|\Phi(x-t) - \sum_{\ell=0}^{p+k} P_\ell^{(k)}(t^2+\tau^2, -2\langle t, x\rangle, x^2)/|x|^{2\ell-k}\right|$$
$$\leq \begin{cases} \left(2\sqrt{t^2+\tau^2}\right)^k \left(\dfrac{\sqrt{t^2+\tau^2}}{|x|}\right)^{p+1} \dfrac{|x|}{|x|-\sqrt{t^2+\tau^2}}, & \text{if } k > 0 \\[2ex] \begin{pmatrix} p \\ p+k+1 \end{pmatrix} \left(\sqrt{t^2+\tau^2}\right)^k \left(\dfrac{\sqrt{t^2+\tau^2}}{|x|}\right)^{p+1} \\ \qquad \times \left(\dfrac{|x|}{|x|-\sqrt{t^2+\tau^2}}\right)^{-k}, & \text{if } k < 0. \end{cases}$$

Proof. Consider firstly the case when $\tau > 0$. Let $a = t^2+\tau^2$, $b = -2\langle t, x\rangle$ and $c = x^2$. Then

$$\Phi(x-t) = \left(x^2 - 2\langle t, x\rangle + t^2 + \tau^2\right)^{k/2} = f_k(1),$$

where f_k is the function defined in (2.1). Since $a, c > 0$, $b^2 \leq 4ac$, and $1 = |z| < \sqrt{c/a} = |x|/\sqrt{t^2+\tau^2}$, Lemma 2.3 may be applied with $\nu = p+k$ to yield the desired results when we recall the bound on F given by Equation (2.6).

This completes the proof when $\tau > 0$. For the remaining case fix x with $|x| > |t|$. Note that $0 < \widetilde{\tau} < \sqrt{|x|^2 - |t|^2}$ implies $|x| > \sqrt{t^2 + \widetilde{\tau}^2}$. Hence the previous case can be applied to the expansion of

$$\Phi(x - t; k, \widetilde{\tau}) = \left((x-t)^2 + \widetilde{\tau}^2\right)^{k/2}$$

for all sufficiently small positive $\widetilde{\tau}$. Taking the limit as $\widetilde{\tau}$ goes to zero from above, and using the continuity of all the relevant quantities as as functions of $\widetilde{\tau}$, gives the result for $\tau = 0$. ∎

EXAMPLE 3.2: In the 1-dimensional case it is convenient to rewrite the series in the simpler form

$$\Phi(x-t) = \operatorname{sign}(x) \sum_{\ell=0}^{\infty} P_\ell^{(k)}(t^2 + \tau^2, -2t, 1)/x^{\ell-k},$$

which becomes, in the important special case ($k = 1$) of the ordinary multiquadric,

$$\begin{aligned}\sqrt{(x-t)^2+\tau^2} = \operatorname{sign}(x)\Big\{ & x - t + \frac{1}{2}\tau^2 x^{-1} + \frac{1}{2} t\tau^2 x^{-2} \\ & + \frac{1}{8}(4t^2\tau^2 - \tau^4)x^{-3} + \frac{1}{8}(4t^3\tau^2 - 3t\tau^4)x^{-4} \\ & + \frac{1}{16}\tau^2(8t^4 - 12t^2\tau^2 + \tau^4)x^{-5} + \cdots + q_\ell(t,\tau)x^{1-\ell} + \cdots \Big\}.\end{aligned}$$

EXAMPLE 3.3: To display the componentwise form of the expansion in two dimensions we will temporarily adopt the notation $x = (x_1, x_2)$ and $t = (t_1, t_2)$. The far field expansion about zero of a single ordinary multiquadric basic function centred at t is then

$$\begin{aligned}&\sqrt{|x-t|^2+\tau^2} \\ &= |x| - \frac{t_1x_1 + t_2x_2}{|x|} + \frac{1}{2}\frac{(t_2^2+\tau^2)x_1^2 + (t_1^2+\tau^2)x_2^2 - 2t_1t_2x_1x_2}{|x|^3} \\ &\quad + \frac{1}{2}\frac{(t_1x_1+t_2x_2)\left\{(t_2^2+\tau^2)x_1^2 + (t_1^2+\tau^2)x_2^2 - 2t_1t_2x_1x_2\right\}}{|x|^5} + \cdots\end{aligned}$$

Since the bound of Lemma 3.1 is increasing in $|t|$ we can apply it to each centre in a cluster and sum obtaining the following expansion of the generalised multiquadric radial basis function associated with a cluster of centres. The geometry of the source cluster and the evaluation region is shown in Figure 1 above.

THEOREM 3.4: Suppose $t_i \in \mathbb{R}^n$, $|t_i| \le r$ and $d_i \in \mathbb{R}$ for each $1 \le i \le N$. Let k be odd, $\tau \ge 0$, and s be the generalised multiquadric spline

$$s(x) = \sum_{i=1}^{N} d_j \Phi(x - t_i) = \sum_{i=1}^{N} d_i \left(\sqrt{(x-t_i)^2 + \tau^2}\right)^k.$$

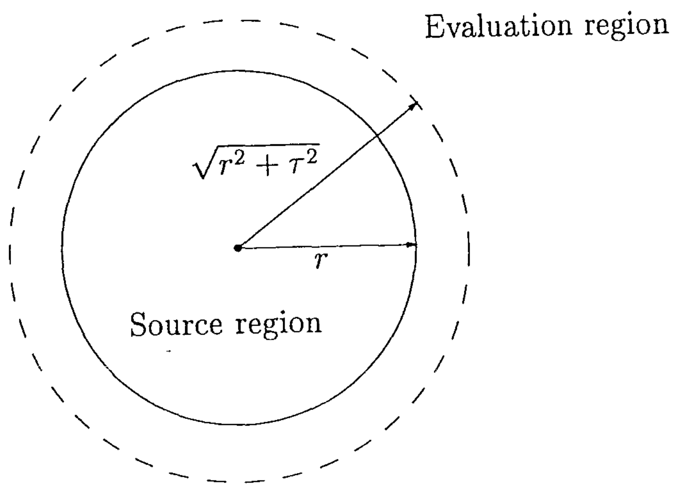

Figure 1: Region of validity of the far field expansion of a cluster.

