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Kernel Based Quadrature on Spheres and Other Homogeneous Spaces

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Abstract

Quadrature formulas for spheres, the rotation group, and other compact, homogeneous manifolds are important in a number of applications and have been the subject of recent research. The main purpose of this paper is to study coordinate independent quadrature (or cubature) formulas associated with certain classes of positive definite and conditionally positive definite kernels that are invariant under the group action of the homogeneous manifold. In particular, we show that these formulas are accurate – optimally so in many cases – and stable under an increasing number of nodes and in the presence of noise, provided the set X of quadrature nodes is quasi-uniform. The stability results are new in all cases. In addition, we may use these quadrature formulas to obtain similar formulas for manifolds diffeomorphic to $\mathbb{S}^n$, oblate spheroids for instance. The weights are obtained by solving a single linear system. For $\mathbb{S}^2$, and the restricted thin plate spline kernel $r^2 \log r$, these weights can be computed for two-thirds of a million nodes, using a preconditioned iterative technique introduced by us.

1 Introduction

Quadrature formulas for spheres, the rotation group, and other compact, homogeneous manifolds are important in many applications and have been the subject of recent research [9, 17–19, 28, 33, 34, 36]. In particular, numerical integration on spheres is an indispensable tool in applications ranging from spectral analysis of experimental data to boundary integral methods for solving partial differential equations [1, Chapter 5 and 6]. Often these applications demand quadrature formulas that are accurate, computationally cheap to generate, stable in the presence of noise, and flexible in terms of locations where data is given. The generation and analysis of such formulas are the focus of this paper.

The quadrature (or cubature) formulas we study are associated with certain classes of positive definite and conditionally positive definite kernels that are invariant under the group action of the homogeneous manifold. The invariance of these kernels leads to simple, easy to construct linear systems that determine the weights. In particular for $\mathbb{S}^2$, techniques that we have developed in [12] allow us to solve these systems when the number of nodes varies over a substantial range, from a few thousand to two-thirds of a million. Numerical tests validating this are described in section 5.

In the course of studying the accuracy of these formulas for various spaces, we obtain new error estimates for interpolation/reproduction problems on two-point homogeneous manifolds. First, for a general such manifold, the estimates hold for $f \in W_2^m(\mathbb{M})$, which is the reproducing Hilbert space (native space) of the kernel. Second, for spheres and real projective spaces, the estimates apply to $f \in W_2^\mu$, with $n/2 < \mu \leq m$. Thus the estimates allow an "escape" from the native space, in the sense that they are for functions *not* smooth enough to be in that space.

The quadrature formulas developed here are for the general setting of a compact, homogeneous, n-dimensional manifold $\mathbb{M}$ that is equipped with a group invariant Riemannian metric g_{ij} and its associated invariant measure $d\mu(x) = \sqrt{\det(g_{ij}(x))}dx$; namely,

$$\int_{\mathbb{M}} f(x)d\mu(x) \doteq \sum_{\xi \in X} c_\xi f(\xi) =: Q(f), \ f \in C(\mathbb{M}). \tag{1.1}$$

The finite set $X \subset \mathbb{M}$ is composed of centers/nodes, and the weights $\{c_\xi\}_{\xi \in X}$ are chosen so that Q integrates exactly a given finite dimensional space of continuous functions, V.

In the case of $\mathbb{S}^n$ and $SO(3)$, popular choices for V are spaces of spherical harmonics [18, 28, 33, 34], and Wigner D-functions [19]. Work also has been done on compact two-point homogeneous manifolds [6] and on general compact homogeneous manifolds [36], with V being chosen to be a set of eigenfunctions of a manifold's Laplace-Beltrami operator. We will use the term *polynomial quadrature* for methods that integrate such spaces exactly; this is because, for spheres and a few other spaces, V consists of restrictions of harmonic polynomials.

The quadrature methods developed here are *kernel* methods; they use a space V consisting of linear combinations of kernels. In [42], Sommariva and Womersley used spaces of rotationally invariant radial basis functions (RBFs) and spherical basis functions (SBFs) to derive a linear system of equations for the weights c_ξ. However, neither accuracy, control over the size of the weights, nor stability was addressed in [42]. In this paper these and other issues are dealt with employing recent results developed by us in [12, 21, 22].

There are situations where the manifold $\mathbb{M}$ involved is *not* a homogeneous space, but quadrature formulas can still be obtained. If $\mathbb{M}$ is diffeomorphic to a homogeneous space, then it is possible to obtain quadrature weights for $\mathbb{M}$ from the ones for the corresponding homogeneous space. In section 6, we will show how this can be done for $\mathbb{S}^n$. We will then apply this to the specific case where $\mathbb{M}$ is an oblate spheroid (e.g., earth with flattening accounted for), which is of course diffeomorphic to $\mathbb{S}^2$.

Accuracy is measured in terms of the mesh norm h, which is defined in section 2. All the kernels we deal with are associated with a Sobolev space W_2^m, for some m in $\mathbb{N}$. Previous error estimates for quadrature with positive definite kernels on $\mathbb{S}^2$ were given in [28]. For the general case of a homogeneous manifold, the error we obtained is $\mathcal{O}(h^m)$, for functions in W_2^m. However, on $\mathbb{S}^n$ or $SO(3)$, we get even better rates, in fact optimal: if a function is in C^{2m}, then the order is $\mathcal{O}(h^{2m})$. For example, the thin-plate spline kernel restricted to $\mathbb{S}^2$ (i.e., surface spline) has $m = 2$, so, for a function in $C^4(\mathbb{S}^2)$, the error would be $\mathcal{O}(h^4)$.

These quadrature formulas are stable both under an increase in the number of points and in the presence of noise. If the number of points is increased, then the norm of the quadrature operator remains uniformly bounded, as long as the level of quasi-uniformity is maintained. Thus there is no oscillatory "Runge phenomenon." To examine the effect of noise, we assume the measured function values differ from the actual ones by independent, identically distributed, zero mean random variables. Under these conditions, the standard deviation of the quadrature formula decreases as $\mathcal{O}(N^{-1/2})$.

The paper is organized this way. Section 2 begins with a brief discussion of positive definite/conditionally positive definite kernels, notation, and, in section 2.1, interpolation. Section 2.2 contains a derivation and discussion of kernel quadrature formulas, with special emphasis on the role played by group invariance of the kernel employed in the formula. In section 2.3, the questions of accuracy and stability mentioned in the introduction are taken up. The results obtained there are aimed at invariant kernels, such as Sobolev and polyharmonic kernels discussed in sections 3 and 4.

Sobolev kernels on a compact manifold are positive definite reproducing kernels for the Sobolev space W_2^m, $m > n/2$. In section 3, we study these in terms of their invariance, interpolation errors, and properties of their Lagrange functions and Lebesgue constants. Finally, in section 3.4 we look at their use in quadrature formulas.

Section 4 is devoted to a very important class of kernels on a compact, two-point homogeneous manifold: the polyharmonic kernels. These kernels, which may be either positive definite or conditionally positive definite, are Green's functions for operators that are polynomials in the the Laplace-Beltrami operator. On spheres, they include restricted surface splines, and on $SO(3)$ similar kernels. All of these are given in terms of simple, explicit formulas. The whole section is a self-contained discussion of these kernels, culminating in their application to quadrature formulas.

The results of various numerical tests that we conducted are discussed in detail in section 5. They were carried out for $\mathbb{M} = \mathbb{S}^2$, in connection with the restricted thin-plate spline. The sets of quasi-uniform nodes were generated via three different, commonly used methods.. The number of nodes employed varied from a few thousand to two-thirds of a million. Weights corresponding to these nodes were computed using a pre-conditioning method developed in [12]. The tests themselves focus on the accuracy and stability of the method, and give excellent results, in agreement with the theory.

