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Fast evaluation of polyharmonic splines in three dimensions

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Abstract: This paper concerns the fast evaluation of radial basis functions. It describes the mathematics of hierarchical and fast multipole methods for fast evaluation of splines of the form

$$s(\mathbf{x}) = p(\mathbf{x}) + \sum_{j=1}^{N} d_j \, |\mathbf{x} - \mathbf{x}_j|^{2\nu-1}, \qquad \mathbf{x} \in \mathcal{R}^3,$$

where ν is a positive integer, and p is a low degree polynomial. Splines s of this form are polyharmonic splines in $\mathcal{R}^3$ and have been found to be very useful for providing solutions to scattered data interpolation problems in $\mathcal{R}^3$. As is now well known hierarchical methods reduce the incremental cost of a single extra evaluation from $\mathcal{O}(N)$ to $\mathcal{O}(\log N)$ operations, and reduce the cost of a matrix vector product (evaluation of s at all the centres) from $\mathcal{O}(N^2)$ to $\mathcal{O}(N \log N)$ operations. We give appropriate far and near field expansions, together with error estimates, uniqueness theorems, and translation formulae. A hierarchical code based on these formulae is detailed and some numerical results are given.

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1 Introduction

Polyharmonic splines in $\mathcal{R}^3$ are functions of the form

$$s(\boldsymbol{x}) = p(\boldsymbol{x}) + \sum_{j=1}^{N} d_j \, |\boldsymbol{x} - \boldsymbol{x}_j|^{2\nu-1}, \tag{1}$$

with ν a positive integer and p a polynomial of degree at most ν. One justification for the name polyharmonic spline is that $|\boldsymbol{x}|^{2\nu-1}$ is a multiple of a fundamental solution Φ to the distributional equation

$$\triangle^{\nu+1}\Phi = \delta_0,$$

where $\triangle$ denotes the Laplacian and δ_0 is the Dirac measure at the origin. One of the attractions of polyharmonic splines is their smoothest interpolation property. Focusing on the $\mathcal{R}^3$ case, given a set of distinct points $\{\boldsymbol{x}_j\}_{j=1}^N$ in $\mathcal{R}^3$ unisolvent for π_ν^3, and corresponding function values $f_j \in \mathcal{R}$, there is a unique $(\nu+1)$-harmonic spline s of the form (1) satisfying the interpolation conditions

$$s(\boldsymbol{x}_j) = f_j, \qquad j = 1, \ldots, N,$$

and the side conditions

$$\sum_{j=1}^{N} d_j \, q(\boldsymbol{x}_j) = 0, \quad \text{for all } q \in \pi_\nu^3.$$

Moreover, this interpolant minimizes the energy functional

$$\sum_{|\boldsymbol{\alpha}|=\nu+1} \frac{(\nu+1)!}{\alpha_1! \, \alpha_2! \, \alpha_3!} \int_{\mathcal{R}^3} \left(D^{\boldsymbol{\alpha}} g(\boldsymbol{x})\right)^2 d\boldsymbol{x}$$

over all suitably smooth interpolants g. In part because of this property 3D polyharmonic splines have been employed in a variety of applications including surface reconstruction from laser and lidar scans (see e.g. [4]), and modeling ore grade from drill hole data.

One obstacle to the widespread use of polyharmonic splines is speed of evaluation. Thus, at first sight, evaluating the spline (1) at a single point $\boldsymbol{x}$ appears to require $\mathcal{O}(N)$ flops. Similarly the matrix-vector product task of evaluating s at all the centres $\boldsymbol{x}_j$ appears to require $\mathcal{O}(N^2)$ flops. This task is very important as iterative methods for finding the coefficients of an interpolant require repeated evaluation of matrix-vector products (see e.g. [7]). Therefore fast evaluators are essential if polyhharmonic splines are to be used in applications involving large data sets. Fortunately, there are now several different fast evaluation methods that can be applied. This paper concerns hierarchical and fast multipole evaluators.

Far field (multipole) and near field expansions of functions, particularly harmonic functions, are well known in Potential Theory, Physics and Quantum Chemistry (see e.g. Jackson [11]). More recently methods for fast evaluation of functions have been built by coupling hierarchical subdivisions of space with these expansions. The resulting numerical methods have dramatically lower operation counts than direct evaluation. Typically the incremental cost of a single extra evaluation is reduced to $\mathcal{O}(\log N)$ or $\mathcal{O}(1)$, and the work of a matrix vector product is reduced to $\mathcal{O}(N \log N)$ or $\mathcal{O}(N)$. The hidden order constants depend on many factors including the precision of evaluation, and the dimension. These fast methods were initially developed for electrostatic potentials in 2-dimensions and gravitational potentials in 3-dimensions. Pioneering work can be found in Barnes and Hut [1], and Greengard and Rokhlin [9, 10]. Algorithms of this type have become known as fast multipole methods. The methods to be developed in this paper are of this type.

This paper is organised as follows. In section 2 the far field expansions are developed for the simple special case of biharmonic splines. In section 3 the particular forms of spherical harmonics and inner and outer functions used here are detailed. In section 4 the outer expansions are developed in the general case of a $(\nu+1)$-harmonic spline. In section 5 translation formulae are developed for outer expansions. In section 6 a uniqueness lemma is given which enables indirect calculation of outer expansions from expansions for child panels. In section 7 a hierarchical code based on the outer expansions is detailed and some numerical results given. In Appendix A outer to inner and inner to inner translation formulae are developed for a full fast multipole code.

2 The biharmonic case

In this section far field expansions are developed for biharmonic splines in $\mathcal{R}^3$, which is the $\nu = 1$ case of expression (1).

A general point $\boldsymbol{x} \in \mathcal{R}^3$ can be expressed in both Cartesian coordinates (x, y, z) and in spherical polar coordinates $[r, \theta, \phi]$. The Cartesian and spherical polar representations are related by

$$(x, y, z) = (r \sin\theta \cos\phi, r \sin\theta \sin\phi, r \cos\theta), \qquad 0 \le \theta \le \pi, \quad -\pi < \phi \le \pi.$$

Consider now points $\boldsymbol{x}$ and $\boldsymbol{x}_<$ in $\mathcal{R}^3$ with Cartesian coordinates (x, y, z) and $(x_<, y_<, z_<)$ and spherical polar coordinates $[r, \theta, \phi]$ and $[r_<, \theta_<, \phi_<]$ respectively. Assume $|\boldsymbol{x}_<| < |\boldsymbol{x}|$ which implies $h = r_</r < 1$. Let γ be the angle between $\boldsymbol{x}$ and

$\boldsymbol{x}_<$. Then

$$\cos\gamma = \cos\theta\cos\theta_< + \sin\theta\sin\theta_<\cos(\phi - \phi_<).$$

Writing $u = \cos\gamma$, we find by the cosine rule

$$\frac{1}{|\boldsymbol{x} - \boldsymbol{x}_<|} = \frac{1}{r\sqrt{1 - 2uh + h^2}}\,.$$

Now $1/\sqrt{1 - 2uh + h^2}$ is the generating function for the Legendre polynomials, which gives

$$\begin{aligned}\frac{1}{|\boldsymbol{x} - \boldsymbol{x}_<|} &= \frac{1}{r}\sum_{n=0}^{\infty} h^n P_n(u)\ , \quad h < 1, \\ &= \sum_{n=0}^{\infty} r^{-n-1}\, r_<^n\, P_n(u), \quad r_< < r, \end{aligned} \tag{2}$$

where as usual P_n denotes the Legendre polynomial of degree n normalised so that $P_n(1) = 1$. Expression (2) can be usefully employed to form the farfield expansion of a cluster when all the sources $\boldsymbol{x}_j$ and the evaluation point $\boldsymbol{x}$ lie on a single straight line through the origin. For more general arrangements of sources and evaluation point, it is necessary to separate the influence of sources and evaluation point which can be achieved by using the addition formula for the Legendre polynomials (See for example Jackson [11] and Greengard and Rokhlin [10]).

There are many different ways to define a collection $\{Y_n^m\}$ of spherical harmonics for the unit sphere $\mathcal{S}^2 \subset \mathcal{R}^3$. Our choice is that of Epton and Dembart [5] and is specified in the second paragraph of section 3. In this case, the addition formula for the Legendre polynomials takes the form

$$P_n(\cos\gamma) = \sum_{m=-n}^{n} Y_n^{-m}(\theta_<, \phi_<)\, Y_n^m(\theta, \phi). \tag{3}$$

Furthermore, the addition formula can be rewritten in terms of inner and outer harmonic functions, also defined in section 3, as

$$r^{-n-1}\, r_<^n\, P_n(\cos\gamma) = (-1)^n \sum_{m=-n}^{n} \mathcal{I}_n^{-m}(\boldsymbol{x}_<)\, O_n^m(\boldsymbol{x}). \tag{4}$$

It follows from expressions (2) and (4) that

$$\frac{1}{|\boldsymbol{x} - \boldsymbol{x}_<|} = \sum_{n=0}^{\infty}(-1)^n \sum_{m=-n}^{n} \mathcal{I}_n^{-m}(\boldsymbol{x}_<)\; O_n^m(\boldsymbol{x}), \qquad |\boldsymbol{x}| > |\boldsymbol{x}_<|\,. \tag{5}$$

This double sum is absolutely convergent in the case $|\boldsymbol{x}| > |\boldsymbol{x}_<|$ because inequality (19) implies the bound

$$\left|\mathcal{I}_n^{-m}(\boldsymbol{x}_<)\,\mathcal{O}_n^m(\boldsymbol{x})\right| \le |\boldsymbol{x}_<|^n\,|\boldsymbol{x}|^{-n-1}\,,$$

for all the integers m and n that occur.

Summing over a cluster of sources $\{\boldsymbol{x}_j\}$ with associated weights $\{d_j\}$ gives the expansion

$$\sum_{j=1}^{N} \frac{d_j}{|\boldsymbol{x}-\boldsymbol{x}_j|} = \sum_{n=0}^{\infty}\sum_{m=-n}^{n} M_n^m\, O_n^m(\boldsymbol{x}), \tag{6}$$

valid everywhere outside the smallest ball about the origin containing all the sources, where

$$M_n^m = (-1)^n \sum_{j=1}^{N} d_j\, \mathcal{I}_n^{-m}(\boldsymbol{x}_j). \tag{7}$$

Applying the same idea to $|\boldsymbol{x}-\boldsymbol{x}_<|$, we find

$$\begin{aligned}
|\boldsymbol{x}-\boldsymbol{x}_<| &= r\sqrt{1-2uh+h^2}\,, \quad h<1\,,\\
&= \frac{r(1-2uh+h^2)}{\sqrt{1-2uh+h^2}}\\
&= r(1-2uh+h^2)\sum_{n=0}^{\infty} h^n P_n(u)\\
&= r\sum_{n=0}^{\infty} h^n\left[P_n(u) - 2u\,P_{n-1}(u) + P_{n-2}(u)\right],
\end{aligned}$$

where $P_{-1}=P_{-2}=0$. Hence, noting the recurrence relation

$$(2k+1)u\,P_k(u) = (k+1)\,P_{k+1}(u) + k\,P_{k-1}(u), \quad k\ge 0\,,$$

for the Legendre polynomials, we derive the formula

$$|\boldsymbol{x}-\boldsymbol{x}_<| = r\sum_{n=0}^{\infty}\frac{-h^n}{2n-1}\left[P_n(u) - P_{n-2}(u)\right], \tag{8}$$

retaining $P_{-1}=P_{-2}=0$.