If $P_\ell^{(k)}$, $\ell \in \mathbb{N}_0$, are the polynomials defined by Equation (1.4), then the polynomials

$$Q_\ell(x) = \sum_{i=1}^{N} d_i P_\ell^{(k)}(t_i^2 + \tau^2, -2\langle t_i, x\rangle, x^2) \qquad \ell \in \mathbb{N}_0,$$

have the following property: Let $p \in \mathbb{N}_0$ and set

$$s_p(x) = \sum_{\ell=0}^{p+k} Q_\ell(x)/|x|^{2\ell-k}, \tag{3.1}$$

$x \in \mathbb{R}^n \backslash \{0\}$. Then for all x with $|x| > R = \sqrt{r^2+\tau^2}$

$$\left|s(x) - s_p(x)\right| \le \begin{cases} 2^k M R^k \left(\dfrac{1}{c}\right)^{p+1} \dfrac{1}{1-1/c}, & \text{if } k > 0 \\ \dbinom{p}{p+k+1} M R^k \left(\dfrac{1}{c}\right)^{p+1} \left(\dfrac{1}{1-1/c}\right)^{-k}, & \text{if } k < 0, \end{cases}$$

where $M = \sum_{i=1}^{N} |d_i|$ and $c = |x|/R$.

4 The Uniqueness of Expansions

The uniqueness of far field expansions is important for two reasons. First, redundant coefficients could mean that a small value is represented as the difference of two large values leading to numerical instability. Second, if the far field expansion of a fixed function, $s(x) = \sum_{i=1}^{N} \Phi(x - t_i)$, is unique then it is often possible to shift the centre of a truncated expansion indirectly without using any knowledge of the underlying centres and weights.

The advantage of such indirect shifting over direct series formation is a flop count which depends only on the number of terms in the expansion, and not on the number of centres in the cluster. This can result in significantly faster code. Furthermore, since the uniqueness implies the indirectly obtained series is identical with that which would have been obtained directly, the indirectly obtained series enjoys the same error bound as the directly obtained one.

We will now prove a general uniqueness lemma from which uniqueness of series expansions of the form (3.1) follows as a special case. Recall that a function g defined for all x in some subset $D \subset \mathbb{R}^n$ is said to be homogeneous of degree γ on D if

$$g(\lambda x) = \lambda^\gamma g(x)$$

for all $\lambda > 0$ and $x \in \mathbb{R}^n$ such that both x and $\lambda x \in D$. (Some authors use the term positively homogeneous of degree γ for this property).

LEMMA 4.1: Suppose $\gamma, R \in \mathbb{R}$ and that a function $f : D \subset \mathbb{R}^n \to \mathbb{R}$ can be expanded in two ways

$$\sum_{\ell=0}^{\infty} U_\ell(x) = f(x) = \sum_{\ell=0}^{\infty} V_\ell(x),$$

both series converging absolutely and uniformly to $f(x)$ for all $|x| \geq R$, where for each ℓ , U_ℓ and V_ℓ are continuous homogeneous functions of degree $\gamma - \ell$. Then for each ℓ, $U_\ell(x) = V_\ell(x)$ for all $|x| \geq R$.

Proof. Since the absolute series converge uniformly on $|x| = R$ there exists an $M < \infty$ such that

$$\max_{|x|=R} \{\max\{|U_\ell(x)|,\ |V_\ell(x)|\}\} \leq M,$$

for all $\ell \in \mathbb{N}_0$. Hence, using the homogeneity,

$$\max\{|U_\ell(x)|,\ |V_\ell(x)|\} \leq M|x|^{\gamma-\ell}/R^{\gamma-\ell}, \tag{4.1}$$

for all x such that $|x| \geq R$, and all $\ell \in \mathbb{N}_0$.

Now suppose U_ℓ and V_ℓ differ for some ℓ's. Let j be the first index for which they differ. Then for all $|x| \geq R$

$$\begin{aligned} 0 &= \left(\frac{|x|}{R}\right)^{j-\gamma} \{f(x) - f(x)\} \\ &= \left(\frac{|x|}{R}\right)^{j-\gamma} \{U_j(x) - V_j(x)\} + \sum_{\ell>j} \left(\frac{|x|}{R}\right)^{j-\gamma} \{U_\ell(x) - V_\ell(x)\}. \end{aligned} \tag{4.2}$$

But from (4.1)

$$\left|\sum_{\ell>j}\left(\frac{|x|}{R}\right)^{j-\gamma}\{U_\ell(x)-V_\ell(x)\}\right| \leq 2M\sum_{\ell>j}\left(\frac{|x|}{R}\right)^{j-\ell}$$
$$= o(1) \qquad \text{as } |x|\to\infty.$$

Hence from (4.2)

$$|U_j(x)-V_j(x)| = o(|x|^{\gamma-j}) \quad \text{as } |x|\to\infty.$$

Since $U_j - V_j$ is homogeneous of degree $\gamma - j$ on D this implies that it is identically zero on D. ∎

5 Efficient formation of the far field series

In the previous sections we have developed far field expansions with the intention of using them for fast evaluation of generalised multiquadric RBF's. In order that these expansions be suitable for this task they must be inexpensive both to form and to evaluate. The purpose of this section is to show that the expansions can be formed in an efficient recursive manner.