In section 6 we discuss ways of using quadrature weights for a compact, homogeneous manifold $\mathbb{M}$ to obtain invariant, coordinate independent weights for manifolds diffeomorphic to $\mathbb{M}$. As an example, we show how to obtain quadrature formulas for oblate spheroids – i.e., the approximate shape of the surface of a planet. Finally, in section 7 we summarize the results of the paper.

2 Interpolation and Quadrature via Kernels

One of the key ingredients in constructing our quadrature formulas on homogeneous manifolds is interpolation via positive definite or conditionally positive definite kernels. However, for kernel interpolation generally we need very little in the way of structure. In fact, we could take our underlying space $\mathbb{M}$ to be a metric space.

Throughout the sequel, we will let $X \subset \mathbb{M}$ denote a finite set of distinct points. In interpolation or approximation problems, points in X are called centers or nodes. Its *mesh norm* (or *fill distance*) $h := \sup_{x \in \mathbb{M}} \mathrm{dist}(x, X)$ measures the density of X in $\mathbb{M}$, while the *separation radius* $q := \frac{1}{2} \inf_{\substack{\xi, \zeta \in X \\ \xi \neq \zeta}} \mathrm{dist}(\xi, \zeta)$ determines the spacing of X. The *mesh ratio* $\rho := h/q$ measures the uniformity of the distribution of X in $\mathbb{M}$.

We say that a continuous kernel $\kappa : \mathbb{M} \times \mathbb{M} \to \mathbb{R}$ is (strictly) *positive definite* on $\mathbb{M}$ if, for every subset $X \subset \mathbb{M}$, the matrix A with entries $A_{\xi,\eta} := \kappa(\xi, \eta)$, $\xi, \eta \in X$, is positive definite.

Conditionally (strictly) positive definite kernels are defined with respect to a finite dimensional space $\Pi := \mathrm{span}\{\psi_k : \mathbb{M} \to \mathbb{R}\}_{k=1}^M$, where the ψ_k's are linearly independent, continuous functions on $\mathbb{M}$. we say that the kernel κ is *conditionally (strictly) positive definite* if for every X and every

nonzero set $\{a_\xi \in \mathbb{R}\}_{\xi \in X}$ such that $\sum_\xi a_\xi \psi_k(\xi) = 0$, $k = 1, \ldots, M$, one has

$$\sum_{\xi, \eta \in X} a_\xi a_\eta \kappa(\xi, \eta) > 0. \tag{2.1}$$

Given a finite set of centers $X \subset \mathbb{M}$, where we let $N := \#X$ be the cardinality of X, we say that Π is *unisolvent* on X if the only function $\psi \in \Pi$ for which $\psi|_X = 0$ is $\psi \equiv 0$. This means that $\{\psi_k|_X\}_{k=1}^m$ is a linearly independent set in $\mathbb{R}^N$. Unisolvancy is a mild condition, but it is necessary in interpolation problems involving conditionally positive definite kernels.

2.1 Interpolation

Positive definite and conditionally positive definite kernels can be used to interpolate a continuous function $f : \mathbb{M} \to \mathbb{R}$, given the data $f|_X$, by means of a function of the form

$$s = \sum_{\xi \in X} a_\xi \kappa(\cdot, \xi) + \sum_{k=1}^M b_k \psi_k, \text{ where } \sum_{\xi \in X} a_\xi \psi_k(\xi) = 0, \ k = 1, \ldots, M. \tag{2.2}$$

We will denote the space of such functions by V_X.

In the case where the kernels are RBFs or SBFs, the space Π is usually taken to be either the polynomials or spherical harmonics with degree less than some fixed number.

We now turn to the interpolation problem. Let $\Psi_k = \psi_k|_X$, $k = 1, \ldots, M$, and define the $N \times M$ matrix $\Psi = [\Psi_1 \ \Psi_2 \cdots \Psi_M]$. In addition, let $a = (a_\xi)_{\xi \in X}$ and $b = (b_1 \ \cdots b_M)^T$. The constraint condition that $\sum_\xi a_\xi \psi_k(\xi) = 0$ can now be stated as $\Psi^T a = 0$. Requiring that s interpolate a function $f \in C(\mathbb{M})$ on X is then $f|_X = s|_X = Aa + \Psi b$, where $A_{\xi, \eta} = \kappa(\xi, \eta)$. Written in matrix form, the interpolation equations are

$$\underbrace{\begin{pmatrix} A & \Psi \\ \Psi^T & 0_{M \times M} \end{pmatrix}}_{\mathbf{A}} \begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} f|_X \\ 0_{m \times 1} \end{pmatrix}. \tag{2.3}$$

Using the constraint condition $\Psi^T a = 0$ and the positivity condition (2.1), one can show that the matrix $\mathbf{A}$ on the left above is invertible [47, Section 8.5]. In addition, the interpolation process reproduces Π; that is, if $f \in \Pi$, then $s = f$. Finally, much is known about how well s fits f. In many cases, the approximation is excellent (cf. [47] and references therein).

In the sequel, we will need the *Lagrange function* centered at $\xi \in X$, $\chi_\xi \in V_X$. We define χ_ξ to be the unique function in V_X that satisfies $\chi_\xi(\eta) = \delta_{\xi, \eta}$; that is, χ_ξ is 1 when $x = \xi$ and 0 when $x = \eta \in X$, $\eta \neq \xi$.

2.2 Quadrature

We will now develop our quadrature formula for a C^∞, n-dimensional Riemannian manifold $\mathbb{M}$ that is a *homogeneous* space for a Lie group $\mathcal{G}$ [46]. This just means that $\mathcal{G}$ acts *transitively* on $\mathbb{M}$: for two points $x, y \in \mathbb{M}$ there is a $\gamma \in \mathcal{G}$ such that $y = \gamma x$. Equivalently, $\mathbb{M}$ is a left coset of $\mathcal{G}$ for a closed subgroup.

$\mathbb{S}^2$ is a homogeneous space for $SO(3)$. In fact, the Lie group $\mathcal{G}$ is a homogeneous space for itself. Thus, $SO(3)$ is its own homogeneous space. Homogeneous spaces also include Stiefel manifolds, Grassmann manifolds an many others. All spheres and projective spaces belong to a special class known as *two-point* homogeneous spaces. Such spaces are characterized by the property that if two

4

pairs of points x, y and x', y' satisfy $\text{dist}(x, y) = \text{dist}(x', y')$, then there is a group element $\gamma \in \mathcal{G}$ such that $x' = \gamma x$ and $y' = \gamma y$. While spheres and projective spaces are compact, there are also non compact spaces: $\mathbb{R}^n$ and certain hyperbolic spaces also belong to the class.

Invariance under $\mathcal{G}$ plays an important here. We will assume throughout that the kernel κ is invariant [45, §I.3.4] (also see [7]), under $\mathcal{G}$. Moreover, we will take $d\mu$ to be the $\mathcal{G}$-invariant measure associated with the Riemannian metric tensor for $\mathbb{M}$ [45, §I.2.3]. Thus, for all $x, y \in \mathbb{M}$, $\gamma \in \mathcal{G}$, and $f \in L_1(\mathbb{M})$ we have

$$\kappa(\gamma x, \gamma y) = \kappa(x, y) \quad \text{and} \quad \int_{\mathbb{M}} f(x) d\mu(x) = \int_{\mathbb{M}} f(\gamma x) d\mu(x). \tag{2.4}$$

In particular, all SBF kernels on $\mathbb{S}^n$, which have the form $\phi(x \cdot y)$, are invariant, as is the standard measure on $\mathbb{S}^n$. The following lemma is a consequence of κ and $d\mu$ being invariant.

Lemma 2.1. *The integral* $J(y) := \int_{\mathbb{M}} \kappa(x, y) d\mu(x)$ *is independent of* y.