We approximate the influence of clusters of sources by far field series based on this expansion. Consider therefore truncating it by neglecting all terms of order $\mathcal{O}(r^{-p})$ or smaller as $r\to\infty$, obtaining

$$|\boldsymbol{x}-\boldsymbol{x}_<| \approx r\sum_{n=0}^{p}\frac{-h^n}{2n-1}\left[P_n(u) - P_{n-2}(u)\right]. \tag{9}$$

From above, and using $|P_n(u)| \le 1$, $-1 \le u \le 1$, the error of the approximation (9) is bounded by

$$\begin{aligned}
&\left| |\boldsymbol{x} - \boldsymbol{x}_<| - r \sum_{n=0}^{p} \frac{-h^n}{2n-1} \Big[P_n(u) - P_{n-2}(u) \Big] \right| \\
&\quad = \left| r \sum_{n=p+1}^{\infty} \frac{h^n}{2n-1} \Big[P_n(u) - P_{n-2}(u) \Big] \right| \\
&\quad \le \frac{2r}{2p+1} h^{p+1} \frac{1}{1-h} \le \left(\frac{2r}{2p+1} \right) \left(\frac{1}{1-\frac{R}{r}} \right) \left(\frac{R}{r} \right)^{p+1}, \qquad (10)
\end{aligned}$$

for any R that satisfies $|\boldsymbol{x}_<| \le R < |\boldsymbol{x}| = r$.

Again the addition formula (4) for Legendre polynomials gives a form that is useful for clusters of sources in general position. Specifically, we write (9) as the estimate

$$\begin{aligned}
|x - x_<| &\approx r^2 \left[-\sum_{n=0}^{p} \frac{r^{-1-n}\, r_<^n}{2n-1} P_n(u) \right] + \left[\sum_{n=0}^{p-2} \frac{r^{-1-n}\, r_<^{n+2}}{2n+3} P_n(u) \right] \\
&= r^2 \left\{ \sum_{n=0}^{p} \sum_{m=-n}^{n} N_{nm}\, \mathcal{O}_n^m(\boldsymbol{x}) \right\} + \left\{ \sum_{n=0}^{p-2} \sum_{m=-n}^{n} M_{nm}\, \mathcal{O}_n^m(\boldsymbol{x}) \right\}, \qquad (11)
\end{aligned}$$

where

$$N_{nm} = -(-1)^n \frac{1}{2n-1} \mathcal{I}_n^{-m}(\boldsymbol{x}_<) \quad \text{and} \quad M_{nm} = (-1)^n \frac{r_<^2}{2n+3} \mathcal{I}_n^{-m}(\boldsymbol{x}_<). \qquad (12)$$

Thus, by superposition, a biharmonic radial function of the form

$$s(\boldsymbol{x}) = \sum_{j=1}^{N} d_j\, |\boldsymbol{x} - \boldsymbol{x}_j|, \qquad (13)$$

can be approximated by the truncated expansion

$$r^2 \left\{ \sum_{n=0}^{p} \sum_{m=n}^{n} N_{nm}\, \mathcal{O}_n^m(\boldsymbol{x}) \right\} + \left\{ \sum_{n=0}^{p-2} \sum_{m=-n}^{n} M_{nm}\, \mathcal{O}_n^m(\boldsymbol{x}) \right\} \qquad (14)$$

where now the coefficients N_{nm} and M_{nm} are the complex numbers

$$N_{nm} = -\frac{(-1)^n}{2n-1} \sum_{j=1}^{N} d_j\, \mathcal{I}_n^{-m}(\boldsymbol{x}_j) \quad \text{and} \quad M_{nm} = \frac{(-1)^n}{2n+3} \sum_{j=1}^{N} d_j\, r_j^2\, \mathcal{I}_n^{-m}(\boldsymbol{x}_j), \qquad (15)$$

which do not depend on $\boldsymbol{x}$. In view of the error bound (10), the expansion (14) converges to $s(\boldsymbol{x})$ as $p \to \infty$ for all $\boldsymbol{x}$ outside the smallest closed ball about the origin containing all the centres $\boldsymbol{x}_j, 1 \le j \le N$.

This paper concerns the application of the expansion (14) and of the analogous truncated expansions of $(\nu+1)$–harmonic splines

$$s(\boldsymbol{x}) = \sum_{j=1}^{N} d_j\,|\boldsymbol{x}-\boldsymbol{x}_j|^{2\nu-1} \tag{16}$$

$$\approx \sum_{k=0}^{\nu} r^{2\nu-2k} \sum_{n=0}^{p-2k} \sum_{m=-n}^{n} N_{nm}^{(k)}\,\mathcal{O}_n^m(\boldsymbol{x}), \tag{17}$$

to the fast evaluation of polyharmonic splines in $\mathcal{R}^3$. Error estimates, uniqueness theorems, translation theorems, and some numerical results will be given in the sections to follow.

3 Spherical harmonics, associated Legendre functions, etc

There are many different formulations and normalizations of spherical harmonics and associated Legendre functions. Consequently one has to be very careful when combining formulae from different sources. We follow Epton and Dembart [5] as their choice helps to simplify the translation formulae.

They employ the associated Legendre functions

$$P_n^m(u) = \frac{(n+m)!}{2^n n!\,(n-m)!}(1-u^2)^{-m/2}\,\frac{d^{n-m}}{du^{n-m}}(u^2-1)^n, \quad -1 \le u \le 1,$$

for $-n \le m \le n$, $n \ge 0$. For all other values of n and m, P_n^m is taken to be the zero function. This specification of the associated Legendre function implies

$$P_n^{-m}(u) = (-1)^m\,\frac{(n-m)!}{(n+m)!}\,P_n^m(u), \qquad -n \le m \le n.$$

Epton and Dembart then define spherical harmonics Y_n^m by

$$Y_n^m(\theta,\phi) = \epsilon_m \sqrt{\frac{(n-m)!}{(n+m)!}}\,P_n^m(\cos\theta)\,e^{im\phi}, \quad -n \le m \le n,$$

where

$$\epsilon_m = \begin{cases} (-1)^m, & m \ge 0 \\ 1, & m \le 0. \end{cases}$$

Their properties include conjugate symmetry

$$Y_n^{-m}(\theta,\phi) = \overline{Y_n^m(\theta,\phi)},$$

and the orthogonality relation

$$\int_0^{\pi}\int_{-\pi}^{\pi} Y_n^m(\theta,\phi)\, Y_k^{-j}(\theta,\phi)\sin\theta\, d\phi\, d\theta = \frac{4\pi}{2n+1}\,\delta_{mj}\,\delta_{nk}. \tag{18}$$

The conjugate symmetry with the addition formula (3) gives the identity

$$1 = P_n(1) = \sum_{m=-n}^{n} \left|Y_n^m(\theta,\phi)\right|^2,$$

for all θ and ϕ in $\mathcal{R}$. It follows that

$$|Y_n^m(\theta,\phi)| \le 1, \tag{19}$$

for all θ, ϕ, n and m. Further Epton and Dembart define outer spherical harmonics (harmonic functions well behaved away from zero)

$$\mathcal{O}_n^m(\boldsymbol{x}) = \mathcal{O}_n^m(r,\theta,\phi) = \frac{\mathfrak{i}^{|m|}(-1)^n}{A_n^m}\,\frac{Y_n^m(\theta,\phi)}{r^{n+1}} \tag{20}$$

and inner spherical harmonics (harmonic functions well behaved away from infinity)

$$\mathcal{I}_n^m(\boldsymbol{x}) = \mathcal{I}_n^m(r,\theta,\phi) = \mathfrak{i}^{-|m|} A_n^m\, r^n\, Y_n^m(\theta,\phi)$$

where

$$A_n^m = A_n^{-m} = \frac{(-1)^n}{\sqrt{(n-m)!\,(n+m)!}},$$

and where $\mathfrak{i}$ denotes the square root of -1. These remarks imply the symmetries

$$\overline{\mathcal{O}_n^m(\boldsymbol{x})} = (-1)^m \mathcal{O}_n^{-m}(\boldsymbol{x}) \quad \text{and} \quad \overline{\mathcal{I}_n^m(\boldsymbol{x})} = (-1)^m \mathcal{I}_n^{-m}(\boldsymbol{x}). \tag{21}$$

It is important that $O_n^m(\boldsymbol{x})$ is of exact order $|\boldsymbol{x}|^{-n-1}$ as $|\boldsymbol{x}| \to \infty$, and that $\mathcal{I}_n^m(\boldsymbol{x})$, $\boldsymbol{x} \in \mathcal{R}^3$, is a homogeneous polynomial of degree n. Define

$$E_n^m = (-\mathfrak{i})^m (n-m)! = \frac{(-1)^n(-\mathfrak{i})^m}{A_n^m}\sqrt{\frac{(n-m)!}{(n+m)!}}, \tag{22}$$

and

$$F_n^m = \frac{(-1)^n\,\mathfrak{i}^m}{(n+m)!} = \mathfrak{i}^m A_n^m \sqrt{\frac{n-m)!}{(n+m)!}}. \tag{23}$$

Then easy calculations provide the formulae

$$\mathcal{O}_n^m(\boldsymbol{x}) = E_n^m\, r^{-n-1}\, P_n^m(\cos\theta)\, e^{\mathfrak{i}m\phi} \quad \text{and} \quad \mathcal{I}_n^m(\boldsymbol{x}) = F_n^m\, r^n\, P_n^m(\cos\theta) e^{\mathfrak{i}m\phi}, \tag{24}$$

which show the homogeneities explicitly.

4 Expansions and error estimates

The following theorem is a generalisation of the expansions (2) and (8) of section 2. Those expansions can be applied to fast evaluation of harmonic and biharmonic splines on $\mathcal{R}^3$, while the theory below covers the general $(\nu+1)$-harmonic spline case on $\mathcal{R}^3$.