Given a single centre $t \in \mathbb{R}^n$, with unit weight, the corresponding truncated expansion of Section 3 is

$$\Phi(x-t) = \left((x-t)^2+\tau^2\right)^{k/2} = \sum_{\ell=0}^{\infty} P_\ell^{(k)}(t^2+\tau^2, -2\langle t,x\rangle, x^2)/|x|^{2\ell-k} \tag{5.1}$$

Writing $G_\ell(x) = P_\ell^{(k)}(t^2+\tau^2,-2\langle t,x\rangle,x^2)$, G_ℓ is a homogeneous polynomial of degree ℓ in x, with coefficients depending on k, τ and t. The expansion for a single centre, with corresponding weight d, then becomes

$$\sum_{\ell=0}^{p+k} dG_\ell(x)/|x|^{2\ell-k}. \tag{5.2}$$

The expansion of a cluster is formed by summing the expansions (5.2) corresponding to each centre, and has the form

$$\sum_{\ell=0}^{p+k} Q_\ell(x)/|x|^{2\ell-k}, \tag{5.3}$$

where each Q_ℓ is a homogeneous polynomial of degree ℓ. Lemma 2.5 implies that the polynomials G_ℓ satisfy the three term recurrence

$$G_\ell(x) = \begin{cases} 1, & \ell=0, \\ -k\langle x,t\rangle, & \ell=1, \\ A_\ell\langle x,t\rangle G_{\ell-1}(x) + B_\ell\, x^2(t^2+\tau^2)\, G_{\ell-2}(x), & \ell\geq 2, \end{cases}$$

where

$$A_\ell = -2\frac{k/2 - \ell + 1}{\ell}, \qquad B_\ell = -\frac{\ell - k - 2}{\ell}.$$

The recurrence is very simple to implement as is demonstrated by the following code fragment for the special case of 2-dimensions. The code fragment employs the notation of Example 3.3.

Code fragment to generate the numerator polynomial coefficients in the expansion of a generalised multiquadric in 2-dimensions.

INPUTS

A centre $t \in \mathbb{R}^2$, the corresponding weight d, the generalised multiquadric parameters k and τ, and the desired order of expansion p.

OUTPUTS

The code fragment generates the coefficients $G(\ell, j)$ of the homogeneous numerator polynomials in the expansion of this single centre. On output $G(\ell, j)$ is the coefficient of $x_1^{\ell-j} x_2^j$ in the homogeneous polynomial dG_ℓ of Equation (5.2).

CODE

$G(0,0) = d$, $G(1,0) = -d * k * t_1$, $G(1,1) = -d * k * t_2$.
for $\ell = 2$ **to** $p + k$
  $a = A_\ell$, $b = B_\ell * (|t|^2 + \tau^2)$
  $tmp = a * G(\ell - 1, 0)$
  $G(\ell, 0) = tmp * t_1$
  $G(\ell, 1) = tmp * t_2$
  for $j = 0$ **to** $\ell - 2$
    $tmp = b * G(\ell - 2, j)$
    $G(\ell, j) = G(\ell, j) + tmp$
    $G(\ell, j + 2) = tmp$
    $tmp = a * G(\ell - 1, j + 1)$
    $G(\ell, j + 1) = G(\ell, j + 1) + tmp * t_1$
    $G(\ell, j + 2) = G(\ell, j + 2) + tmp * t_2$
  end for
end for

Recall that the $\binom{\ell+n-1}{\ell}$ monomials of exact degree ℓ, $\{x^\alpha : \alpha \in \mathbb{N}_0^n, \alpha \geq 0, \alpha_1 + \alpha_2 + \cdots + \alpha_n = \ell\}$, form a basis for the homogeneous polynomials of degree ℓ on $\mathbb{R}^n$. Represent the polynomials G_ℓ in terms of these monomials. Then, from the recurrence, each coefficient of G_ℓ can be calculated using at most n coefficients of $G_{\ell-1}$ and at most n coefficients of $G_{\ell-2}$.

It follows that all the numerator polynomials Q_ℓ in the truncated expansion (5.3) of an m centre cluster can be formed (that is their $\binom{n+p+k}{p+k}$ coefficients calculated) in $\mathcal{O}\big(mn\binom{n+p+k}{p+k}\big)$ floating point operations. This quantity is $\mathcal{O}(mn(p+k)^n)$ when the dimension n is less than the degree $p+k$.

6 A Subspace of Polynomials

In this section we will investigate a subspace of polynomials in n variables. This space will arise in Section 7 and the aim of that section will be to translate a member of this subspace. It will shown that, modulo a low degree polynomial, this subspace is closed under translation of the underlying Cartesian coordinate system.

Throughout this section and the next n will be fixed and any complexity estimates will be expressed as a function of polynomial degree only. Thus a typical estimate might take the form $\mathcal{O}((p+k)^n)$. In such expressions multiplicative order constants depending on n have been suppressed, and we will be interested in the estimate only when the argument $p+k$ is bigger than n.

The following standard spaces will be used.

- π_j^n Polynomials of total degree not exceeding j in n variables.
- $\mathcal{H}_j^n$ homogeneous polynomials of degree j in n variables.

Also, for given function spaces S and T, define new spaces as follows.

$$\begin{aligned} ST &= \{s(\cdot)\,t(\cdot) \ : \ s\in S,\ t\in T\}, & & \\ S\oplus T &= \{s(\cdot)+t(\cdot) \ : \ s\in S,\ t\in T\}, & & S\cap T=\{0\}, \\ sT &= \{s(\cdot)\,t(\cdot) \ : \ t\in T\}, & & s\in S. \end{aligned}$$

The subspaces of polynomials that are the subject of this section are defined by

$$S_j^n = \left\{ q\in\pi_{2j}^n : q(\cdot)=\sum_{\ell=0}^{j} q_\ell(\cdot)|\cdot|^{2(j-\ell)}, q_\ell\in\mathcal{H}_\ell^n \right\}. \tag{6.1}$$

Apart from 0, the polynomials of S_j^n have total degree no greater than $2j$ and no less than j. It follows from Lemma 4.1 that $q\in S_n^j$ is uniquely determined by the homogeneous polynomials $\{q_\ell\}_{\ell=0}^j$ and thus by the coefficients of those polynomials with respect to some appropriate basis. Hence

$$\dim S_j^n = \sum_{\ell=0}^{j}\dim H_\ell^n. \tag{6.2}$$

THEOREM 6.1: S_j^n in invariant under orthogonal transformation of the underlying coordinate system, i.e., if $q\in S_j^n$ then $q(Q\,\cdot)\in S_j^n$ for orthogonal Q.