Proof. Take $z \in \mathbb{M}$ to be fixed. Because of the group action on $\mathbb{M}$, we may find $\gamma \in \mathcal{G}$ such that $z = \gamma y$. From the invariance of κ under γ, we have $\kappa(x, y) = \kappa(\gamma x, z)$. Hence, $J(y) = \int_{\mathbb{M}} \kappa(\gamma x, z) d\mu(x)$. However, the integral being invariant under $\mathcal{G}$ then yields

$$J(y) = \int_{\mathbb{M}} \kappa(\gamma x, z) d\mu(x) = \int_{\mathbb{M}} \kappa(x, z) d\mu(x) = J(z),$$

which completes the proof. $\qquad\qquad\square$

Since $J(y)$ is independent of y, we may drop y and denote it by J_0, which we will do throughout the sequel. Note that J_0 may be 0. In addition, we define these quantities.

$$\begin{cases} J_k & := & \int_{\mathbb{M}} \psi_k(x) d\mu(x), \ k = 1, \dots, M; \\ J & := & (J_1 \cdots J_M)^T; \\ \mathbf{1} & := & 1|_X. \end{cases}$$

We point out that, for the constant function 1 on $\mathbb{M}$, $\mathbf{1} = 1|_X$ is the column vector in $\mathbb{R}^N$ with all entries equal to 1.

The result below gives a formula for the integral of a function $s \in V_X$ and provides a system of equations that determine the quadrature weights. It follows the one given in [42], with rotational invariance replaced by the invariance under $\mathcal{G}$ proved in Lemma 2.1.

Proposition 2.2. *Let* κ *and* $d\mu$ *satisfy (2.4) and suppose that* c *and* d *are the* $N \times 1$ *and* $M \times 1$ *column vectors that uniquely solve the* $(N + M) \times (N + M)$ *system of equations*

$$Ac + \Psi d = J_0 \mathbf{1} \ \text{and} \ \Psi^T c = J. \tag{2.5}$$

If $s \in V_X$, *then*

$$\int_{\mathbb{M}} s(x) d\mu(x) = c^T s|_X = \sum_{\xi \in X} c_\xi s(\xi) \tag{2.6}$$

In addition, if $\chi_\xi \in V_X$ *is the Lagrange function centered at* ξ, *then we also have*

$$c_\xi = \int_{\mathbb{M}} \chi_\xi(x) d\mu(x) \ \text{and} \ |c_\xi| \le \|\chi_\xi\|_{L_1(\mathbb{M})} \tag{2.7}$$

Proof. Integrating $s(x)$ from (2.2) results in this chain of equations:

$$
\begin{aligned}
\int_{\mathbb{M}} s(x) d\mu(x) &= \sum_{\xi \in X} a_\xi \underbrace{\int_{\mathbb{M}} \kappa(x, \xi) d\mu(x)}_{J_0} + \sum_{k=1}^{M} b_k \underbrace{\int_{\mathbb{M}} \psi_k(x) d\mu(x)}_{J_k} \\
&= J_0 \mathbf{1}^T a + J^T b \\
&= (J_0 \mathbf{1}^T \ \ J^T) \begin{pmatrix} a \\ b \end{pmatrix}.
\end{aligned}
\tag{2.8}
$$

Using (2.3), with $f|_X$ replaced by $s|_X$, together with the invertibility and self adjointness of $\mathbf{A}$, we obtain

$$
(J_0 \mathbf{1}^T \ \ J^T) \begin{pmatrix} a \\ b \end{pmatrix} = \left\{ \underbrace{\mathbf{A}^{-1} \begin{pmatrix} J_0 \mathbf{1} \\ J \end{pmatrix}}_{\begin{pmatrix} c \\ d \end{pmatrix}} \right\}^T \begin{pmatrix} s|_X \\ 0_{m \times 1} \end{pmatrix} = c^T s|_X.
$$

Multiplying $\begin{pmatrix} c \\ d \end{pmatrix}$ by $\mathbf{A}$ and writing out the equations for c, d yields the system (2.5). Combining the two previous equations then yields (2.6). Moreover, from (2.6), with s replaced by χ_ξ and the values of $s|_X$ replaced by those of χ_ξ on the set X, we obtain the formula for c_ξ in (2.7). Finally, the bound on the right in (2.7) follows immediately from the integral formula for c_ξ. $\qquad \square$

As we mentioned earlier, the quadrature formula for $f \in C(\mathbb{M})$ is obtained by replacing f with its interpolant in V_X. To that end, we define the linear functional $Q_{V_X}(f)$ that will play the role of our quadrature operator.

Definition 2.3. *Let $f \in C(\mathbb{M})$ and let $s_f \in V_X$ be the unique interpolant for f, so that $s_f|_X = f|_X$. Then, we define the linear functional $Q_{V_X} : C(\mathbb{M}) \to \mathbb{R}$ via*

$$
Q_{V_X}(f) := \int_{\mathbb{M}} s_f(x) d\mu(x) = \sum_{\xi \in X} c_\xi f(\xi),
\tag{2.9}
$$

where the c_ξ's, the weights, are given in Proposition 2.2.

The invariance assumption on the kernel κ produces a system with the same attractive feature as one for an SBF $\phi(x \cdot y)$. The integral J_0 depends only on κ and $\mathbb{M}$; it is entirely independent of X. This is also true of the other J_k's. As a result the equations (2.5) defining the weight vector c only depend on X through function evaluations. The integrals $J_0, J_1, \ldots, J_M$ are all known in advance and are *independent* of X.

It is important to note that, *without* the invariance of κ, obtaining the system for c would require computing integrals of the form $\int_{\mathbb{M}} \kappa(x, \xi) d\mu(x)$ for each $\xi \in X$. This follows just by looking at equation (2.8) in the derivation of (2.5). This would make finding c numerically very expensive, not only because each integral would have to be computed for every $\xi \in X$, but also because the whole set would have to be recomputed whenever X was changed.

2.2.1 Weights

In many cases, the weights appearing in the quadrature formula above may be interpreted as coming from simple interpolation problems. In particular, if κ is strictly positive definite and

$\Pi = \{0\}$, then the system (2.5) becomes $Ac = J_0 \mathbf{1}$. This is the set of equations for interpolating the function $f(x) \equiv 1/J_0$. To obtain the interpolation problem for quadrature with κ being merely conditionally positive definite with respect to Π requires manipulating the saddle point system (2.5) as follows (see [4] for background). First, let $\Psi^T c = J$. This equation completely determines the orthogonal projection of c, $c_\parallel := Pc$, onto the range of Ψ: The standard normal equations give $c_\parallel = Pc = \Psi(\Psi^T \Psi)^{-1} \Psi^T c = \Psi(\Psi^T \Psi)^{-1} J$. Thus, $c_\parallel$ is known. Next, let $c_\perp := P^\perp c$, which obviously satisfies $Pc_\perp = 0$, so $\Psi^T c_\perp = 0$, and, consequently, the following system:

$$Ac_\perp + \Psi d = J_0 \mathbf{1} - A\Psi(\Psi^T \Psi)^{-1} J \text{ and } \Psi^T c_\perp = 0. \tag{2.10}$$

This is the interpolation problem (2.3), with $f_X = J_0 \mathbf{1} - A\Psi(\Psi^T \Psi)^{-1} J$. The final weights are then

$$c = c_\perp + \underbrace{\Psi(\Psi^T \Psi)^{-1} J}_{c_\parallel}. \tag{2.11}$$

Note that (2.10) may be solved for $c_\perp$, without also having to solve for d as follows. Start by eliminating d from (2.10). Multiply both sides of (2.10) by $P^\perp$. Since $P^\perp c_\perp = c_\perp$ and $P^\perp \Psi = 0$, we get

$$P^\perp A P^\perp c_\perp = J_0 P^\perp \mathbf{1} - P^\perp A \Psi(\Psi^T \Psi)^{-1} J. \tag{2.12}$$

Because κ is conditionally positive definite relative to Π, $P^\perp A P^\perp$ is positive definite on the orthogonal complement of the range of Ψ. Restricted to that space, it is invertible. Carrying out the inverse gives us $c_\perp$.