Theorem 4.1. (Generalized Legendre expansion)
Let h and u be real numbers that satisfy $0 \le h < 1$, $-1 \le u \le 1$, and let ν be any positive integer. Then

$$\left(1 - 2hu + h^2\right)^{\nu - \frac{1}{2}} = \sum_{n=0}^{\infty} h^n \sum_{k=0}^{\nu} \alpha_{\nu,k}(n)\, P_{n-2k}(u), \tag{25}$$

where the coefficients have the values

$$\alpha_{\nu,k}(n) = (-1)^{\nu+k}\,(2\nu-1)!!\binom{\nu}{k} \prod_{\ell=0,\ \ell\neq k}^{\nu} \frac{1}{2n - 2k - 2\ell + 1}, \tag{26}$$

and where, for $n < 2k$, we set $P_{n-2k}(u) = 0$. The term $(2\nu-1)!!$ is the product $\prod_{j=1}^{\nu}(2j-1)$.

Note: For each choice of ν and for $k = 0, 1, \ldots, \nu$, the coefficient $\alpha_{\nu,k}(n)$ is of magnitude $n^{-\nu}$ for large n. Also the modulus of $P_{n-2k}(u)$, $-1 \le u \le 1$, is at most one. It then follows from $|h| < 1$ that the double sum on the right of (25) is absolutely convergent. All double sums in the proof below have this property.

Proof. When $\nu = 1$, expression (26) gives the coefficients

$$\alpha_{1,0}(n) = \frac{-1}{2n-1} \quad \text{and} \quad \alpha_{1,1}(n) = \frac{1}{2n-1}. \tag{27}$$

Therefore, after dividing both sides of (8) by $r = |\boldsymbol{x}|$, we find that the theorem is true for the biharmonic case $\nu = 1$.

We complete the proof by induction on ν. Let equation (25) hold for the current ν, beginning with $\nu = 1$. We show that the equation remains true if ν is increased by one. Starting with (25) we obtain

$$\begin{aligned}\left(1 - 2hu + h^2\right)^{\nu + \frac{1}{2}} &= \sum_{n=0}^{\infty} h^n \sum_{k=0}^{\nu} \left(1 - 2hu + h^2\right) \alpha_{\nu,k}(n)\, P_{n-2k}(u) \\ &= \sum_{n=0}^{\infty} h^n \sum_{k=0}^{\nu} \{\alpha_{\nu,k}(n)\, P_{n-2k}(u) - 2u\, \alpha_{\nu,k}(n-1)\, P_{n-2k-1}(u) \\ &\qquad + \alpha_{\nu,k}(n-2)\ P_{n-2k-2}(u)\}\,. \end{aligned} \tag{28}$$

The three term recurrence relation for the Legendre polynomials provides the identity

$$2u\,P_{n-2k-1}(u) = \frac{2n-4k}{2n-4k-1}\,P_{n-2k}(u) + \frac{2n-4k-2}{2n-4k-1}\,P_{n-2k-2}(u), \qquad (29)$$

even if some of the subscripts of P are negative. Thus we deduce the expression

$$\left(1-2hu+h^2\right)^{\nu+\frac{1}{2}} = \sum_{n=0}^{\infty} h^n \sum_{k=0}^{\nu+1} \widehat{\alpha}_{\nu,k}(n)\,P_{n-2k}(u), \qquad (30)$$

where the new coefficients are the numbers

$$\widehat{\alpha}_{\nu,0}(n) = \alpha_{\nu,0}(n) - \frac{2n}{2n-1}\,\alpha_{\nu,0}(n-1), \qquad (31a)$$

$$\widehat{\alpha}_{\nu,\nu+1}(n) = \alpha_{\nu,\nu}(n-2) - \frac{2n-4\nu-2}{2n-4\nu-1}\,\alpha_{\nu,\nu}(n-1), \quad \text{and} \qquad (31b)$$

$$\widehat{\alpha}_{\nu,k}(n) = \alpha_{\nu,k}(n) - \frac{2n-4k}{2n-4k-1}\,\alpha_{\nu,k}(n-1) \qquad (31c)$$
$$+\,\alpha_{\nu,k-1}(n-2) - \frac{2n-4k+2}{2n-4k+3}\,\alpha_{\nu,k-1}(n-1), \quad 1 \le k \le \nu.$$

It remains to establish algebraically that $\widehat{\alpha}_{\nu,k}(n) = \alpha_{\nu+1,k}(n)$.

When $k=0$, we find the value

$$\begin{aligned}\widehat{\alpha}_{\nu,0}(n) &= (-1)^\nu \left\{\prod_{\ell=1}^{\nu} \frac{2\ell-1}{2n-2\ell+1} - \frac{2n}{2n-1}\prod_{\ell=1}^{\nu}\frac{2\ell-1}{2n-2\ell-1}\right\} \\ &= (-1)^\nu \left\{\prod_{\ell=1}^{\nu} \frac{2\ell-1}{2n-2\ell+1}\right\}\left\{1-\frac{2n}{2n-2\nu-1}\right\} \\ &= (-1)^{\nu+1} \prod_{\ell=1}^{\nu+1} \frac{2\ell-1}{2n-2\ell+1} = \alpha_{\nu+1,0}(n), \end{aligned} \qquad (32)$$

and, when $k=\nu+1$,

$$\begin{aligned}\widehat{\alpha}_{\nu,\nu+1}(n) &= \frac{2n-4\nu-3}{2n-2\nu-3}\prod_{\ell=1}^{\nu}\frac{2\ell-1}{2n-2\nu-2\ell-3} - \frac{2n-4\nu-2}{2n-2\nu-1}\prod_{\ell=1}^{\nu}\frac{2\ell-1}{2n-2\nu-2\ell-1} \\ &= \left\{\prod_{\ell=1}^{\nu}\frac{2\ell-1}{2n-2\nu-2\ell-1}\right\}\left\{1-\frac{2n-4\nu-2}{2n-2\nu-1}\right\} \\ &= \frac{2n-4\nu-3}{2n-2\nu-1}\prod_{\ell=1}^{\nu+1}\frac{2\ell-1}{2n-2\nu-2\ell-1} = \alpha_{\nu+1,\nu+1}(n). \end{aligned} \qquad (33)$$

Therefore, in the remainder of the proof, k is any integer from the interval $[1, \nu]$.

We substitute the values

$$\alpha_{\nu,k}(n) = -\frac{\nu-k+1}{k}\,\frac{2n-4k+1}{2n-4k+3}\,\alpha_{\nu,k-1}(n-1) \tag{34a}$$

$$\alpha_{\nu,k}(n-1) = -\frac{\nu-k+1}{k}\,\frac{2n-4k-1}{2n-4k+3}\,\frac{2n-2k+1}{2n-2k-2\nu-1}\,\alpha_{\nu,k-1}(n-1) \tag{34b}$$

$$\alpha_{\nu,k-1}(n-2) = \frac{2n-4k+1}{2n-4k+3}\,\frac{2n-2k+1}{2n-2k-2\nu-1}\,\alpha_{\nu,k-1}(n-1) \tag{34c}$$

into (31c), in order to express $\widehat{\alpha}_{\nu,k}(n)$ as a multiple of $\alpha_{\nu,k-1}(n-1)$. We merge the second and fourth terms that occur making use of the identity

$$\begin{aligned}(\nu-k+1)(n-2k)(2n-2k+1) - k(2n-2k-2\nu-1)(n-2k+1)\\ = (2n-4k+1)(n\nu+2k^2-2kn-k+n),\end{aligned} \tag{35}$$

because the factor $(2n-4k+1)$ occurs in the other two terms. Thus $\widehat{\alpha}_{\nu,k}(n)$ is the product of the expressions

$$(2n-4k+1)\,\alpha_{\nu,k-1}(n-1)/\,\{k(2n-4k+3)(2n-2k-2\nu-1)\} \tag{36}$$

and

$$\begin{aligned}-(\nu-k+1)(2n-2k-2\nu-1) + 2(n\nu+2k^2-2kn-k+n)\\ + k(2n-2k+1) = 2\nu^2+3\nu+1.\end{aligned} \tag{37}$$

It follows from the identity

$$\frac{\alpha_{\nu+1,k}(n)}{\alpha_{\nu,k-1}(n-1)} = \frac{\nu+1}{k}\,\frac{2n-4k+1}{2n-4k+3}\,\frac{2\nu+1}{2n-2k-2\nu-1} \tag{38}$$

that the theorem is true. □

We are going to estimate $(1-2hu+h^2)^{\nu-1/2}$ by truncating the infinite sum (25). The inequality

$$\left| h^n \sum_{k=0}^{\nu} \alpha_{\nu,k}(n)\, P_{n-2k}(u) \right| \;\le\; h^n \sum_{k=0}^{\nu} |\alpha_{\nu,k}(n)| \;=\; h^n\, C_\nu(n),$$

say, is going to provide a useful bound on the terms that are dropped from the infinite sum. The definition (26) implies the formula

$$C_\nu(n) \;=\; \sum_{k=0}^{\nu} |\alpha_{\nu,k}(n)| \;=\; \frac{(2\nu-1)!!\,2^\nu}{(2n-1)(2n-5)\cdots(2n-4\nu+3)}, \quad n \ge 2\nu-1, \tag{39}$$

which was found originally by straightforward algebra for $\nu = 1, 2, 3$, and 4. Then, by invoking special functions, Iserles (private communication) established the formula for all positive integers ν, and later the authors devised a proof by induction. The latter proof is available in the *Publications and Downloads* section of the web page www.math.canterbury.ac.nz/~rkb29.

The next theorem addresses the truncation of the infinite sum involving inner and outer functions derived from (25) by use of the addition formula.