Proof. Since Q is orthogonal the range of $Q\cdot$ is all of $\mathbb{R}^n$. Hence, for each i, the component function $f_i(x) = (Qx)_i$ is homogeneous in x of exact degree 1. Thus

$$(Qx)^\alpha = (Qx)_1^{\alpha_1}(Qx)_2^{\alpha_s}\ldots(Qx)_n^{\alpha_n}$$

is homogeneous of exact degree $|\alpha|$. It follows that $q_\ell(Q\cdot)$ is homogeneous of degree ℓ if q_ℓ is. Finally, since Q is orthogonal,

$$|Q\cdot| = |\cdot|,$$

and the result follows. ∎

Before we prove translation invariance of S_j^n we will make a few simple observations regarding these spaces.

LEMMA 6.2: The spaces S_j^n satisfy the following relations.

(i). $S_{j+1}^n = \left(|\cdot|^2 S_j^n\right) \oplus \mathcal{H}_{j+1}^n$,

(ii). $\mathcal{H}_1^n S_j^n \subset S_{j+1}^n$,

(iii). $S_j^n \subset S_{j+1}^n \oplus \mathcal{H}_j^n$.

Proof. Let $q \in S_{j+1}^n$ and let $\{q_\ell\}_{\ell=0}^j$ be the polynomials such that

$$q = \sum_{\ell=0}^{j} |\cdot|^{2(j-\ell)} q_\ell, \qquad q_\ell \in \mathcal{H}_\ell^n.$$

The observation that

$$q = |\cdot|^2 h + q_{j+1}$$

where

$$h = \left(\sum_{\ell=0}^{j-1} |\cdot|^{2(j-1-\ell)} q_\ell\right) \in S_j^n$$

proves part (i).

Now let $p \in \mathcal{H}_1^n$. Then for each ℓ, $0 \le \ell \le j$, the product $\tilde{q}_{\ell+1} = pq_\ell \in \mathcal{H}_{\ell+1}^n$. Thus

$$pq = \sum_{\ell=0}^{j} |\cdot|^{2(j-\ell)} \tilde{q}_{\ell+1} = \sum_{k=1}^{j+1} |\cdot|^{2(j+1-k)} \tilde{q}_k \in S_{j+1}^n,$$

which shows part(ii).

For part (iii),

$$q(x) = \sum_{\ell=0}^{j} q_\ell(x)|x|^{2(j-\ell)} = q_j(x) + \sum_{\ell=0}^{j-1} q_\ell(x)|x|^2\,|x|^{2(j-1-\ell)}$$

$$= q_j(x) + \sum_{\ell=0}^{j-1} \tilde{q}_{\ell+2}(x)\, |x|^{2(j-1-\ell)}$$

$$= q_j(x) + \sum_{\ell=2}^{j+1} \tilde{q}_{\ell}(x)\, |x|^{2(j+1-\ell)} \in \mathcal{H}_j^n \oplus S_{j+1}^n,$$

since the polynomials $\tilde{q}_{\ell+2}(\cdot) = q_\ell(\cdot)|\cdot|^2$ are homogeneous of degree $\ell+2$. ∎

THEOREM 6.3: S_j^n is translation invariant modulo polynomials of degree $j-1$, i.e., for any $q \in S_j^n$ and $u \in \mathbb{R}^n$, $q(\cdot - u) \in S_j^n \oplus \pi_{j-1}^n$.

Proof. The proof is by induction on j. The result is trivially true in the case $j = 0$ since S_0^n is the space of constants and π_{-1}^n is the singleton $\{0\}$.

Now assume the result for $k = 0, 1, 2, \ldots, j$, let $q \in S_{j+1}^n$ and let $u \in \mathbb{R}^n$. Then by Lemma 6.2, part (i),

$$q(x-u) = |x-u|^2\, h(x-u) + q_{j+1}(x-u) \tag{6.3}$$

where $h \in S_j^n$ and $q_{j+1} \in \mathcal{H}_{j+1}^n$. By the induction hypothesis, $h(\cdot - u) \in S_j^n \oplus \pi_{j-1}^n$. Thus

$$h(x-u) = \tilde{h}_j(x) + \tilde{h}_{j-1}(x) + \tilde{h}_<(x) \tag{6.4}$$

where $\tilde{h}_j \in S_j^n$, $\tilde{h}_{j-1} \in \mathcal{H}_{j-1}^n$ and $\tilde{h}_< \in \pi_{j-2}^n$. Since $q_{j+1} \in \mathcal{H}_{j+1}^n$,

$$q_{j+1}(x-u) = q_{j+1}(x) - \tilde{q}_<(x) \tag{6.5}$$

where $\tilde{q}_<(x) \in \pi_j^n$. Expand (6.3) to get

$$q(x-u) = \left(|x|^2 - 2\langle x, u\rangle + |u|^2\right)\left(\tilde{h}_j(x) + \tilde{h}_{j-1} + \tilde{h}_<\right) + q_{j+1}(x) + \tilde{q}_<(x). \tag{6.6}$$

Consider each term of this sum:

$\lvert\cdot\rvert^2 \tilde{h}_j \in S_{j+1}^n$	by Lemma 6.2, part (i)
$-2\langle \cdot, u\rangle \tilde{h}_j \in S_{j+1}^n$	by Lemma 6.2, part (ii)
$\lvert u\rvert^2 \tilde{h}_j \in S_j^n \subset S_{j+1}^n \oplus \mathcal{H}_j^n$	by Lemma 6.2, part (iii)
$\lvert\cdot\rvert^2 \tilde{h}_{j-1} \in S_{j+1}^n$	by definition of S_{j+1}^n
$-2\langle \cdot, u\rangle \tilde{h}_{j-1} \in \mathcal{H}_j^n$	
$\lvert u\rvert^2 \tilde{h}_{j-1} + \lvert\cdot - u\rvert^2 \tilde{h}_< \in \pi_j^n.$	

Thus it follows that $q(\cdot - u) \in S_{j+1}^n \oplus \pi_j^n$. The result follows by induction. ∎

In computations, a polynomial $p \in S_j^n$ may be known in terms of the monomial basis, but what is actually required are the polynomials $\{q_\ell\}_{\ell=0}^{j}$ such that

$$p(x) = \sum_{\ell=0}^{j} q_\ell(x)|x|^{2(j-\ell)} \tag{6.7}$$

Since the polynomials $\{q_\ell\}$ are homogeneous, for a given ℓ, q_ℓ must be determined entirely by those terms of p that are homogeneous of degree $2j-\ell$. Thus the problem of determining $\{q_\ell\}$ may be broken down into homogeneous parts. Hence, without loss of generality, assume that p is a given homogeneous polynomial of degree $\ell + 2k$ such that

$$p(x) = |x|^{2k} q(x) \tag{6.8}$$

with q unknown and to be determined from p. Since

$$p(x) = |x|^{2k} q(x) = |x|^2 \big(|x|^{2(k-1)} q(x)\big),$$

if q can be determined in the case where $k = 1$, the more general problem may be solved in an inductive manner.

Let $\{p_j\}_{j=0}^{\ell+2}$ and $\{q_i\}_{i=0}^{\ell}$ be homogeneous polynomials in $x_2, \dots, x_n$ such that

$$p(x) = \sum_{j=0}^{\ell+2} x_1^{\ell+2-j} p_j(\bar{x}), \quad q(x) = \sum_{i=0}^{\ell} x_1^{\ell-i} q_i(\bar{x}), \quad \text{and} \quad p(x) = |x|^2 q(x),$$

where, if $x = (x_1, \dots, x_n)$ then $\bar{x} = (x_2, \dots, x_n)$. Using this same notation,

$$|x|^2 = x_1^2 + |\bar{x}|^2$$

and hence

$$\begin{aligned}\sum_{j=0}^{\ell+2} x_1^{\ell+2-j} p_j(\bar{x}) &= \big(x_1^2 + |\bar{x}|^2\big) \sum_{i=0}^{\ell} x_1^{\ell-i} q_i(\bar{x}) \\ &= x_1^{\ell+2} q_0(\bar{x}) + x_1^{\ell+1} q_1(\bar{x}) + \left\{ \sum_{i=2}^{\ell} x_1^{\ell+2-i} \big(q_i(\bar{x}) + |\bar{x}|^2 q_{i-2}(\bar{x})\big) \right\} \\ &\qquad + x_1 |\bar{x}|^2 q_{\ell-1}(\bar{x}) + |\bar{x}|^2 q_\ell(\bar{x}).\end{aligned}$$

Equating coefficients the polynomials q_i may now be written in terms of the polynomials p_j.

$$\begin{aligned} q_0(\bar{x}) &= p_0(\bar{x}), \\ q_1(\bar{x}) &= p_1(\bar{x}), \\ q_2(\bar{x}) &= p_2(\bar{x}) - |\bar{x}|^2 q_0(\bar{x}), \end{aligned}$$

$$\begin{aligned} q_3(\bar{x}) &= p_3(\bar{x}) - |\bar{x}|^2 q_1(\bar{x}), \\ &\vdots \\ q_{\ell-1}(\bar{x}) &= p_{\ell-1}(\bar{x}) - |\bar{x}|^2 q_{\ell-3}(\bar{x}), \\ q_\ell(\bar{x}) &= p_\ell(\bar{x}) - |\bar{x}|^2 q_{\ell-2}(\bar{x}). \end{aligned}$$

Multiplication of a polynomial by a monomial corresponds to a relabelling of coefficients and computationally corresponds to assignment or addition. Since,

$$|\bar{x}|^2 = x_2^2 + \cdots + x_n^2$$

is just the sum of $n-1$ monomials, for fixed i the product $|\cdot|^2 q_i(\cdot)$ may calculated with $\mathcal{O}(nC_i)$ additions, where $C_i = \dim \mathcal{H}_i^{n-1}$. It is well known that

$$\begin{aligned} \dim \mathcal{H}_i^n = \binom{i+n-1}{n-1} &= \frac{(i+n-1)!}{i!(n-1)!} \\ &= \frac{1}{(n-1)!}\big((i+n-1)\cdots(i+1)\big) = \mathcal{O}(i^{n-1}), \end{aligned}$$

and hence $|\cdot|^2 q_i(\cdot)$ may be calculated in $\mathcal{O}(i^{n-2})$ operations. It now follows that all of the polynomials $\{q_i\}_{i=0}^{\ell}$ may be calculated in $\mathcal{O}(\ell^{n-1})$ operations.

Since the more general problem of (6.8) may be solved by k applications of this simpler case, $q(x) = p(x)/|x|^{2k}$ may be calculated in

$$\sum_{i=0}^{k-1} \mathcal{O}\big((\ell+2i)^{n-1}\big) = \mathcal{O}\big((\ell+2k)^n\big)$$

operations. Applying this to each homogeneous part of (6.7) gives the following lemma.

LEMMA 6.4: Let $n \in \mathbb{Z}$. There exists a constant C depending only on n with the following property. Given any polynomial $p \in S_j^n$ the polynomials $\{q_\ell\}_{\ell=0}^{j}$ such that $q_\ell \in \mathcal{H}_\ell^n$ and

$$p = \sum_{\ell=0}^{j} |\cdot|^{2(j-\ell)} q_\ell \ ,$$

may be determined in no more than Cj^{n+1} operations.