Often, the space Π contains the constant function; that is, $1 \in \Pi$. When this happens, the term with J_0 drops out of (2.12), which then becomes

$$P^\perp A P^\perp c_\perp = -P^\perp A c_\parallel = -P^\perp A \Psi(\Psi^T \Psi)^{-1} J.$$

This equation is homogeneous in A and is therefore independent of J_0. This implies that $c_\perp$ can be determined *independently* of J_0.

There is another consequence of having $1 \in \Pi$. First, the column vector $\mathbf{1}$ is in the range of Ψ, so $P\mathbf{1} = \mathbf{1}$. Let $\langle c_\perp \rangle$ be the average of $c_\perp$. Since $Pc_\perp = 0$, we have $N\langle c_\perp \rangle = \mathbf{1}^T c_\perp = (P\mathbf{1})^T c_\perp = 0$. Second, since $1 \in \Pi$, we also have that the quadrature formula is exact for it, and so $Q(1) = \text{vol}(\mathbb{M}) = \mathbf{1}^T c = N\langle c \rangle$. Using $c = c_\perp + c_\parallel$, along with a little algebra, yields

$$\langle c_\perp \rangle = 0, \ \langle c \rangle = \langle c_\parallel \rangle = \frac{\text{vol}(\mathbb{M})}{N}, \ \text{ provided } 1 \in \Pi. \tag{2.13}$$

Weights in quadrature formulas are usually positive. This is true for the polynomial quadrature formulas developed for spheres [33] and for two-point homogeneous manifolds [6]. Numerical experiments by Sommariva and Womersley [42] produced negative weights for kernels formed by restricting Gaussians to $\mathbb{S}^2$. On the other hand, their experiments involving the thin-plate splines (cf. section 4) restricted to $\mathbb{S}^2$ resulted in only positive weights.

Determining for what kernels and with what restrictions on X all of the weights are positive is an open problem.

2.3 Accuracy and Stability of Q_{V_X}

There are two important questions that arise concerning the quadrature method that we have been discussing. First, how accurate is it? Second, how stable is it?

The *accuracy* of Q_{V_X} depends on how well the underlying space of functions, V_X in our case, reproduces functions from the class to be integrated. Specifically, we have the following standard estimate:

$$\left| Q_{V_X}(f) - \int_{\mathbb{M}} f(x)d\mu(x) \right| \leq \|s_f - f\|_{L_1(\mathbb{M})} \leq (\text{vol}(\mathbb{M}))^{1/2}\|s_f - f\|_{L_2(\mathbb{M})}. \qquad (2.14)$$

This inequality converts estimates of the accuracy of $Q_{V_X}(f)$ to error bounds for kernel interpolation. These are known in many cases of importance.

Stability is related to how well the quadrature formula performs under the presence of noise. Lack of stability can amplify the effect that noise in $f|_X$ will have on the value of $Q_{V_X}(f)$. Stability also relates to performance as the number of data sites increases. Standard one-dimensional equally spaced quadrature formulas that reproduce polynomials can be quite unstable, due to the well-known Runge phenomenon.

A measure of stability is the $C(\mathbb{M})$ norm of the quadrature operator. From the definition of Q_{V_X} in (2.9) and equation (2.7), we have that

$$\|Q_{V_X}\|_{C(\mathbb{M})} = \sum_{\xi \in X} |c_\xi| \leq \sum_{\xi \in X} \|\chi_\xi\|_{L_1(\mathbb{M})}. \qquad (2.15)$$

When $\mathbb{M}$ is a compact manifold, this bound can be given in terms of the Lebesgue constant, $\Lambda_{V_X} = \max_{x \in \mathbb{M}} \sum_{\xi \in X} |\chi_\xi(x)|$. The reason is that

$$\|Q_{V_X}\|_{C(\mathbb{M})} \leq \sum_{\xi \in X} \|\chi_\xi\|_{L_1(\mathbb{M})} \leq \sum_{\xi \in X} \int_{\mathbb{M}} |\chi_\xi(x)|d\mu(x) \leq \text{vol}(\mathbb{M})\Lambda_{V_X}. \qquad (2.16)$$

Let us briefly see how noise affects $Q_{V_X}(f)$. Suppose that at each of the sites ξ we measure $f(\xi) + \nu_\xi$, where ν_ξ is a zero mean random variable. Further, we suppose that the ν_ξ's are independent and identically distributed, with variance σ_ν^2. Our quadrature formula gives us $Q_{V_X}(f + \nu)$ rather than $Q_{V_X}(f)$. Because the ν_ξ's have zero mean, we have that the mean $E\{Q_{V_X}(f + \nu)\} = Q_{V_X}(f)$. The variance of $Q_{V_X}(f + \nu)$ is thus

$$\sigma_Q^2 = E\{\left(Q_{V_X}(f + \nu) - Q_{V_X}(f)\right)^2\} = E\{Q_{V_X}(\nu)^2\}. \qquad (2.17)$$

We can both calculate and estimate σ_Q:

Proposition 2.4. *Let ν_ξ be independent, identically distributed, zero mean random variables having standard deviation σ_ν. Then the standard deviation σ_Q satisfies*

$$\sigma_Q^2 = \sigma_\nu^2\|c\|_2^2 \leq \sigma_\nu^2\|c\|_1\|c\|_\infty \leq \text{vol}(\mathbb{M})\sigma_\nu^2\Lambda_{V_X}\max_{\xi \in X}\|\chi_\xi\|_{L_1(\mathbb{M})} \qquad (2.18)$$

Proof. We begin by evaluating the term on the right in (2.17). to do this, we need to compute $E\{\nu_\xi\nu_\eta\}$. Since the ν_ξ's are i.i.d., we have $E\{\nu_\xi\nu_\eta\} = \sigma_\nu^2\delta_{\xi,\eta}$. It follows that $\sigma_Q^2 = E\{Q_{V_X}(\nu)^2\} = \sigma_\nu^2\|c\|_2^2$. Moreover, $\|c\|_2^2 \leq \|c\|_\infty\|c\|_1$. Combining this with (2.7) and the previous equation results in (2.18). $\square$

3 Sobolev Kernels

There are two classes of kernels that we will discuss here. The first class was introduced in [21, § 3.3], in the context of a compact n-dimensional Riemannian manifold[1] $\mathbb{M}$ equipped with a metric g. This

---

[1]See [21] for a discussion of the Riemannian geometry involved, including metrics, tensors, covariant derivatives, *etc.*

class comprises positive definite reproducing kernels for the Sobolev spaces $W_2^m(\mathbb{M})$, as defined in [2, 26]. For $\mathbb{M}$ a homogeneous space with g being the invariant metric that $\mathbb{M}$ inherits from a Lie group $\mathcal{G}$, we will show below that these kernels are invariant under the action of $\mathcal{G}$.

The second class, which was introduced and studied in [22], comprises polyharmonic kernels on two-point manifolds – spheres, projective spaces, which include $SO(3)$, along with a few others. These kernels are conditionally positive definite with respect to finite dimensional subspaces of eigenfunctions of the Laplace-Beltrami operator and they are invariant under appropriate transformations. We will discuss these in section 4 below.