Theorem 4.2. *Let $\nu \in \mathcal{N}$ be fixed, and let N centres $\boldsymbol{x}_j \in \mathcal{R}^3$, $1 \leq j \leq N$, with $|\boldsymbol{x}_j| \leq R$, and N corresponding real coefficients d_j be given. Then, whenever $r = |\boldsymbol{x}| > R$, the $(\nu+1)$-harmonic spline*

$$s(\boldsymbol{x}) = \sum_{j=1}^{N} d_j \, |\boldsymbol{x} - \boldsymbol{x}_j|^{2\nu-1}, \qquad \boldsymbol{x} \in \mathcal{R}^3 \ , \tag{40}$$

can be written as the convergent series

$$s(\boldsymbol{x}) = \sum_{k=0}^{\nu} |\boldsymbol{x}|^{2\nu-2k} \sum_{n=0}^{\infty} \sum_{m=-n}^{n} N_{nm}^{(k)} \, \mathcal{O}_n^m(\boldsymbol{x}), \tag{41}$$

the coefficients being

$$N_{nm}^{(k)} = (-1)^n \, \alpha_{\nu,k}(n+2k) \sum_{j=1}^{N} d_j \, r_j^{2k} \, \mathcal{I}_n^{-m}(\boldsymbol{x}_j), \quad 0 \leq |m| \leq n, \quad 0 \leq k \leq \nu, \tag{42}$$

where $\alpha_{\nu,k}(n+2k)$ is defined in Theorem 4.1 and $r_j = |\boldsymbol{x}_j|$. Furthermore, if $p \in \mathcal{N}$ and $p \geq 2\nu - 1$, then

$$\begin{aligned} \Big| \sum_{j=1}^{N} d_j |\boldsymbol{x} - \boldsymbol{x}_j|^{2\nu-1} \ &- \ \sum_{k=0}^{\nu} |\boldsymbol{x}|^{2\nu-2k} \sum_{n=0}^{p-2k} \sum_{m=-n}^{n} N_{nm}^{(k)} \, \mathcal{O}_n^m(\boldsymbol{x}) \Big| \\ &\leq \ M r^{2\nu-1} \, C_\nu(p+1) \left(\frac{R}{r} \right)^{p+1} \left(\frac{1}{1 - \frac{R}{r}} \right) \end{aligned} \tag{43}$$

where $M = \sum_{j=1}^{N} |d_j|$ and $C_\nu(p+1)$ is defined by (39).

Remark: An empty sum of the form $\sum_{n=0}^{-1} \sum_{m=-n}^{n} \ldots$ occurs in (43) when $p = 2\nu - 1$ and $k = \nu$. All such empty sums are to be taken as zero.

Proof. Consider the special case of a single centre at $\boldsymbol{x}_<$ and weight unity

$$s(\boldsymbol{x}) = |\boldsymbol{x} - \boldsymbol{x}_<|^{2\nu-1} \ .$$

As before, we write h for $|\boldsymbol{x}_<|/|\boldsymbol{x}| < 1$ and u for $\cos\gamma$, where γ is the angle between $\boldsymbol{x}_<$ and $\boldsymbol{x}$. Then by the cosine formula

$$\begin{aligned}
|\boldsymbol{x}-\boldsymbol{x}_<|^{2\nu-1} &= \left(|\boldsymbol{x}|^2 - 2|\boldsymbol{x}||\boldsymbol{x}_<|\cos\gamma + |\boldsymbol{x}_<|^2\right)^{\nu-\frac{1}{2}} \\
&= r^{2\nu-1}\left(1-2hu+h^2\right)^{\nu-\frac{1}{2}} \\
&= r^{2\nu-1}\sum_{n=0}^{\infty} h^n \sum_{k=0}^{\nu} \alpha_{\nu,k}(n)\, P_{n-2k}(u) \\
&= \sum_{k=0}^{\nu} r^{2\nu-2k}\, r_<^{2k} \sum_{n=0}^{\infty} \alpha_{\nu,k}(n+2k)\, r^{-n-1}\, r_<^n\, P_n(u) \\
&= \sum_{k=0}^{\nu} r^{2\nu-2k}\, r_<^{2k} \sum_{n=0}^{\infty} (-1)^n\, \alpha_{\nu,k}(n+2k) \sum_{m=-n}^{n} \mathcal{I}_n^{-m}(\boldsymbol{x}_<)\, \mathcal{O}_n^m(\boldsymbol{x}), \quad (44)
\end{aligned}$$

where we have used Theorem 4.1, the note following it, the property $P_{n-2k}(u) = 0$, $n < 2k$, and equation (4). This shows (41) and (42) in the special case. They follow by superposition for the general case.

We now turn to the error estimate. Consider again the special case $s(\boldsymbol{x}) = |\boldsymbol{x}-\boldsymbol{x}_<|^{2\nu-1}$ where $r = |\boldsymbol{x}| > R \geq |\boldsymbol{x}_<|$. From the reasoning leading to (44), the left hand side of (43) is

$$\left| r^{2\nu-1} \sum_{n=p+1}^{\infty} \left(\frac{|\boldsymbol{x}_<|}{r}\right)^n \sum_{k=0}^{\nu} \alpha_{\nu,k}(n)\, P_{n-2k}(u) \right| =: E.$$

Recalling $|P_n(u)| \leq 1$ and (39), we obtain

$$E \leq r^{2\nu-1} \sum_{n=p+1}^{\infty} \left(\frac{R}{r}\right)^n \sum_{k=0}^{\nu} |\alpha_{\nu,k}(n)| = r^{2\nu-1} \sum_{n=p+1}^{\infty} \left(\frac{R}{r}\right)^n C_\nu(n), \qquad (45)$$

for $p \geq 2\nu - 1$, which gives the bound

$$E \leq r^{2\nu-1}\, C_\nu(p+1) \left(\frac{R}{r}\right)^{p+1} \frac{1}{1-\left(\frac{R}{r}\right)}\ , \qquad (46)$$

because expression (39) is a decreasing function of n.

This shows (43) in the special case. Since the right hand side of the error estimate (46) is increasing in $h = R/r$, the error estimate (43) for the general case follows by superposition. □

5 Uniqueness of outer expansions

This section contains a uniqueness result for truncated outer expansions. It shows that the truncated expansion of equation (43) is the only expansion of that form achieving asymptotic accuracy $o\left(|\boldsymbol{x}|^{(2\nu-1)-p}\right)$ for large $|\boldsymbol{x}|$. This result will later allow coefficients of the outer series for a panel to be calculated from the outer series for child panels by an indirect method that is inexpensive.

Lemma 5.1. *Let ν and p be any nonnegative integers, and let a function g_p, defined for all $\boldsymbol{x} \in \mathcal{R}^3\backslash\{\mathbf{0}\}$, be written in the form*

$$g_p(\boldsymbol{x}) = \sum_{k=0}^{\nu} |\boldsymbol{x}|^{2\nu-2k} \sum_{n=0}^{p-2k} \sum_{m=-n}^{n} N_{nm}^{(k)}\, \mathcal{O}_n^m(\boldsymbol{x}), \tag{47}$$

for some complex coefficients $\left\{N_{nm}^{(k)}\right\}$, the inner double sum being taken as zero whenever $2k > p$ occurs. Then

(i) the coefficients $\left\{N_{nm}^{(k)}\right\}$ are uniquely determined by the function g_p,

(ii) if $|g_p(\boldsymbol{x}|) = o\left(|\boldsymbol{x}|^{(2\nu-1)-p}\right)$ as $|\boldsymbol{x}| \to \infty$, then g_p is the zero function.

Proof of (i). Recall from (18) that the functions $\{Y_n^m : -n \le m \le n,\ 0 \le n \le p\}$ are an orthogonal set of nontrivial spherical harmonics on the unit sphere $\mathcal{S}^2$ with respect to the inner product

$$\langle f, g\rangle = \int_{\mathcal{S}^2} f(\boldsymbol{x})\, \overline{g(\boldsymbol{x})}\, d\sigma(\boldsymbol{x})\,.$$

Further recall from (20) that $\mathcal{O}_n^m$ is homogeneous of degree $-n-1$ on $\mathcal{R}^3\backslash\{0\}$, meaning

$$\mathcal{O}_n^m(\lambda\boldsymbol{x}) = \lambda^{-n-1}\mathcal{O}_n^m(\boldsymbol{x}), \quad \text{for all } \boldsymbol{x} \neq \mathbf{0} \text{ and } \lambda > 0.$$

It follows, from this homogeneity property and expression (47) for g_p, that the decay rates of the terms of $g_p(\boldsymbol{x})$ as $|\boldsymbol{x}| \to \infty$ are between $|\boldsymbol{x}|^{2\nu-1}$ and $|\boldsymbol{x}|^{2\nu-1-p}$. Therefore g_p can be decomposed into an expansion

$$g_p(\boldsymbol{x}) = T_0(\boldsymbol{x}) + T_1(\boldsymbol{x}) + \cdots + T_p(\boldsymbol{x}),$$

where each function T_q is either identically zero or nonzero and homogeneous of degree $(2\nu-1)-q$. For $\boldsymbol{u}$ with $|\boldsymbol{u}| = 1$ the T_q's are given by the recurrence

$$T_q(\boldsymbol{u}) = \lim_{\lambda\to\infty} \frac{g_p(\lambda\boldsymbol{u}) - \sum_{k=0}^{q-1} T_k(\lambda\boldsymbol{u})}{\lambda^{(2\nu-1)-q}}, \quad q = 0, 1, \ldots, p.$$

Now fix q, $0 \le q \le p$. Then expression (47) for g_p gives the formula

$$T_q(\boldsymbol{x}) = \sum_{k=0}^{\min\{\nu,[q/2]\}} r^{2\nu-2k} \sum_{m=-(q-2k)}^{q-2k} N_{q-2k,m}^{(k)} \mathcal{O}_{q-2k}^{m}(\boldsymbol{x}), \quad r = |\boldsymbol{x}| > 0, \tag{48}$$

where $[q/2]$ is the integer part of $q/2$. In this expression each $\mathcal{O}_n^m$ occurs at most once. Hence, taking $r = |\boldsymbol{x}| = 1$, the orthogonality of the $\{\mathcal{O}_n^m\}$ on $\mathcal{S}^2$ implies that the coefficients $\left\{N_{q-2k,m}^{(k)}\right\}$ occurring on the right of (48) are uniquely determined by T_q. Combining this with the recursive definition of the T_q's from limits of g_p, we find that the first claim of the lemma is true.

Proof of (ii) From the proof of part (i) of the lemma $g_p = T_0 + T_1 + \cdots + T_p$, where each T_q is homogeneous of degree $(2\nu-1)-q$. The decay of g_p at infinity is dominated by the first nonzero term of this expansion. Hence $|g_p(\boldsymbol{x})| = o\left(|\boldsymbol{x}|^{(2\nu-1)-p}\right)$ as $|\boldsymbol{x}| \to \infty$ implies $T_0, T_1, \ldots, T_p$ are all identically zero. Hence g_p also is identically zero. □

6 Outer to outer translation formulae

This section concerns translation formulae for various truncated outer function expansions. For a $(\nu+1)$-harmonic spline

$$\sum_{j=1}^{N} d_j |\boldsymbol{x} - \boldsymbol{x}_j|^{2\nu-1},$$

s they allow the truncated expansion about one origin, say $\mathbf{0}$, to be derived from the truncated expansion about another origin $\boldsymbol{t}$. It is important that the operation count for the translation depends only on the number of terms in the original expansion and not on the number of centres/sources underlying it. Such indirect calculation of series can be very efficient when the number of centres is large. In the algorithm to come a panel $\mathcal{T}$ is an object, or structure, with many characteristics, foremost amongst which is its correspondence to a rectangular subset of $\mathcal{R}^3$. Subpanels formed by partitioning the rectangular subset are called the children of $\mathcal{T}$. The translation formulae of this section can be applied to obtain outer, or far field, expansions for a parent panel $\mathcal{T}$ inexpensively from those of $\mathcal{T}$'s children.