7 Translation of a far field expansion

The uniqueness of the far field expansions makes it is possible to shift the centre of a truncated expansion knowing only its coefficients, and without any direct knowledge of the underlying centres and weights. As the operation count for indirect translation depends on the length of the series, not the number of centres, indirect translation can be significantly faster than direct formation of series for clusters with many centres.

The precise problem we address is the following. Let

$$s_p(x) = \sum_{\ell=0}^{p+k} Q_\ell(y)/|y|^{2\ell-k}, \qquad y = x - u \neq 0, \tag{7.1}$$

where Q_ℓ are homogeneous polynomials of degree ℓ, be an expansion similar to (3.1) or (5.3), but centred at $u \neq 0$ rather than 0. We wish to shift the centre of expansion to the origin. That is we seek homogenous polynomials $\{\widehat{Q}_\ell\}$, $\widehat{Q}_\ell$ being of degree ℓ, so that

$$s_p(x) = \sum_{\ell=0}^{p+k} \widehat{Q}_\ell(x)/|x|^{2\ell-k} + \mathcal{O}(1/|x|^{p+1}), \tag{7.2}$$

as $|x| \to \infty$. We will show that translations of truncated expansions of the form (7.1) into expansions of the form (7.2) may be performed in $\mathcal{O}\left((p+k)^{n+1}\right)$ operations using simple polynomial manipulations.

7.1 The cost of multiplication

In this subsection it will be shown that the product of two homogeneous polynomials of degree ℓ in n variables may be computed in $\mathcal{O}(\ell^{n-1}\log \ell)$ operations.

Let p be a homogeneous polynomial of degree ℓ. Since p is homogeneous,

$$p(x) = p(x_1, x_2, \ldots, x_n) = x_n^\ell p\left(\frac{x_1}{x_n}, \frac{x_2}{x_n}, \ldots, \frac{x_{n-1}}{x_n}, 1\right), \qquad x_n \neq 0.$$

Furthermore given $x_n^\ell p(\ldots)$ for all x with $x_n \neq 0$, $p(x)$ can be recovered on the hyperplane $x_n = 0$ by continuity. Thus for the purposes of the multiplication and division that are the subject of this section, we may consider multiplication and division of general, that is probably inhomogeneous, polynomials of degree ℓ in $n-1$ variables rather than of homogeneous polynomials of degree ℓ in n variables.

Let p and q be two polynomials of degree ℓ in $n-1$ variables. Then their product is

$$p(x)q(x) = \left(\sum_{|\alpha|\le\ell} a_\alpha x^\alpha\right)\left(\sum_{|\beta|\le\ell} b_\beta x^\beta\right) = \sum_{|\alpha|\le 2\ell}\left(\sum_{0\le\beta\le\alpha} a_\beta b_{\alpha-\beta}\right)x^\alpha,$$

the Cauchy product. The convolution producing the coefficients of the product can be computed in $\mathcal{O}(\ell^{n-1}\log \ell)$ operations by FFTs. It now follows that the homogeneous polynomial multiplication above can also be carried out in $\mathcal{O}(\ell^{n-1}\log \ell)$ operations.

7.2 Translation by convolution

In this subsection it will be shown that translation of the far field series may be performed by convolution.

Throughout this subsection when we speak of forming a polynomial we mean finding its coefficients with respect to a basis, usually the monomial basis. When we speak of forming a truncated expansion of the type (5.3), we mean finding the coefficients of all the relevant numerator polynomials.

First we set

$$Q(y) = \sum_{\ell=0}^{p+k} Q_\ell(y)|y|^{2(p+k-\ell)}. \tag{7.3}$$

Then

$$s_p(x) = Q(y)/|y|^{2p+k}, \qquad y = x - u \neq 0. \tag{7.4}$$

Since we already have all of the Q_ℓ, all we need to do to form Q is form the polynomials $|\cdot|^{2(p+k-\ell)}$ and then form the products $Q_\ell(\cdot)|\cdot|^{2(p+k-\ell)}$. Form $|\cdot|^{2j}$, $j = 0, \dots, p+k$ once and store. Each $|\cdot|^{2j-2}$ is homogeneous of degree $2j-2$ and therefore involves $\mathcal{O}(j^{n-1})$ coefficients. The polynomial $|\cdot|^{2j}$ may be obtained from $|\cdot|^{2j-2}$ with n additions for each coefficient in $|\cdot|^{2j-2}$. Hence the cost of forming the $|\cdot|^{2j}$'s is $\mathcal{O}((p+k)^n)$ operations. Each of the products $Q_\ell(\cdot)|\cdot|^{2(p+k-\ell)}$ is the product of two homogeneous polynomials and is of degree no greater than $2(p+k)$. Hence we can calculate each product in $\mathcal{O}\big((p+k)^{n-1}\log(p+k)\big)$ operations. As there are $p+k+1$ of these products in Q, forming Q takes $\mathcal{O}\big((p+k)^n\log(p+k)\big)$ operations.

We proceed to shift the centre of expansion of Q by setting

$$\widetilde{Q}(x) = Q(x-u), \qquad x \in \mathcal{R}^n. \tag{7.5}$$

A translation of this sort can be done simply and quickly by convolution. For example, using the scaled monomial basis $V_\alpha(x) = x^\alpha/\alpha!$ (α a multi-index), we have

$$\begin{aligned}
p(x-u) &= \sum_{|\alpha|<k} a_\alpha V_\alpha(x-u) \\
&= \sum_{|\alpha|<k} a_\alpha \frac{(x-u)^\alpha}{\alpha!} \\
&= \sum_{|\alpha|<k} \frac{a_\alpha}{\alpha!} \sum_{\beta<\alpha} \binom{\alpha}{\beta} x^\beta (-u)^{(\alpha-\beta)} \\
&= \sum_{|\alpha|<k} a_\alpha \sum_{\beta<\alpha} \frac{x^\beta}{\beta!} \frac{(-u)^{(\alpha-\beta)}}{(\alpha-\beta)!} \\
&= \sum_{|\beta|<k} \frac{x^\beta}{\beta!} \sum_{\alpha<\beta} a_\alpha \frac{(-u)^{(\alpha-\beta)}}{(\alpha-\beta)!}.
\end{aligned}$$

Thus an n-dimensional convolution of $\{a_\alpha\}$ and $\{(-u)^\alpha/\alpha!\}$ gives the coefficients of the translated polynomial. Again this can be computed in $\mathcal{O}\big((p+k)^n \log(p+k)\big)$ operations by an FFT method. This gives us $\widetilde{Q}$ in terms of the monomial or scaled monomial basis.