The Sobolev space $W_2^m(\mathbb{M})$, $m \in \mathbb{N}$, is defined as follows. Let $\langle \cdot, \cdot \rangle_{g,x}$ be the inner product for a Riemannian metric g defined on $T\mathbb{M}_x$, the tangent space at $x \in \mathbb{M}$. The norm associated with this inner product will be denoted by $|\cdot|_{g,x}$. This inner product can also be applied to spaces of tensors at x, via $\langle S, T \rangle_{g,x} = \sum S^{i_1,\ldots,i_k} \overline{T}_{i_1,\ldots,i_k}$. We denote by ∇^k the kth order covariant derivative associated with the metric g, and let $d\mu$ be the measure associated with g. For $W_2^m(\mathbb{M})$, define the inner product

$$\langle f, h \rangle_{m,\mathbb{M}} := \langle f, h \rangle_{W_2^m(\mathbb{M})} := \sum_{k=0}^{m} \int_{\mathbb{M}} \langle \nabla^k f, \nabla^k h \rangle_{g,x} \, d\mu(x), \tag{3.1}$$

and norm $\|f\|_{m,\mathbb{M}}^2 := \langle f, f \rangle_{m,\mathbb{M}}$, where $f, h : \mathbb{M} \to \mathbb{R}$ are assumed smooth enough for their W_2^m norms to be finite. The advantage of this definition is that it yields Sobolev spaces that are coordinate independent and can also be defined on measurable regions $\Omega \subseteq \mathbb{M}$. Using the Sobolev embedding theorem for manifolds [2, §2.7], one can show that if $m > n/2$ these spaces are reproducing kernel Hilbert spaces, with κ_m being the unique, strictly positive definite reproducing kernel for $W_2^m(\mathbb{M})$; that is,

$$f(x) = \langle f(\cdot), \kappa_m(x, \cdot) \rangle_{m,\mathbb{M}}$$

In the remainder of this section we will discuss invariance, interpolation error estimates, Lagrange functions, Lebesgue constants, and quadrature formulas derived from κ_m.

For completeness sake, we define norms for $W_p^m(\mathbb{M})$, $1 \le p \le \infty$:

$$\|f\|_{W_{\mathsf{p}}^m(\mathbb{M})} := \begin{cases} \left(\sum_{k=0}^{m} \int_{\mathbb{M}} |\nabla^k f|_{g,p}^{\mathsf{p}} \, d\mu(p) \right)^{1/\mathsf{p}}, & 1 \le \mathsf{p} < \infty; \\ \max_{0 \le k \le m} \left\| |\nabla^k f|_{g,p} \right\|_{L_\infty(\mathbb{M})}, & \mathsf{p} = \infty. \end{cases} \tag{3.2}$$

3.1 Invariance of κ_m

We now turn to a discussion of the invariance of κ_m under the action of a diffeomorphism that is also an isometry. We will then apply this to the case of a homogeneous space. Here is what we will need.

Proposition 3.1. *Let $\mathbb{M}$ be a compact Riemannian manifold of dimension n with metric g. If $\Phi : \mathbb{M} \to \mathbb{M}$ is a diffeomorphism that is also an isometry, then the kernel κ_m satisfies $\kappa_m(\Phi(x), \Phi(y)) = \kappa_m(x, y)$ and $d\mu(\Phi(x)) = d\mu(x)$.*

Proof. The proof proceeds in two steps. The first is showing this. Let $f : \mathbb{M} \to \mathbb{R}$ and let $f^\Phi = f \circ \Phi$ be the pullback of f by Φ. Then,

$$\langle \nabla^k f^\Phi, \nabla^k h^\Phi \rangle_{g,x} = \langle \nabla^k f, \nabla^k h \rangle_{g,\Phi(x)}. \tag{3.3}$$

We will follow a technique used in [27, Proposition 2.4, p. 246] and in [22]. Let $(\mathfrak{U}, \phi)$ be a local chart, with coordinates $u^j = \phi^j(x)$, $j = 1, \ldots, n$ for $x \in \mathfrak{U}$. Since Φ is a diffeomorphism, $(\Phi(\mathfrak{U}), \phi \circ \Phi^{-1})$

is also a local chart. Let $\psi = \phi \circ \Phi^{-1}$, and use the coordinates $v^j = \psi^j(y)$ for $y \in \Phi(\mathfrak{U})$. The choice of coordinates has the effect of assigning the *same* point in $\mathbb{R}^n$ to x and y, provided $y = \Phi(x)$ – i.e., $u^j(x) = v^j(y)$. Thus, relative to these coordinates the map Φ is the identity, and consequently, the two tangent vectors $(\frac{\partial}{\partial v^j})_y \in T_y\mathbb{M}$ and $(\frac{\partial}{\partial u^j})_x \in T_x\mathbb{M}$ are related via

$$\left(\frac{\partial}{\partial v^j}\right)_{\Phi(x)} = d\Phi_x \left(\frac{\partial}{\partial u^j}\right)_x.$$

So far, we have only used the fact that Φ is a diffeomorphism. The map Φ being in addition an isometry then implies that

$$\left\langle \frac{\partial}{\partial v^j}, \frac{\partial}{\partial v^k} \right\rangle_{\Phi(x)} = \left\langle d\Phi_x \left(\frac{\partial}{\partial u^j}\right), d\Phi_x \left(\frac{\partial}{\partial u^k}\right) \right\rangle_{\Phi(x)} = \left\langle \frac{\partial}{\partial u^j}, \frac{\partial}{\partial u^k} \right\rangle_x.$$

The expressions on the left and right are the metric tensors at $y = \Phi(x)$ and x; the equation implies that, as functions of v and u, $g_{jk}(v) = g_{jk}(u)$. From this it follows that the expressions for the Christoffel symbols, covariant derivatives and various expressions formed from them also will be the same, as functions of local coordinates. In addition, note that the local forms for f^Φ and h^Φ at $u = u(x)$ are $f^\Phi \circ \phi^{-1}$ and $h^\Phi \circ \phi^{-1}$, respectively, and those for f and h at $v = v(y)$ are $f \circ \psi^{-1}$ and $h \circ \psi^{-1}$. At $u = u(x)$ and $v = v(y)$, $y = \Phi(x)$, $f \circ \psi^{-1}(v) = f \circ \Phi \circ \phi^{-1}(v) = f^\Phi \circ \phi^{-1}(v)$, and similarly for h. Again, this is functional equality in local coordinates, so matching partial derivatives are also equal. Consequently, (3.3) holds.

The equality of the coordinate forms of the metric g_{jk}, which was established above, implies invariance of the Riemannian measure:

$$d\mu(x) = \sqrt{\det(g_{jk}(u))}d^n u = \sqrt{\det(g_{jk}(v))}d^n v = d\mu(\Phi(x)). \tag{3.4}$$

Using this we see that

$$\begin{aligned}
\int_\mathbb{M} \langle \nabla^k f^\Phi, \nabla^k h^\phi \rangle_{g,x} d\mu(x) &= \int_\mathbb{M} \langle \nabla^k f, \nabla^k h \rangle_{g,\Phi(x)} d\mu(x) \\
&= \int_\mathbb{M} \langle \nabla^k f, \nabla^k h \rangle_{g,\Phi(x)} d\mu(\Phi(x)) \\
&= \int_\mathbb{M} \langle \nabla^k f, \nabla^k h \rangle_{g,y} d\mu(y)
\end{aligned}$$

Finally, from this and (3.1), we have invariance of the Sobolev inner product:

$$\langle f^\Phi, h^\Phi \rangle_{m,\mathbb{M}} = \langle f, h \rangle_{m,\mathbb{M}} \tag{3.5}$$

The second step is to show that the kernel is invariant. Since κ_m is a reproducing kernel, we have $f(x) = \langle f(\cdot), \kappa_m(x, \cdot) \rangle_{m,\mathbb{M}}$. By (3.5), we also have $f(x) = \langle f^\Phi(\cdot), \kappa_m(x, \Phi(\cdot)) \rangle_{m,\mathbb{M}}$. Replacing x by $\Phi(x)$ then yields

$$f(\Phi(x)) = f^\Phi(x) = \langle f^\Phi(\cdot), \kappa_m(\Phi(x), \Phi(\cdot)) \rangle_{m,\mathbb{M}}.$$

Finally, replacing f by $f^{\Phi^{-1}}$ above gives us

$$f(x) = \langle f(\cdot), \kappa_m(\Phi(x), \Phi(\cdot)) \rangle_{m,\mathbb{M}},$$

from which it follows that $\kappa_m(\Phi(x), \Phi(y))$ is also a reproducing kernel for $W_2^m(\mathbb{M})$. But, reproducing kernels are unique, so $\kappa_m(\Phi(x), \Phi(y)) = \kappa_m(x, y)$. Thus κ_m is invariant. $\square$

Homogeneous spaces have two properties that allow us to use the proposition just proved. First, they inherit a Riemannian metric invariant under the action of the Lie group $\mathcal{G}$. Second, the action of a group element produces an isometric diffeomorphism [27, 45]. These observations then yield this:

Corollary 3.2. *Let $\mathbb{M}$ be a homogeneous space for a Lie group $\mathcal{G}$ and suppose that $\mathbb{M}$ is equipped with an invariant metric g from $\mathcal{G}$. Then the reproducing kernel κ_m for $W_2^m(\mathbb{M})$ is invariant under the action of $\gamma \in \mathcal{G}$.*

3.2 Error estimates for interpolation via κ_m

Recall that the accuracy of the quadrature formula associated with κ_m is directly dependent on error estimates for interpolation via κ_m. To obtain these, we will first state a theorem that provides estimates on functions with many zeros, quasi-uniformly distributed over a compact manifold.