Consider a harmonic function s expressed as an outer series about $\boldsymbol{t}$,

$$s(\boldsymbol{x}) = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} C_n^m \, \mathcal{O}_n^{-m}(\boldsymbol{x} - \boldsymbol{t}), \qquad |\boldsymbol{x} - \boldsymbol{t}| > R \ge 0, \tag{49}$$

where the convergence is uniform on the set $\mathcal{U}_{R+\epsilon} := \{\boldsymbol{x} : |\boldsymbol{x} - \boldsymbol{t}| \ge R + \epsilon\}$ for any $\epsilon > 0$. Then from Epton and Dembart [5, Section 2.3] and well known homogeneity arguments, $s(\boldsymbol{x})$ can be rewritten as an outer series about $\mathbf{0}$,

$$s(\boldsymbol{x}) = \sum_{\ell=0}^{\infty} \sum_{j=-\ell}^{\ell} D_j^{\ell}\, \mathcal{O}_{\ell}^{-j}(\boldsymbol{x}), \qquad |\boldsymbol{x}| > R + |\boldsymbol{t}|, \tag{50}$$

where now the convergence is uniform on the set $\{\boldsymbol{x} : |\boldsymbol{x}| \geq R + |\boldsymbol{t}| + \epsilon\}$ for any $\epsilon > 0$ and where

$$D_{\ell}^{j} = \sum_{n=0}^{\ell} \sum_{m=-n}^{n} C_n^m\, \mathcal{I}_{\ell-n}^{j-m}(-\boldsymbol{t}). \tag{51}$$

Now consider a truncated outer series for s,

$$h_p(\boldsymbol{x}) = \sum_{k=0}^{\nu} |\boldsymbol{x} - \boldsymbol{t}|^{2\nu-2k} \sum_{n=0}^{p-2k} \sum_{m=-n}^{n} M_{nm}^{(k)}\, \mathcal{O}_n^m(\boldsymbol{x} - \boldsymbol{t}), \tag{52}$$

formed as in Theorem 4.2 but with the origin shifted to $\boldsymbol{t}$. According to Theorem 4.2 this series about $\boldsymbol{t}$ approximates $s(\boldsymbol{x})$ with error $|s(\boldsymbol{x}) - h_p(\boldsymbol{x})| = \mathcal{O}\left(|\boldsymbol{x}|^{\ell}\right)$ as $|\boldsymbol{x}| \to \infty$, the value of ℓ being $(2\nu - 1) - (p + 1)$. Applying (49), (50) and (51), h_p can be expressed in the partially translated form

$$h_p(\boldsymbol{x}) = \sum_{k=0}^{\nu} |\boldsymbol{x} - \boldsymbol{t}|^{2\nu-2k} \sum_{n=0}^{\infty} \sum_{m=-n}^{n} \widetilde{M}_{nm}^{(k)}\, \mathcal{O}_n^m(\boldsymbol{x}), \quad |\boldsymbol{x}| > |\boldsymbol{t}|.$$

We drop all terms in this expression of magnitude at most $|\boldsymbol{x}|^{\ell}$ for large $|\boldsymbol{x}|$, which gives the truncated expansion

$$\widetilde{g}_p(\boldsymbol{x}) = \sum_{k=0}^{\nu} |\boldsymbol{x} - \boldsymbol{t}|^{2\nu-2k} \sum_{n=0}^{p-2k} \sum_{m=-n}^{n} \widetilde{M}_{nm}^{(k)}\, \mathcal{O}_n^m(\boldsymbol{x}), \tag{53}$$

again approximating $s(\boldsymbol{x})$ with accuracy $\mathcal{O}\left(|\boldsymbol{x}|^{\ell}\right)$ as $|\boldsymbol{x}| \to \infty$.

Formulae will now be developed that express the function

$$q(\boldsymbol{x}) = |\boldsymbol{x} - \boldsymbol{t}|^2 \sum_{n=0}^{j} \sum_{m=-n}^{n} A_{nm}\, \mathcal{O}_n^m(\boldsymbol{x}), \tag{54}$$

in the form

$$\sum_{n=0}^{j-2} \sum_{m=-n}^{n} U_{nm}\, \mathcal{O}_n^m(\boldsymbol{x}) + |\boldsymbol{x}|^2 \sum_{n=0}^{j} \sum_{m=-n}^{n} V_{nm}\, \mathcal{O}_n^m(\boldsymbol{x}) + \mathcal{O}(|\boldsymbol{x}|^{-j}), \quad |\boldsymbol{x}| > |\boldsymbol{t}|. \tag{55}$$

By applying this remark $\nu - k$ times to the factor $|\boldsymbol{x}-\boldsymbol{t}|^{2\nu-2k}$ in (53), we complete the translation of the truncated outer series (52) about $\boldsymbol{t}$, into a truncated outer series about $\mathbf{0}$, of form (47). The final truncated expansion approximates $s(\boldsymbol{x})$ with accuracy $\mathcal{O}\left(|\boldsymbol{x}|^{\ell}\right)$ as $|\boldsymbol{x}| \to \infty$. Moreover, according to Theorem 4.2 the truncated expansion obtained by direct calculation of coefficients gives the same order of convergence. Therefore, by the uniqueness result of Lemma 5.1, the two truncated expansions are identical.

It remains only to describe the process for rewriting expression (54) in the form (55). We employ some recurrence relations, taken from [6, Section 3.8], namely that the associated Legendre functions satisfy

$$\cos\theta\, P_n^m(\cos\theta) = \left(\frac{n+m}{2n+1}\right) P_{n-1}^m(\cos\theta) + \left(\frac{n-m+1}{2n+1}\right) P_{n+1}^m(\cos\theta)\,, \tag{56}$$

$$\sin\theta\, P_n^m(\cos\theta) = \frac{1}{2n+1}\left\{P_{n-1}^{m+1}(\cos\theta) - P_{n+1}^{m+1}(\cos\theta)\right\}, \tag{57}$$

and

$$\begin{aligned}\sin\theta\, P_n^m(\cos\theta) \;=\; \frac{1}{2n+1}\Big\{&(n-m+1)(n-m+2)P_{n+1}^{m-1}(\cos\theta) \\ &-(n+m)(n+m-1)P_{n-1}^{m-1}(\cos\theta)\Big\},\end{aligned} \tag{58}$$

where $-n \le m \le n$. We deduce from (56), (57), (58), (22) and the first part of (24) that

$$r\cos\theta\, \mathcal{O}_n^m(\boldsymbol{x}) = \frac{1}{2n+1}\left\{(n+m)(n-m)\,\mathcal{O}_{n-1}^m(\boldsymbol{x}) + r^2\,\mathcal{O}_{n+1}^m(\boldsymbol{x})\right\}, \tag{56$'$}$$

$$r\sin\theta\, e^{\mathrm{i}\phi}\, \mathcal{O}_n^m(\boldsymbol{x}) = \frac{\mathrm{i}}{2n+1}\left\{(n-m)(n-m-1)\,\mathcal{O}_{n-1}^{m+1}(\boldsymbol{x}) - r^2\,\mathcal{O}_{n+1}^{m+1}(\boldsymbol{x})\right\}, \tag{57$'$}$$

and

$$r\sin\theta\, e^{-\mathrm{i}\phi}\, \mathcal{O}_n^m(\boldsymbol{x}) = \frac{\mathrm{i}}{2n+1}\left\{(n+m)(n+m-1)\,\mathcal{O}_{n-1}^{m-1}(\boldsymbol{x}) - r^2\,\mathcal{O}_{n+1}^{m-1}(\boldsymbol{x})\right\}, \tag{58$'$}$$

where $\mathcal{O}_\ell^k(\boldsymbol{x})$ is defined to be zero for all integers k and ℓ that satisfy $|k| > \ell$.

Then, letting $\boldsymbol{t}$ have spherical polar coordinates $[\rho, \alpha, \beta]$ and $\boldsymbol{x}$ have spherical polar coordinates $[r, \theta, \phi]$, we use the cosine formula

$$|\boldsymbol{x}-\boldsymbol{t}|^2 = r^2 + \rho^2 - 2r\rho\cos\gamma\,, \tag{59}$$

where γ is the angle between vectors $\boldsymbol{x}$ and $\boldsymbol{t}$. Substituting (59) into (54), and recalling that $\mathcal{O}_n^m(\boldsymbol{x})$ is $\mathcal{O}(|\boldsymbol{x}|^{-n-1})$ as $|\boldsymbol{x}| \to \infty$, the terms arising from multiplication by r^2 and ρ^2 are already in the desired form (55), because when $n = j-1$ and $n = j$, we include $\rho^2 A_{nm}\mathcal{O}_n^m(\boldsymbol{x})$ in the $\mathcal{O}\left(|\boldsymbol{x}|^{-j}\right)$ term of (55). The product

$$-2r\rho\cos\gamma\left\{\sum_{n=0}^{j}\sum_{m=-n}^{n} A_{nm}\,\mathcal{O}_n^m(\boldsymbol{x})\right\}, \tag{60}$$

however, gives rise to terms that require further attention. By substituting the identity

$$\begin{aligned}\cos\gamma &= \cos\theta\cos\alpha + \sin\theta\sin\alpha\cos(\phi-\beta)\\ &= \cos\theta\cos\alpha + \sin\theta\sin\alpha\left[\frac{e^{\mathrm{i}(\phi-\beta)} + e^{-\mathrm{i}(\phi-\beta)}}{2}\right],\end{aligned} \tag{61}$$

into (60), we obtain a series in which the dependence on $\boldsymbol{x}$ of each term is a linear combination of (56′), (57′), or (58′). Using these last three equations recasts the sum into the required form (55).

Combining the results above, we deduce the fully translated form (55) from the partially translated series (54), where the new coefficients take the values

$$\begin{aligned}U_{nm} &= \rho^2 A_{nm} - \frac{2\rho\cos\alpha}{2n+3}(n+m+1)(n-m+1)A_{n+1,m}\\ &\quad -\frac{\mathrm{i}\,\rho\sin\alpha\,e^{-\mathrm{i}\beta}}{2n+3}(n-m+2)(n-m+1)A_{n+1,m-1}\\ &\quad -\frac{\mathrm{i}\,\rho\sin\alpha\,e^{\mathrm{i}\beta}}{2n+3}(n+m+2)(n+m+1)A_{n+1,m+1},\end{aligned} \tag{62}$$

and

$$\begin{aligned}V_{nm} &= A_{nm} - \frac{2\rho\cos\alpha}{2n-1}A_{n-1,m} + \frac{\mathrm{i}\,\rho\sin\alpha\,e^{-\mathrm{i}\beta}}{2n-1}A_{n-1,m-1}\\ &\quad +\frac{\mathrm{i}\,\rho\sin\alpha\,e^{\mathrm{i}\beta}}{2n-1}A_{n-1,m+1},\end{aligned} \tag{63}$$

where $A_{\ell k}$ is defined to be zero for all integers k and ℓ that satisfy $|k| > \ell$.