The next task is to recast $\widetilde{Q}$ into a sum of products of powers of $|x|$ and homogeneous polynomials. By Theorem 6.3 we know that

$$\widetilde{Q}(x) = \sum_{\ell=0}^{p+k} q_\ell(x)|x|^{2(p+k-\ell)} + q_{\text{low}}(x) \tag{7.6}$$

where the q_ℓ are homogeneous of degree ℓ and q_{low} is some polynomial of degree $p+k-1$ or less. By Lemma 6.4, these homogeneous polynomials q_ℓ can be calculated from $\widetilde{Q}$ in $\mathcal{O}\big((p+k)^{n+1}\big)$ operations.

Combining equations (7.4) and (7.5) and appealing to Lemma 3.1 gives

$$\begin{aligned}
s_p(x) &= Q(x-u)/|x-u|^{2p+k} \\
&= \widetilde{Q}(x)/|x-u|^{2p+k} \qquad\qquad (7.7)\\
&= \widetilde{Q}(x) \sum_{m=0}^{\infty} P_m^{(-2p-k)}(u^2, -2\langle x,u\rangle, x^2)/|x|^{2p+k+2m} \\
&= \left(\sum_{\ell=0}^{p+k} q_\ell(x)|x|^{2(p+k-\ell)} + q_{\text{low}}(x)\right) \\
&\quad \times \left(\sum_{m=0}^{\infty} P_m^{(-2p-k)}(u^2, -2\langle x,u\rangle, x^2)/|x|^{2p+k+2m}\right) \\
&= \sum_{\ell=0}^{p+k} \sum_{m=0}^{\infty} q_\ell(x) P_m^{(-2p-k)}(u^2, -2\langle x,u\rangle, x^2)/|x|^{2(m+\ell)-k} + \mathcal{O}(1/|x|^{p+1}) \\
&= \sum_{\ell=0}^{p+k} \left(\sum_{j=0}^{\ell} q_j(x) P_{\ell-j}^{(-2p-k)}(u^2, -2\langle x,u\rangle, x^2)\right) /|x|^{2\ell-k} + \mathcal{O}(1/|x|^{p+1}) \\
&= \sum_{\ell=0}^{p+k} \widehat{Q}_\ell(x)/|x|^{2\ell-k} + \mathcal{O}(1/|x|^{p+1}).
\end{aligned}$$

The sums of products

$$\widehat{Q}_\ell(x) = \sum_{j=0}^{\ell} q_j(x) P_{\ell-j}^{(-2p-k)}(u^2, -2\langle x,u\rangle, x^2), \quad 0 \le \ell \le p+k, \tag{7.8}$$

can be computed simultaneously as homogeneous parts of the product

$$\left[\sum_{j=0}^{p+k} q_j(\cdot)\right] \left[\sum_{m=0}^{p+k} P_m^{-2p+k}\left(u^2, -2\langle \cdot, u\rangle, (\cdot)^2\right)\right].$$

Hence they can be computed by a single FFT convolution in $\mathcal{O}\left((p+k)^n \log(p+k)\right)$ operations.

8 Conversion to a near field series

The final step in the process of forming expansions for the FMM is to convert the far field series into a near field, or Taylor, series. At the implementation level, this step is almost identical to the first part of the translation of the far field series.

Define two non-intersecting discs:

$$D_{\text{eval}} = \{x : |x| \leq r\},$$
$$D_{\text{src}} = \{x : |x - u| \leq \sqrt{(\theta r)^2 - \tau^2}\}, \qquad \theta > 0.$$

Let

$$s_p(x) = \sum_{\ell=0}^{p+k} Q_\ell(y)/|y|^{2\ell-k}, \qquad y = x - u \neq 0,$$

be a far field series, such as (3.1) or (7.1), of $s(x) = \sum_{i=1}^{N} d_i \Phi(x - t_i)$ due to a cluster of centres $\{t_i\}$ located inside D_{src}. Then by Theorem 3.4, s_p approximates s well on D_{eval}. We wish find to a near field series that approximates s_p, and thus s, on D_{eval}.

Proceeding in an identical fashion to Section 7.2, we see that we may calculate the polynomial $\widetilde{Q}$ such that

$$s_p(x) = \widetilde{Q}(x)/|x - u|^{2p+k}$$

in $\mathcal{O}\left((p+k)^n \log(p+k)\right)$ operations. When translating the far field expansion to another far field expansion, we essentially convolved $\widetilde{Q}$ with the far field series for $|\cdot - u|^{-(2p+k)}$. To get the near field, all we need do is convolve $\widetilde{Q}$ with the near field series for $|\cdot - u|^{-(2p+k)}$.

The next result gives an explicit expression for the Maclaurin series of $\Phi(\cdot - u) = \left((\cdot - u)^2 + \tau^2\right)^{k/2}$ together with an estimate of the error in approximation by truncating this series. Specialising to the case $\tau = 0$ in this lemma gives the Maclaurin series for $|\cdot - u|^k$.