Theorem 3.3 ([22, Corollary A.13] "Zeros Lemma"). *Suppose that $\mathbb{M}$ is a C^∞, compact, n-dimensional manifold, that $1 \le p \le \infty$, $m \in \mathbb{N}$, and also that $u \in W_p^m(\mathbb{M})$. Assume that $m > n/p$ when $p > 1$, and $m \ge n$ when $p = 1$. Then there are constants $C_0 = C_0(\mathbb{M})$ and $C_1 = C_1(m, k, \mathbb{M})$ such that if $u|_X = 0$ and $X \subset \mathbb{M}$ has mesh norm $h \le C_0/m^2$, then*

$$\|u\|_{W_p^k(\mathbb{M})} \le C_1 h^{m-k} \|u\|_{W_p^m(\mathbb{M})}. \tag{3.6}$$

Using this "zeros lemma" we are able obtain an estimate for $\|s_f - f\|_{L_2(\mathbb{M})}$, provided $f \in W_2^m(\mathbb{M})$ and s_f is the interpolant for f.

Proposition 3.4. *Let $m > n/2$, $f \in W_2^m(\mathbb{M})$, and let s_f be the κ_m-interpolant for f from V_X. Then, with the notation from Theorem 3.3, if $h \le C_0/m^2$, we have*

$$\|s_f - f\|_{L_2(\mathbb{M})} \le C_1 h^m \|f\|_{W_2^m(\mathbb{M})}. \tag{3.7}$$

Proof. Clearly $s_f - f \in W_2^m$ and $(s_f - f)|_X = f|_X - f_X = 0$. Applying Theorem 3.3 to $s_f - f$ with $k = 0$ yields $\|s_f - f\|_{L_2(\mathbb{M})} \le C_1 h^m \|s_f - f\|_{W_2^m(\mathbb{M})}$. Since the space $W_2^m(\mathbb{M})$ is the reproducing Hilbert space for κ_m, the interpolant s_f minimizes $\|g - f\|_{W_2^m(\mathbb{M})}$ among all $g \in W_2^m(\mathbb{M})$ (see [47, Section 10.1]). Thus, taking $g = 0$ yields $\|s_f - f\|_{W_2^m(\mathbb{M})} \le \|0 - f\|_{W_2^m(\mathbb{M})} = \|f\|_{W_2^m(\mathbb{M})}$, from which the inequality (3.7) follows immediately. $\square$

The bounds in (3.7) hold whether or not $\mathbb{M}$ is homogeneous. In one respect, the bounds are not as strong as we would like. The assumption that f is in the reproducing kernel space W_2^m precludes estimates for less smooth f, in $W_2^k(\mathbb{M})$, with $k < m$. Stronger bounds do hold in important cases, though. For example, in section 4, we will see that the stronger result for $f \in W_2^k$ holds for the class of "polyharmonic" kernels, where $\mathbb{M}$ can be a sphere or some other two-point homogeneous space. We conjecture that, at least for κ_m, the stronger result holds for general C^∞ compact, Riemannian manifolds.

3.3 Lagrange functions and Lebesgue constants

The Lagrange functions $\{\chi_\xi\}_{\xi \in X}$ associated with κ_m have remarkable properties. For quasi-uniform sets of centers, Lebesgue constants are bounded independently of the number of points and the L_1 norms of the Lagrange functions are nicely controlled. Specifically, we have the result below, which holds for a general C^∞ metric g.

Theorem 3.5 ([21, Theorem 4.6] [20, Proposition 3.6]). *Let $\mathbb{M}$ be a compact Riemannian manifold of dimension n, and assume $m > n/2$. For a quasi-uniform set $X \subset \mathbb{M}$, with mesh ratio $h/q \le \rho$, there exist constants $C_{\mathbb{M}}$ and $C_{\mathbb{M},m}$ such that if $h \le C_{\mathbb{M}}/m^2$, then the Lebesgue constant $\Lambda_{V_X} = \max_{x \in \mathbb{M}} \sum_{\xi \in X} |\chi_\xi(x)|$ associated with κ_m satisfies*

$$\Lambda_{V_X} \le C_{\mathbb{M},m}\rho^n.$$

In addition, we have this uniform bound on the L_1-norm of the Lagrange functions:

$$\max_{\xi \in X} \|\chi_\xi\|_{L_1(\mathbb{M})} \le C_{\rho,m,\mathbb{M}}q^n.$$

Proof. In the statement of the theorem used above, we have made explicit the ρ dependence of the bound on Λ_{V_X} found in the proof of [21, Theorem 4.6]. We have also adapted the notation there to that used here. The bound on $\|\chi_\xi\|_{L_1(\mathbb{M})}$ follows from [20, Proposition 3.6], with $s = \chi_\xi$ and $p = 1$. In that proposition, the coefficients $A_{p,\eta} = q^{n/p}\delta_{\xi,\eta}$ and so $\|A_{p,.}\|_p = q^{n/p}$. For $p = 1$, $\|A_{1,.}\|_1 = q^d$, and so $\|\chi_\xi\|_{L_1(\mathbb{M})} \le C_{\rho,m}q^n$. □

3.4 Kernel quadrature via κ_m

The positive definite Sobolev kernel κ_m is invariant under the action of $\mathcal{G}$, by Corollary 3.2. This is the bare minimum requirement for a kernel to be able to give rise to a computable quadrature formula. The other properties of κ_m established in the previous sections give us the result below concerning accuracy and stability.

Theorem 3.6. *Let $X \subset \mathbb{M}$ be a finite set having mesh norm $\rho_X \le \rho$. Take $A = (\kappa_m(\xi,\eta))|_{\xi,\eta \in X}$ and suppose $f \in W_2^m(\mathbb{M})$. Then the vector of weights in Q_{V_X} is $c = J_0 A^{-1}\mathbf{1}$, the error for Q_{V_X} satisfies $|Q_{V_X}(f) - \int_{\mathbb{M}} f d\mu| \le h^m\|f\|_{W_2^m(\mathbb{M})}$, and the norm of Q_{V_X} is bounded by $\|Q_{V_X}\|_{C(\mathbb{M})} \le C_{\mathbb{M},m}\rho^n$. Finally, the standard deviation defined in Proposition 2.4 satisfies the bound $\sigma_Q \le C_{\rho,m,\mathbb{M}}\sigma_\nu h^{n/2}$.*

Proof. The formula for the weights is a consequence of two things. First, by Corollary 3.2 the kernel is invariant and so by Lemma 2.1 the integral $\int_{\mathbb{M}} \kappa_m(x,\cdot)d\mu(x)$ is a constant, namely J_0. Second, since the kernel is positive definite, Proposition 2.2 provides the desired formula for the weights. The error estimate is a consequence of (2.14) and Proposition 3.7, and the norm estimate follows from (2.16) and Proposition 3.5. Finally, the bound on σ_Q is a consequence of Proposition 2.4, Proposition 3.5, and of the fact that $\rho^n q^n = h^n$. □

There are two significant implications of this result. The first is just what was noted in section 2.2; namely, the weights are obtained by directly solving a linear system of equations. The second is that the measures of accuracy and stability hold for any X with mesh ratio less than a fixed ρ.