7 A binary tree based hierarchical fast evaluator

In this section we outline a simple binary tree based hierarchical fast evaluator for the $(\nu+1)$-harmonic spline

$$s(\boldsymbol{x}) = \sum_{j=1}^{N} d_j\,|\boldsymbol{x}-\boldsymbol{x}_j|^{2\nu-1}. \tag{64}$$

This evaluator is built upon the far field expansions developed in the previous sections. Hierarchical fast evaluators are relatively easy to implement, and are also suitable for nonuniform distributions of centres. Nonuniform distributions occur in many applications, including surface reconstruction from laser and lidar scans and modeling ore grade from drill hole data. Powell [12] describes a hierarchical fast evaluator for biharmonic splines in $\mathcal{R}^2$.

The key to the fast evaluator is a tree data structure. Each node of the tree corresponds to a rectangular panel in $\mathcal{R}^3$ containing centres/sources. The root node is placed at the top of the tree and is a panel containing all the centres. The relevant information for each node will be stored in a structure containing at least the following items:

- $\boldsymbol{c} \in \mathcal{R}^3$ contains the midpoint of the axis oriented rectangular panel.
- $\boldsymbol{h} \in \mathcal{R}^3$ contains the half side lengths of the panel.
- `child` either contains pointers to two child panels, `child[0]` and `child[1]`, or is `null` if the current panel has no children.
- `leftcent`, `rightcent`: Two integers indicating which centres lie in the panel, their values being the start and end index (plus one) in a final sorted list of centres, which evolves as the tree is created.
- `far_series`: An array containing the coefficients $N_{nm}^{(k)}$ of a far field expansion about the midpoint $\boldsymbol{c}$ of the panel of the form specified in Theorem 4.2. The expansion takes the form

$$r_{\mathcal{T},p}(\boldsymbol{x}) = \sum_{k=0}^{\nu} |\boldsymbol{x}-\boldsymbol{c}|^{2\nu-2k} \sum_{n=0}^{p-2k} \sum_{m=-n}^{n} N_{nm}^{(k)}\, \mathcal{O}_n^m(\boldsymbol{x}-\boldsymbol{c}), \tag{65}$$

  which is an approximation to

$$s_{\mathcal{T}}(\boldsymbol{x}) = \sum_{j:\boldsymbol{x}_j \in \mathcal{T}} d_j\, |\boldsymbol{x}-\boldsymbol{x}_j|^{2\nu-1},$$

  where $\mathcal{T} \subset \mathcal{R}^3$ is the current panel. According to Theorem 4.2, the error $|s_{\mathcal{T}}(\boldsymbol{x}) - r_{\mathcal{T},p}(\boldsymbol{x})|$ is $\mathcal{O}\left(|\boldsymbol{x}-\boldsymbol{c}|^{(2\nu-1)-(p+1)}\right)$ as $|\boldsymbol{x}| \to \infty$.
- `use_at_dist_sq`: A vector containing entries for some selected positive integers q not exceeding p. The entry corresponding to q is the square of the distance from $\boldsymbol{c}$ at which the truncated series $r_{\mathcal{T},q}$ is estimated to achieve the per panel absolute accuracy δ, when used as an approximation to $s_{\mathcal{T}}(\boldsymbol{x})$. The

per panel accuracy, and its estimation, are described later. Given the desired accuracy δ and $\boldsymbol{x}$, these entries may reduce the work of employing the approximation $r_{\mathcal{T},p}(\boldsymbol{x}) \approx s_{\mathcal{T}}(\boldsymbol{x})$, by allowing the use of the approximation $r_{\mathcal{T},q}$ with $q < p$. This saving is made in the evaluation procedure that is given later.

A hierarchical fast evaluator for polyharmonic splines in $\mathcal{R}^3$

INPUT

Input the set of N nodes $\mathcal{X} = \{\boldsymbol{x}_j\}$, the corresponding coefficients $\{d_j\}$ of $|\boldsymbol{x} - \boldsymbol{x}_j|^{2\nu-1}$, and the expansion order p. Also input the desired absolute accuracy ϵ and a positive integer `threshhold` controlling the splitting of panels. Only panels with more than $2 *$ `threshhold` points will become parents, and all panels created will contain at least `threshhold` centres.

DOWNWARD SWEEP CREATING A BINARY TREE OF SOURCE PANELS

Step 1. Find the smallest axis oriented closed rectangular box containing all the centres. This is the root panel at `level` 0. Associate with this box the full list of centres.

Step 2 For `level`$= 0, 1, 2, \ldots$ in turn.
Work though all the panels at the `level`. Split all of those containing more than `2*threshhold` centres into two child panels, each centre being assigned to just one of the children. Usually child panels are created by splitting the parent panel at the midpoint of its longest side, and assigning the centres of each piece to the appropriate child. However, if this procedure would give a child panel with fewer than `threshhold` points, then the plane boundary between the child panels is moved the minimum amount, so that exactly `threshhold` points are allocated to one of the children. Child panels are then shrunk to become the smallest axis oriented rectangular boxes containing all their centres. After shrinking, the vectors $\boldsymbol{c}$ and `h` are calculated and stored.

The procedure generates a binary tree of `total` panels where `total` lies in the interval $[(N - \texttt{threshold})/\texttt{threshhold}, (2 * N - \texttt{threshhold})/\texttt{threshhold}]$. Details of the method in the $\mathcal{R}^2$ case can be found in Powell [12].

UPWARD SWEEP CALCULATING FAR FIELD EXPANSIONS

Work up the tree level by level, ending at level 1 where there are two panels. For each panel $\mathcal{T}$ at the current `level`:

Step 1 Calculate the far field series (65) for the panel. That is calculate the coefficients for the far field approximation $r_{\mathcal{T}} \approx s_{\mathcal{T}}$. If the panel is childless, the coefficients are given by the formula

$$N_{nm}^{(k)} = (-1)^n \, \alpha_{\nu,k}(n+2k) \sum_{j:\boldsymbol{x}_j \in \mathcal{T}} d_j \, |\boldsymbol{x}_j - \boldsymbol{c}|^{2k} \, \mathcal{I}_n^{-m}(\boldsymbol{x}_j - \boldsymbol{c}),$$

as in Theorem 4.2. Otherwise, if the panel is a parent, then perform the calculation by the more efficient of direct calculation or translation of child panel coefficients, as described in section 6.

Step 2 Calculate `use_at_dist_sq` entries for the panel, the procedure in Section 7.1 being recommended.

EVALUATION AT A POINT $\boldsymbol{x}$

The evaluation of the RBF at a point $\boldsymbol{x}$ can be performed by recursive code. Such a code descends the tree from level one . The approximation associated with a panel is used when it gives sufficient accuracy, but otherwise better accuracy is achieved by descending to the children. Details of such an evaluation algorithm, including `C++` like pseudo code, are given in [3]. Instead we prefer a stack based code that avoids the use of recursive function calls.

Initialize the stack by setting `stack`[0] and `stack`[1] equal to the two panels of the binary tree at level one. Set `count`$=1$ and `val`$=0.0$.

while `count` ≥ 0
 $\mathcal{T}$ = `stack[count]`.
 Calculate the square of the distance from $\boldsymbol{x}$ to the midpoint $\boldsymbol{c}$ of $\mathcal{T}$.
 Compare with the entry in `use_at_dist_sq` corresponding to using the full series (65).
 if (The longest truncated series gives sufficient accuracy) **then**
  Derive an efficient length of series to use from the `use_at_dist_sq` entries.
  Calculate the approximation to $s_{\mathcal{T}}(\boldsymbol{x})$ and add it to `val`.
  Decrease `count` by one.
 else if ($\mathcal{T}$ is childless)
  Calculate $s_{\mathcal{T}}(\boldsymbol{x})$ directly and add it to `val`.
  Decrease `count` by one.
 else (Descent to the children of $\mathcal{T}$)
  Assign the two child panels of $\mathcal{T}$ to `stack[count]` and `stack[count+1]`.

Increase `count` by one.
end if
end while

On exit `val` is the required approximation to $s(\boldsymbol{x})$.

It is easy to see that, throughout this evaluation, the number of elements in the stack is at most the number of levels in the binary tree.

7.1 An adaptive method for accuracy estimation

The error bound (43) of Theorem 4.2 tends to be highly pessimistic when most of the distances $|\boldsymbol{x}_j|$, $j = 1, 2, \ldots, N$ are much less than R. Therefore, in the numerical tests that are reported later, the `use_at_dist_sq` entries are calculated by the following adaptive method.

Consider a panel $\mathcal{T}$ with midpoint $\boldsymbol{c}$ and radius $R = \max\{|\boldsymbol{x}_j - \boldsymbol{c}| : \boldsymbol{x}_j \in \mathcal{T}\}$. The truncated series $r_{\mathcal{T},q}(\boldsymbol{x})$ of (65), $0 < q \le p$, is used as an approximation to the function

$$\begin{aligned} s_{\mathcal{T}}(\boldsymbol{x}) &= \sum_{j:\boldsymbol{x}_j \in \mathcal{T}} d_j\, |\boldsymbol{x} - \boldsymbol{x}_j|^{2\nu-1} \\ &= \sum_{k=0}^{\nu} |\boldsymbol{x} - \boldsymbol{c}|^{2\nu-2k} \sum_{n=0}^{\infty} \sum_{m=-n}^{n} N_{nm}^{(k)}\, \mathcal{O}_n^m(\boldsymbol{x} - \boldsymbol{c}), \quad |\boldsymbol{x} - \boldsymbol{c}| > R. \end{aligned}$$

Denoting $|\boldsymbol{x} - \boldsymbol{c}|$ by r, it follows from the homogeneity of the O_n^m functions that the error $|s_{\mathcal{T}}(\boldsymbol{x}) - r_{\mathcal{T},q}(\boldsymbol{x})|$ is bounded by

$$\sum_{k=0}^{\nu} r^{2\nu-2k} \sum_{n=q+1-2k}^{\infty} \sum_{m=-n}^{n} |N_{nm}^{(k)}|\, \Omega_{nm}\, r^{-n-1},$$

where Ω_{nm} is the number $\max\{|\mathcal{O}_n^m(\boldsymbol{x})| : |\boldsymbol{x}| = 1\}$. We approximate this infinite sum by

$$E_{\mathcal{T},q}(r) = \sum_{k=0}^{\nu} r^{2\nu-2k} \sum_{n=q+1-2k}^{p+3-2k} \sum_{m=-n}^{n} |N_{nm}^{(k)}|\, \Omega_{nm}\, r^{-n-1}, \quad r > R, \tag{66}$$

and use this as our estimate of $|s_{\mathcal{T}}(\boldsymbol{x}) - r_{\mathcal{T},q}(\boldsymbol{x})|$, $0 < q \le p$. It requires the calculation initially of three *safety layers* of coefficients, namely the coefficients $N_{nm}^{(k)}$ of the terms for $p - 2k < n \le p + 3 - 2k$. As with adaptive quadrature rules the error estimation method described above could fail for contrived input data. However, in our computational experience, it has never failed. We also note that the error estimate has the desirable property of being more conservative for smaller values of q, as then it uses many *safety layers* of coefficients $N_{nm}^{(k)}$.