Lemma 8.1: Let $k \in \mathbb{Z}$ be odd, and $u \in \mathbb{R}^n \setminus \{0\}$ and $\tau \geq 0$. For all $x \in \mathbb{R}^n$ with $|x| < \sqrt{u^2 + \tau^2}$,

$$\Phi(x - u) = \left((x - u)^2 + \tau^2\right)^{k/2} = \sum_{\ell=0}^{\infty} P_\ell^{(k)}(x^2, -2\langle u, x\rangle, u^2 + \tau^2)/\left(\sqrt{u^2 + \tau^2}\right)^{2\ell-k} \qquad (8.1)$$

where the polynomials $P_\ell^{(k)}$ are defined in Equation (1.4). Moreover,

$$T_q\left(\Phi(\cdot - u)\right)(x) := \sum_{\ell=0}^{q} P_\ell^{(k)}(x^2, -2\langle u, x\rangle, u^2 + \tau^2)/\left(\sqrt{u^2 + \tau^2}\right)^{2\ell-k}, \qquad (8.2)$$

is the Maclaurin polynomial of degree q of $\Phi(\cdot - u)$. When $|x| < \sqrt{u^2 + \tau^2}$ and $q \in \mathbb{N}$,

$$\left|\Phi(x-u) - \sum_{\ell=0}^{q} P_\ell^{(k)}(x^2, -2\langle u, x\rangle, u^2+\tau^2)/\left(\sqrt{u^2+\tau^2}\right)^{2\ell-k}\right|$$
$$\leq \begin{cases} \left(\sqrt{u^2+\tau^2}\right)^k \left(\dfrac{|x|}{\sqrt{u^2+\tau^2}}\right)^{q+1} \dfrac{\sqrt{u^2+\tau^2}}{\sqrt{u^2+\tau^2}-|x|}, & \text{if } k>0, \\ \dbinom{q-k}{q+1} \left(\sqrt{u^2+\tau^2}\right)^k \left(\dfrac{|x|}{\sqrt{u^2+\tau^2}}\right)^{q+1} \left(\dfrac{\sqrt{u^2+\tau^2}}{\sqrt{u^2+\tau^2}-|x|}\right)^{-k}, & \text{if } k<0. \end{cases} \tag{8.3}$$

Proof. Assume firstly that $x \neq 0$. Let $a = x^2$, $b = -2\langle u, x\rangle$ and $c = u^2 + \tau^2$. Then

$$\Phi(x-u) = \left(x^2 - 2\langle u, x\rangle + u^2 + \tau^2\right)^{k/2} = f_k(1),$$

where f_k is the function that is defined in (2.1). Since $a, c > 0$, $b^2 \leq 4ac$, and $1 = |z| < \sqrt{c/a} = \sqrt{u^2+\tau^2}/|x|$, Lemma 2.3 may be applied with $\nu = q$ to yield Equations (8.1) and (8.3) when $x \neq 0$. The results for $x = 0$ follow by continuity.

It remains to show that $T_q(\Phi(\cdot - u))$ is the Maclaurin polynomial of $\Phi(\cdot - u)$. Observe from (1.4) that

$$P_\ell^{(k)}(a, b, c) = P_\ell^{(k)}(x^2, -2\langle u, x\rangle, u^2 + \tau^2)$$

is either a homogeneous polynomial of exact degree ℓ in x, or is trivial. Hence, by Equation (8.3), $T_q(\Phi(\cdot - u))$ is a polynomial of total degree q in x such that

$$\left|\Phi(x-u) - T_q(\Phi(\cdot - u))(x)\right| = \mathcal{O}(|x|^{q+1}) \text{ as } |x| \to 0.$$

The result follows since the only such polynomial is the Maclaurin polynomial.

9 Numerical Results

In this section we present numerical results generated by an initial, non-optimised, implementation of a hierarchical evaluator for generalised multiquadrics.

The current implementation is based on a hierarchical subdivision of an initial box containing all the centres using a binary tree of panels. Associated with a panel are the centres lying within it, a far field expansion, and a distance from the panel's midpoint at which the far field expansion approximates the influence of the panel to sufficient accuracy. Panels are divided generating children if they contain more than a critical number of centres.

Pseudo code for recursive and non-recursive evaluators appropriate for use with such a binary tree evaluation structure is sketched in [3, pp. 8–11]. Nominally the discussion there is limited to an $\mathbb{R}^1$, rather than $\mathbb{R}^n$, setting but the generalisation is immediate.

N	Direct time	Algorithm time	Ratio
1,000	3.20(-1)	1.30(-1)	2.46
2,000	1.312(0)	3.30(-1)	3.98
4,000	5.358(0)	7.91(-1)	6.77
8,000	2.745(1)	1.762(0)	15.58
16,000	1.098(2)	3.665(0)	29.96
32,000	4.394(2)	8.382(0)	52.42

Table 1: Results of numerical experiments with a generalised multiquadric fast evaluator.

Table 1 above gives times in seconds on an Intel Celeron based machine for various evaluation tasks in $\mathbb{R}^2$. An entry of the form $d_0.d_1d_2d_3(e)$ in the table with d_0, d_1, d_2, d_3 decimal digits represents the number $d_0.d_1d_2d_3 \times 10^e$. In the numerical experiments the centres are uniformly distributed on $[0,1]^2$, the multiquadric parameter τ is taken as $1/\sqrt{N}$, where N is the number of centres, and ϕ is the ordinary multiquadric $\phi(r) = \sqrt{r^2 + \tau^2}$. All the coefficients d_i were taken as 1 and the task was to evaluate the spline at the centres to with an infinity norm relative accuracy of 10^{-6}. The code used was structured as a general evaluator and the symmetry inherent in this matrix-vector product test problem was not exploited.

It can be seen from the table that even this initial, non-optimised, implementation is substantially faster than direct evaluation. Thus the methods of this paper will allow use of multiquadric RBF's in much bigger problems than previously possible. We would expect even better performance as the code is developed to incorporate such features as conversion of far field to local expansions.

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