There are several drawbacks. In the case of a *general* homogeneous space $\mathbb{M}$, the formulas for kernels κ_m are not yet explicitly known. This may be less of a problem when specific cases come up in applications; we will see such explicit formulas in equations (4.3) and (4.4) for spheres and $SO(3)$. Also, the error estimates, which provide the chief measure of accuracy, hold for f in the space $W_2^m(\mathbb{M})$. We would like to "escape" from this "native space" (reproducing kernel space) and have estimates for less smooth f. As we shall see in the next section, the situation is much improved in the case of spheres, projective spaces, and other two-point homogeneous manifolds. In the case of $\mathbb{S}^2$, not only do we have the requisite kernels, but in important cases we can also give fast algorithms for obtaining the weights (cf. section 5).

12

4 Polyharmonic Kernels

In this section we discuss both interpolation and quadrature on two-point homogeneous manifolds, e.g. spheres, $SO(3)$ and similar spaces (see [27, pgs. 167 & 177] for a list), employing *polyharmonic* kernels, which are related to Green's functions for certain differential operators. Important examples include restrictions of thin-plate splines [22] to spheres and certain kernels for $SO(3)$. These kernels are useful because they are given via explicit formulas. Our aim is to get error estimates for the associated interpolation problems and the use them to obtain such estimates for associated quadrature formulas.

The differential operators are polynomials in the Laplace-Beltrami operator. Since, on a compact Riemannian manifold $-\Delta$ is a self adjoint operator with a countable sequence of nonnegative eigenvalues $\lambda_j < \lambda_{j+1}$ having $+\infty$ as the only accumulation point, we can express a polyharmonic kernel in terms of the associated eigenfunctions $-\Delta\phi_{j,s} = \lambda_j\phi_{j,s}$, $s = 1, \ldots, d_j$, d_j being the multiplicity of λ_j. To make this clear, we will need some notation.

Let $m \in \mathbb{N}$ such that $m > n/2$ and let $\pi_m \in \Pi_m(\mathbb{R})$ be of the form $\pi_m(x) = \sum_{\nu=0}^{m} c_\nu x^\nu$, where $c_m > 0$ and let $\mathcal{L}_m$ be the $2m$-order differential operator given by $\mathcal{L}_m = \pi_m(-\Delta)$. We define $\mathcal{J} \subset \mathbb{N}$ to be a finite set that includes all j for which the eigenvalue $\pi_m(\lambda_j)$ of $\mathcal{L}_m$ satisfies $\pi_m(\lambda_j) \leq 0$. (In addition to this finite set, $\mathcal{J}$ may also include a finite number j's for which $\pi_m(\lambda_j) > 0$.) We say that the kernel $\kappa : \mathbb{M} \times \mathbb{M} \to \mathbb{R}$ is *polyharmonic* if it has the eigenfunction expansion

$$\kappa(x,y) := \sum_{j=0}^{\infty} \tilde{\kappa}_j \left(\sum_{s=1}^{d_j} \phi_{j,s}(x)\phi_{j,s}(y) \right), \quad \text{where } \tilde{\kappa}_j := \begin{cases} \pi_m(\lambda_j)^{-1}, & j \notin \mathcal{J}, \\ \text{arbitrary}, & j \in \mathcal{J}. \end{cases} \tag{4.1}$$

The kernel κ is conditionally positive definite with respect to the space $\Pi_{\mathcal{J}} = \text{span}\{\phi_{j,s} : j \in \mathcal{J}, 1 \leq s \leq d_j\}$. In the sequel, we will need eigenspaces, Laplace-Beltrami operators and so on for compact two-point homogenous manifolds. Without further comment, we will use results taken from the excellent summary given in [6]. This paper gives original references for these results.

Polyharmonic kernels are special cases of *zonal* functions, which are invariant kernels that depend only on the geodesic distance $d(x,y)$ between the variables x and y; d is normalized so that the diameter of $\mathbb{M}$ is π — i.e., $0 \leq d(x,y) \leq \pi$. To see that polyharmonic kernels are zonal functions, we need the addition theorem on two-point homogeneous manifolds. If $P_\ell^{(\alpha,\beta)}$ denotes the ℓth degree Jacobi polynomial, normalized so that $P_\ell^{(\alpha,\beta)}(1) = \frac{\Gamma(\ell+\alpha+1)}{\Gamma(\ell+1)\Gamma(\alpha+1)}$, then this theorem states that for any orthonormal basis $\{\phi_{j,s}\}_{s=1}^{d_j}$ of the eigenspace corresponding to λ_j we have

$$\sum_{s=1}^{d_j} \phi_{j,s}(x)\phi_{j,s}(y) = c_{\varepsilon j} P_{\varepsilon j}^{(\frac{n-2}{2},\beta)}(\cos(\varepsilon^{-1}d(x,y))), \quad c_\ell := \frac{(2\ell + \frac{n}{2} + \beta)\Gamma(\beta+1)\Gamma(\ell + \frac{n}{2} + \beta)}{\Gamma(\beta + \frac{n+2}{2})\Gamma(\ell+\beta+1)},$$

where the parameters ε and β, and of course λ_j, depend on the manifold. These are listed in the table below. In summary, every polyharmonic kernel has the form $\kappa(x,y) = \Phi(\cos(\varepsilon^{-1}d(x,y)))$, where

$$\Phi(t) = \sum_{j=0}^{\infty} \tilde{\kappa}_j c_{\varepsilon j} P_{\varepsilon j}^{(\frac{n-2}{2},\beta)}(t), \quad -1 \leq t \leq 1. \tag{4.2}$$

An important class of polyharmonic kernels on $\mathbb{S}^n$ are the surface (thin-plate) splines restricted to the sphere. The surface splines on $\mathbb{R}^n$ are defined in [47, Section 8.3]; their $\tilde{\kappa}_j$'s are computed in [3]. When $m > n/2$, these kernels have expansion coefficients of the form (4.1). Below, we list both kernel and the coefficients $\tilde{\kappa}_j$ in terms of the parameter $s = m - n/2$; they are also normalized

Manifold	ε	β	λ_j
$\mathbb{S}^n$	1	$\frac{n-2}{2}$	$j(j+n-1)$
$\mathbb{RP}^n$	2	$\frac{n-2}{2}$	$2j(2j+n-1)$
$\mathbb{CP}^n$	1	0	$j(j+\frac{n}{2})$
Quaternion $\mathbb{P}^n$	1	1	$j(j+\frac{n+2}{2})$
Cayley $\mathbb{P}^{16}$	1	3	$j(j+12)$

Table 1: Parameters for compact, two-point homogeneous manifolds .

to conventions used here (see also [32]). The first formula is used for odd n and the second for even n. These kernels are conditionally positive definite of order m, meaning that the polynomial operator $\pi_m(-\Delta)$ corresponding to them annihilates eigenfunctions of Δ corresponding to λ_j, with $j \leq m-1$. Thus the corresponding space Π is the span of these eigenfunctions.

$$
\left.
\begin{aligned}
\Phi_s(t) &= \begin{cases} (-1)^{s+\frac{1}{2}}(1-t)^s, & s = m - \frac{n}{2} \in \mathbb{N} + \frac{1}{2} \\ (-1)^{s+1}(1-t)^s \log(1-t), & s = m - \frac{n}{2} \in \mathbb{N}. \end{cases} \\
\tilde{\kappa}_j &= C_{s,n} \frac{\Gamma(j-s)}{\Gamma(j+s+n)}, \text{ where, for even } n, \ j > s.
\end{aligned}
\right\} \tag{4.3}
$$

The factor $C_{s,n}$ is given by

$$
C_{s,n} := 2^{s+n} \pi^{\frac{n}{2}} \Gamma(s+1) \Gamma\left(s + \frac{n}{2}\right) \begin{cases} \frac{\sin(\pi s)}{\pi} & s = m - \frac{n}{2} \in \mathbb{N} + \frac{1}{2} \\ 1, & s \in \mathbb{N}. \end{cases}
$$

For the group $SO(3) \, (= \mathbb{RP}^3)$, the following family of polyharmonic kernels, which are similar to those above, was discussed in [23]:

$$
\kappa(x,y) = \left(\sin\left(\frac{\omega(y^{-1}x)}{2} \right) \right)^{2m-1}, \ m \geq 1. \tag{4.4}
$$

Here $\omega(z)$ is the rotational angle of $z \in SO(3)$. Adjusting the normalization given in [23, Lemma 2] to that used here, the polynomial $\pi(x)$ associated with κ is $\pi(x) = \prod_{\nu=0}^{m}(x+1-4\nu^2)$. We remark that derivation of the kernels given in [23] used the theory of group representations along with a generalized addition formula that holds for any compact homogeneous manifold (see [13]).