Now given a desired overall absolute error ϵ we choose to partially compensate for the number of levels by setting the per panel error tolerance as $\delta = \epsilon / \max(0.3 * \log(\texttt{numbcent}/\texttt{threshold}), 1.0)$. This heuristic has worked well in our numerical experiments. Finding an entry of the `use_at_dist_sq` vector involves solving the equation $E_{\mathcal{T},q}(r) = \delta$ for r, which is easily done by Newton iteration, because the dependence on r of (66) has the form $\sum_{j=2\nu-p-4}^{2\nu-q-2} A_j\, r^j$, $r > R$. Indeed the convexity of $E_{\mathcal{T},q}(r)$ as a function of r implies that this method converges monotonically after the first iteration.

7.2 Exploiting symmetry

In implementing the above code, storage requirements and operation counts can be reduced substantially by exploiting symmetry. We consider the usual case in which all the coefficients d_j of the spline (64) are real. Then (42) and the second part of (21) imply the symmetry

$$N_{n,-m}^{(k)} = (-1)^m \overline{N_{nm}^{(k)}}.$$

It follows that

$$N_{nm}^{(k)} \mathcal{O}_n^m(\boldsymbol{x}) + N_{n,-m}^{(k)} \mathcal{O}_n^{-m}(\boldsymbol{x}) = 2\Re \left\{ N_{nm}^{(k)} \mathcal{O}_n^m(\boldsymbol{x}) \right\}, \quad m > 0,$$

and that $N_{n0}^{(k)}$ and $\mathcal{O}_n^0(\boldsymbol{x})$ are real. Thus the truncated far field expansion (65) can be rewritten in the form

$$r_{\mathcal{T},p}(\boldsymbol{x}) = \sum_{k=0}^{\nu} |\boldsymbol{x}-\boldsymbol{c}|^{2\nu-2k} \sum_{n=0}^{p-2k} \left\{ N_{n0}^{(k)}\, \mathcal{O}_n^0(\boldsymbol{x}-\boldsymbol{c}) + 2\Re \left(\sum_{m=1}^{n} N_{nm}^{(k)}\, \mathcal{O}_n^m(\boldsymbol{x}-\boldsymbol{c}) \right) \right\}.$$

Using this form approximately halves the coefficient storage requirements of the fast evaluator. It also lowers significantly the computational cost of forming and evaluating the series expansions.

7.3 Computing the inner and outer functions

The formation of the far field series, directly or indirectly, requires the calculation of inner functions, and thus of associated Legendre functions. One way to formulate the calculation of the latter functions efficiently and stably is given in Press,

	Achieved accuracy		Fast eval time		Direct
N	$\tau = 10^{-3}$	$\tau = 10^{-6}$	$\tau = 10^{-3}$	$\tau = 10^{-6}$	time
$4,000$	$2.52(-4)$	$2.90(-7)$	$1.36(-1)$	$2.47(-1)$	$2.68(-1)$
$8,000$	$3.86(-4)$	$5.26(-7)$	$3.30(-1)$	$7.09(-1)$	$1.05(0)$
$16,000$	$3.72(-4)$	$3.98(-7)$	$8.06(-1)$	$1.89(0)$	$4.27(0)$
$32,000$	$3.83(-4)$	$4.47(-7)$	$1.67(0)$	$4.45(0)$	$2.20(1)$
$64,000$	$3.75(-4)$	$5.31(-7)$	$3.66(0)$	$1.08(1)$	$9.06(1)$
$128,000$	$3.72(-4)$	$4.57(-7)$	$8.25(0)$	$2.56(1)$	$3.90(2)$

Table 1: Time in seconds to compute a matrix-vector product – centres uniformly distributed within a cube.

Flannery, Teukolsky and Vetterling [13]. They combine a variant of the recurrence relation (56) with the initial value

$$P_m^m(u) = (-1)^m (2m-1)!! \left(1-u^2\right)^{m/2}, \quad u = \cos\theta.$$

Furthermore, the first part of expression (24) shows that the associated Legendre functions $P_n^m(u)$ are also required when formula (65) is used for the evaluation of far field expansions, m and n being from the intervals $[-n, n]$ and $[0, p]$ respectively. Therefore the work of evaluating a truncated far field expansion (65) at a single point $\boldsymbol{x}$ is $\mathcal{O}\left((\nu+1)p^2\right)$ flops. If, however, we find from `use_at_dist_sq` that (65) can be replaced by $r_{\mathcal{T},q}(\boldsymbol{x})$ with $q < p$, then the amount of computation is reduced to $\mathcal{O}((\nu+1)q^2)$ flops.

The evaluation formula (65) exploits polyharmonicity to gain speed. Since the outer harmonic function $\mathcal{O}_n^m(\boldsymbol{x}-\boldsymbol{c})$ is a polynomial of degree n divided by $|\boldsymbol{x}-\boldsymbol{c}|^{2n+1}$, there is an alternative evaluation formula consisting of a single polynomial of degree $2p+2\nu$ in $\boldsymbol{x}$ divided by $|\boldsymbol{x}-\boldsymbol{c}|^{2p+1}$. It would be less efficient than the given method for calculating $r_{\mathcal{T},p}(\boldsymbol{x})$, because it would require $\mathcal{O}(\left(p+\nu\right)^3)$ flops instead of $\mathcal{O}\left((\nu+1)p^2\right)$ flops.

7.4 Numerical experiments

We now present some numerical results obtained by a C implementation of the algorithm above. A very similar C implementation was used for the surface reconstructions reported in Carr et al [4]. In that paper the hierarchical fast evaluation technique was coupled with domain decomposition and a greedy algorithm to fit surfaces to meshes and lidar scans with hundreds of thousands of points.

Our numerical experiments here concern the matrix vector product task, that

N	Achieved accuracy		Fast eval time		Direct time
	$\tau = 10^{-3}$	$\tau = 10^{-6}$	$\tau = 10^{-3}$	$\tau = 10^{-6}$	
4,000	3.44(−4)	3.97(−7)	1.39(−1)	2.47(−1)	2.68(−1)
8,000	3.24(−4)	4.15(−7)	3.02(−1)	6.11(−1)	1.05(0)
16,000	3.26(−4)	3.90(−7)	6.77(−1)	1.47(0)	4.27(0)
32,000	3.05(−4)	4.09(−7)	1.44(0)	3.33(0)	2.20(1)
64,000	2.95(−4)	3.95(−7)	3.11(0)	7.45(0)	9.06(1)
128,000	2.65(−4)	3.83(−7)	6.78(0)	1.66(1)	3.90(2)

Table 2: Time in seconds to compute a matrix-vector product – centres uniformly distributed on the sphere $\mathcal{S}^2$.

is the fast evaluation of the biharmonic spline

$$s(\boldsymbol{x}) = \sum_{j=1}^{N} \lambda_j \, |\boldsymbol{x} - \boldsymbol{x}_j|,$$

at all the centres $\boldsymbol{x}_i$.

Table 1 shows times in seconds for computing matrix vector products for biharmonic splines with N centres distributed uniformly at random in the cube $[-1,1]^3$. The coefficients λ_j were chosen uniformly at random from $[-1,1]$. A timing in the table is the average over 10 replications. In conducting the experiments we compensated for the increasing infinity norm of the spline s as N increased by calculating to given relative accuracy. Thus, given a desired relative accuracy τ, we first computed $\|s\|_\infty = \max_{1\le j\le N} |s(\boldsymbol{x}_j)|$, and then we picked the absolute accuracy $\epsilon = \tau\|s\|_\infty$ for the fast evaluation algorithm. Similarly, letting g be the vector of values computed by the fast evaluation algorithm, the relative accuracy is $\|s - g\|_\infty / \|s\|_\infty$. The achieved accuracy reported in the table is the average relative accuracy over the 10 replications. In no replication did the achieved accuracy exceed the desired relative accuracy τ. The numerical experiments were carried out on a generic Athlon XP 2600 personal computer. In the numerical experiments the parameter p of the far field series (65) was chosen as 15, and the parameter `threshhold` controlling the paneling was chosen as 100. An entry of the form $x.yz(b)$ in the table indicates the number $x.yz \times 10^b$. It is clear from the table that the time for approximate evaluation grows at a rate that is substantially slower than N^2.

Analogous computations were carried out for centres distributed uniformly at random on the 2-sphere $\mathcal{S}^2 = \{\boldsymbol{x} \in \mathcal{R}^3 \, : \, |\boldsymbol{x}| = 1\}$. Once more the coefficients were chosen uniformly at random from $[-1,1]$. The results of these computations are recorded in Table 2.

We note that the timings for the fast method improve considerably in this points on a two dimensional manifold situation. One reason is the curse of dimensionality, which in our case implies that random points are in a sense closer together within a cube than on a two dimensional manifold. For example in a uniform partitioning of a cube into subcubes a typical subcube has 26 neighbours, while in a uniform tiling of a square into subsquares a typical subsquare has 8 neighbours. Thus there is a tendency for more centres to be relatively far away from each centre in the two dimensional manifold situation, which allows the hierarchical evaluator to perform better.

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Appendix A: Outer to inner and inner to inner translation formulae

This appendix gives some mathematics that would be required if one developed the hierarchical code of section 7 into a full fast multipole code. Specifically both outer series about $\boldsymbol{t}$ and inner series about $\boldsymbol{t}$ are translated into inner series about $\mathbf{0}$.

There are two reasons for describing a hierarchical code rather than a full fast multipole code in section 7. Firstly, a hierarchical code is an order of magnitude simpler to write. Secondly, in our scattered data applications, our experience comparing the hierarchical code with an octtree based full fast multipole code is that the latter will only perform significantly better for very large numbers of centres and evaluation points.

The difference between a hierarchical code and a full fast multipole code is that in a full fast multipole code the far field outer expansions are converted to inner expansions in a pass descending down a tree of evaluation panels. Typically, when the distributions of centres and evaluation points are nearly uniform, to achieve accuracy ϵ in a matrix vector product a hierarchical 3D code would require $\mathcal{O}\left((1+|\log\epsilon|)^2 N\log N\right)$ flops while a full fast multipole code would require only $\mathcal{O}\left((1+|\log\epsilon|)^2 N\right)$ flops. Here the factors $(1+|\log\epsilon|)^2$ come from the polyharmonic series, $\mathcal{O}\left((\nu+1)(1+|\log\epsilon|)^2\right)$ terms being sufficient to give the required accuracy. The additional factor $\log N$ in the estimate for the hierarchical code is due to using far field series from $\log N$ different levels for each evaluation, which is avoided in the full fast multipole code by collecting the contributions of all panels sufficiently far from the current evaluation panel into a single inner series (polynomial). Thus, as the number N of centres becomes very large, a full fast multipole code will do better than a hierarchical code. See [3] for details of the difference between hierarchical and full multipole codes. A fast multipole code for biharmonic splines in $\mathcal{R}^2$ is described in [2].

To see why outer to inner conversion can be useful think of a target, or evaluation panel $\mathcal{E}$, at a fine scale. Shift the origin so that this target panel is centered at $\mathbf{0}$. Then the outer series of a distant source panel $\mathcal{T}$, centered at $\boldsymbol{t}$, is very smooth everywhere in the target panel $\mathcal{E}$. Therefore it can be approximated within $\mathcal{E}$ by an inner series valid for small $|\boldsymbol{x}|$. Since the form of the inner series remains constant as the source panel $\mathcal{T}$ changes, we can sum and approximate the influence within $\mathcal{E}$ of many distant panels with a single truncated inner series.

We now discuss some of the details needed to implement the above idea. Epton and Dembart [5] give the outer to inner translation formula

$$\begin{aligned} s(\boldsymbol{x}) &= \sum_{n=0}^{k} \sum_{m=-n}^{n} D_n^m \, \mathcal{O}_n^{-m}(\boldsymbol{x}-\boldsymbol{t}) \\ &= \sum_{\ell=0}^{\infty} \sum_{j=-\ell}^{\ell} E_\ell^j \, \mathcal{I}_\ell^j(\boldsymbol{x}) \,, \quad |\boldsymbol{x}| < |\boldsymbol{t}|, \end{aligned}$$

where

$$E_\ell^j = \sum_{n=0}^{k} \sum_{m=-n}^{n} D_n^m \, \mathcal{O}_{n+\ell}^{-m-j}(-\boldsymbol{t}) \,.$$

When $|\boldsymbol{t}|$ is sufficiently large, we approximate the truncated outer expansion about $\boldsymbol{t} \neq \mathbf{0}$

$$h_p(\boldsymbol{x}) = \sum_{k=0}^{\nu} |\boldsymbol{x}-\boldsymbol{t}|^{2\nu-2k} \sum_{n=0}^{p-2k} \sum_{m=-n}^{n} M_{nm}^{(k)} \, \mathcal{O}_n^m(\boldsymbol{x}-\boldsymbol{t}), \tag{67}$$

by a polynomial of the form

$$\hat{g}_q(\boldsymbol{x}) = \sum_{k=0}^{\nu} |\boldsymbol{x}-\boldsymbol{t}|^{2\nu-2k} \sum_{n=0}^{q} \sum_{m=-n}^{n} \widetilde{M}_{nm}^{(k)} \, \mathcal{I}_n^m(\boldsymbol{x}), \quad |\boldsymbol{x}| < |\boldsymbol{t}|, \tag{68}$$

for a suitable choice of q, the coefficients $\widetilde{M}_{nm}^{(k)}$ being derived from the above definition of E_ℓ^j. Recalling that $\mathcal{I}_n^m(\boldsymbol{x})$ is a homogenous polynomial of degree n, we see that the term multiplying $|\boldsymbol{x}-\boldsymbol{t}|^{2\nu-2k}$ in (68) is a Taylor polynomial approximation to the corresponding term in (67). Hence $\hat{g}_q$ has the property $|h_p(\boldsymbol{x}) - \hat{g}_q(\boldsymbol{x})| =$

$\mathcal{O}\left(|\boldsymbol{x}|^{q+1}\right)$ as $\boldsymbol{x} \to \mathbf{0}$. We are going to deduce from $\hat{g}_q$ a Taylor polynomial approximation to h_p, that retains the $\mathcal{O}\left(|\boldsymbol{x}|^{q+1}\right)$ accuracy, and that has coefficients that include all the dependencies on $\boldsymbol{t}$. A similar task was addressed in section 6, expression (53) being analogous to (68). Therefore now it is sufficient to express the product

$$q(\boldsymbol{x}) = |\boldsymbol{x}-\boldsymbol{t}|^2 \sum_{n=0}^{q} \sum_{m=-n}^{n} A_{nm}\, \mathcal{I}_n^m(\boldsymbol{x}), \tag{69}$$

in the form

$$\sum_{n=0}^{q+1} \sum_{m=-n}^{n} U_{nm}\, \mathcal{I}_n^m(\boldsymbol{x}) + |\boldsymbol{x}|^2 \sum_{n=0}^{q} \sum_{m=-n}^{n} V_{nm}\, \mathcal{I}_n^m(\boldsymbol{x}). \tag{70}$$

This construction can be applied repeatedly to the $(\nu+1)$-harmonic polynomial (68), discarding the $\mathcal{O}\left(|\boldsymbol{x}|^{q+1}\right)$ and $\mathcal{O}\left(|\boldsymbol{x}|^{q+2}\right)$ terms of expression (70), in order to obtain the required Taylor polynomial.

Let $\boldsymbol{x}$ and $\boldsymbol{t}$ be as in the paragraph that includes equations (59) and (61). We recall the identity

$$|\boldsymbol{x}-\boldsymbol{t}|^2 = r^2 + \rho^2 - 2r\rho \left\{ \cos\theta\cos\alpha + \sin\theta\sin\alpha \left[\frac{e^{\mathrm{i}(\phi-\beta)} + e^{-\mathrm{i}(\phi-\beta)}}{2} \right] \right\}.$$

Moreover we deduce from (56), (57), (58), (23) and the second part of (24) that

$$r\cos\theta\, \mathcal{I}_n^m(\boldsymbol{x}) = \frac{-1}{2n+1} \left\{ (n-m+1)(n+m+1)\, \mathcal{I}_{n+1}^m(\boldsymbol{x}) + r^2\, \mathcal{I}_{n-1}^m(\boldsymbol{x}) \right\}, \tag{56''}$$

$$r\sin\theta\, e^{\mathrm{i}\phi}\, \mathcal{I}_n^m(\boldsymbol{x}) = \frac{\mathrm{i}}{2n+1} \left\{ r^2\, \mathcal{I}_{n-1}^{m+1}(\boldsymbol{x}) - (n+m+2)(n+m+1)\, \mathcal{I}_{n+1}^{m+1}(\boldsymbol{x}) \right\}, \tag{57''}$$

and

$$r\sin\theta\, e^{-\mathrm{i}\phi}\, \mathcal{I}_n^m(\boldsymbol{x}) = \frac{\mathrm{i}}{2n+1} \left\{ r^2\, \mathcal{I}_{n-1}^{m-1}(\boldsymbol{x}) - (n-m+1)(n-m+2)\, \mathcal{I}_{n+1}^{m-1}(\boldsymbol{x}) \right\}. \tag{58''}$$

It follows that the coefficients of the form (70) take the values

$$\begin{aligned} U_{nm} \;=\; & \rho^2 A_{nm} + \frac{2\rho\cos\alpha}{2n-1}(n-m)(n+m)A_{n-1,m} \\ & + \frac{\mathrm{i}\,\rho\sin\alpha e^{-\mathrm{i}\beta}}{2n-1}(n+m)(n+m-1)A_{n-1,m-1} \\ & + \frac{\mathrm{i}\,\rho\sin\alpha e^{\mathrm{i}\beta}}{2n-1}(n-m-1)(n-m)A_{n-1,m+1}, \end{aligned} \tag{71}$$

and

$$
\begin{aligned}
V_{nm} \;=\; & A_{nm} + \frac{2\rho\cos\alpha}{2n+3}A_{n+1,m} - \frac{\mathrm{i}\,\rho\sin\alpha\, e^{-\mathrm{i}\beta}}{2n+3}A_{n+1,m-1} \\
& - \frac{\mathrm{i}\,\rho\sin\alpha\, e^{\mathrm{i}\beta}}{2n+3}A_{n+1,m+1},
\end{aligned}
\tag{72}
$$

where $A_{\ell k}$ is defined to be zero for all integers k and ℓ that satisfy $|k| > \ell$.

Inner series about $\boldsymbol{t}$ can be translated to inner series about $\mathbf{0}$, by employing the formula [5],

$$
h(\boldsymbol{x}) = \sum_{n=0}^{q}\sum_{m=-n}^{n} E_{nm}\,\mathcal{I}_n^m(\boldsymbol{x}-\boldsymbol{t}) = \sum_{\ell=0}^{q}\sum_{k=-\ell}^{\ell} F_{\ell k}\,\mathcal{I}_\ell^k(\boldsymbol{x}),
$$

where

$$
F_{\ell k} = \sum_{n=\ell}^{q}\sum_{m=-n}^{n} E_{nm}\,\mathcal{I}_{n-\ell}^{m-k}(-\boldsymbol{t}).
$$

Combining this with the expressions (69), (70), (71) and (72) above allows the translation of an inner series, a $(\nu+1)$-harmonic polynomial, of the form

$$
\sum_{k=0}^{\nu} |\boldsymbol{x}-\boldsymbol{t}|^{2\nu-2k} \sum_{n=0}^{q+2k}\sum_{m=-n}^{n} \widetilde{M}_{nm}^{(k)}\,\mathcal{I}_n^m(\boldsymbol{x}-\boldsymbol{t}),
$$

into an inner series

$$
\sum_{k=0}^{\nu} |\boldsymbol{x}|^{2\nu-2k} \sum_{n=0}^{q+2k}\sum_{m=-n}^{n} M_{nm}^{(k)}\,\mathcal{I}_n^m(\boldsymbol{x}),
$$

centered at $\mathbf{0}$. This inner to inner translation can be used to recenter inner expansions associated with parent panels in order to initialize the inner expansions of children, in a fast multipole implementation.

As was discussed in section 7 for the outer series, in the usual case when the coefficients d_j in the spline (64) are real, symmetry can be exploited to allow carrying only the terms with $m \ge 0$ in a truncated inner series.