Remark 4.1. *For two-point homogeneous manifolds, the Sobolev kernels κ_m are in fact polyharmonic. The reason is that κ_m is the Green's function for the linear operator $\mathcal{L}_m = \sum_{k=0}^{m} \nabla^{k*}\nabla^k$. However, by [22, Lemmas 4.2 & 4.3], $\mathcal{L}_m = \pi_m(-\Delta)$, where $\pi_m(x) = x^m + \sum_{\nu=0}^{m-1} c_\nu x^\nu$, so it has to have the form (4.1). Also, it is easy to show that $\pi_m(\lambda_j) > 0$ for $j = 0, 1, \ldots,$ and that $\kappa_{m,j} = \pi_m(\lambda_j)^{-1} \sim \lambda_j^{-m}$ for j large.*

There are two reproducing kernel Hilbert spaces associated with a polyharmonic kernel κ. We will take $\tilde{\kappa}_j > 0$ for $j \in \mathcal{J}$. These spaces are often called "native spaces," and are denoted by $\mathcal{N}_\kappa$ and $\mathcal{N}_{\kappa,\mathcal{J}}$. Consider the inner products

$$
\langle f, g \rangle_\kappa = \sum_{j=0}^{\infty} \sum_{s=1}^{d_j} \frac{\hat{f}_{j,s} \overline{\hat{g}}_{j,s}}{\tilde{\kappa}_j} \text{ and } \langle f, g \rangle_{\kappa,\mathcal{J}} = \sum_{j \notin \mathcal{J}} \sum_{s=1}^{d_j} \frac{\hat{f}_{j,s} \overline{\hat{g}}_{j,s}}{\tilde{\kappa}_j}.
$$

14

The first of these is the inner product of the reproducing kernel Hilbert space for κ itself, $\mathcal{N}_\kappa$, and the second is the semi-inner product for the Hilbert space modulo $\Pi_\mathcal{J}$, $\mathcal{N}_{\kappa,\mathcal{J}}$. The series form of the inner products above has an important consequence.

Remark 4.2. *The norms for W_2^m and $\mathcal{N}_\kappa$ are equivalent,*

$$\|f\|_\kappa \approx \|f\|_{W_2^m(\mathbb{M})}. \tag{4.5}$$

This follows from two facts. First, by Remark 4.1 the Sobolev kernel κ_m for a two-point homogeneous manifolds the is itself polyharmonic, and so the inner product for W_2^m has the form of the series $\langle f, g \rangle_\kappa$ in the equation above. Second, a polyharmonic kernel κ associated with a polynomial $\pi(x) = c_m x^m + c_{m-1} + \cdots + c_0$ also has an inner product that can be expressed in term of the same type of series. As mentioned above, the coefficients involved are asymptotically equivalent, up to constants. The norms are therefore equivalent. *In fact by the same argument, this will be true for any kernel, polyharmonic or not, having a series expansion similar to (4.1), with coefficients that asymptotically behave like λ_j^{-m} for j large.*

4.1 Interpolation with polyharmonic kernels

If we choose $\tilde{\kappa}_j > 0$ for $j \in \mathcal{J}$, the kernel will be positive definite, and so we can interpolate any $f \in C(\mathbb{M})$ given data on a finite, discrete set $X \subset\in \mathbb{M}$. The form of the interpolant will be

$$I_X f = \sum_{\xi \in X} a_\xi \kappa(x, \xi). \tag{4.6}$$

with the coefficients being obtained by inverting $f|_X = Aa$, where $A = [\kappa_{(\xi, \eta)}]_{\xi, \eta \in X}$ and the components of a are the a_ξ's.

Let's look at error estimates, given that $f \in W_2^m(\mathbb{M})$. Before we start, we begin with the observation that (4.5) and the usual minimization properties of $\| \cdot \|_\kappa$ imply that

$$\|I_X f - f\|_{W_2^m(\mathbb{M})} \leq C_1 \|I_X f - f\|_\kappa \leq C \|f\|_\kappa \leq C_2 \|f\|_{W_2^m(\mathbb{M})}.$$

This inequality was the key to proving Proposition 3.4, where the reproducing kernel Hilbert space was itself $W_2^m(\mathbb{M})$. Hence, repeating the proof of that proposition, with the inequality changed appropriately, we obtain the estimate

$$\|I_X f - f\|_{L_2(\mathbb{M})} \leq C h^m \|f\|_{W_2^m(\mathbb{M})}, \ f \in W_2^m(\mathbb{M}), \tag{4.7}$$

which holds for a polyharmonic kernel (4.1), provided the conditions on X in Proposition 3.4 are satisfied. There are no restrictions on the two-point homogeneous manifold $\mathbb{M}$.

There are, however, restrictions on the smoothness of f – namely, f must be at least as smooth as κ. Put another way, f has to be in the reproducing kernel Hilbert space $\mathcal{N}_\kappa$.

In the case of $\mathbb{S}^n$ or $\mathbb{RP}^n$, it is possible to remove this restriction and "escape" from the "native space" of κ. We will first deal with $\mathbb{S}^n$. From (4.2), we see that polyharmonic kernels on $\mathbb{S}^n$ are *spherical basis functions* (SBFs), provided coefficients with $j \in \mathcal{J}$ are taken to be positive. Moreover, $\tilde{\kappa}_j \sim \lambda_j^{-m}$ for j large. We may then apply [35, Theorem 5.5], with $\phi, \tau, \beta, \mu \to \Phi, m, \mu, 0$, to obtain the estimate below. (Note that for an integer k, the space $H_k(\mathbb{S}^n)$ in [35] is $W_2^k(\mathbb{S}^n)$ here.) This result applies to functions *not* smooth enough enough to be in W_2^m.

Proposition 4.3 (Case of $\mathbb{S}^n$). *Let κ be a polyhamonic kernel of the form (4.2), with $\deg(\pi(x)) = m$, and with $\tilde{\kappa}_j$, $j \in J$, chosen to be positive. Assume that the conditions on $X \subset \mathbb{S}^n$ in Proposition 3.4 are satisfied. If μ is an integer satisfying $m \geq \mu > n/2$ and if $f \in W_2^\mu(\mathbb{S}^n)$, then, provided h is sufficiently small,*

$$\|I_X f - f\|_{L_2(\mathbb{S}^n)} \leq Ch^\mu \|f\|_{W_2^\mu(\mathbb{S}^n)}. \tag{4.8}$$

The n-dimensional, real projective space, $\mathbb{RP}^n$, is the sphere $\mathbb{S}^n$ with antipodal points identified. Thus each $x \in \mathbb{RP}^n$ corresponds to $\{x, -x\}$ on $\mathbb{S}^n$. We will use this correspondence to lift the entire problem to $\mathbb{S}^n$, which is an idea used in [16,23] in connection with approximation on $SO(3)$. As we mentioned earlier, the distance $d(x, y) = d_{\mathbb{RP}^n}(x, y)$ has been normalized so that the diameter of $\mathbb{RP}^n$ is π, rather than the $\pi/2$ one would expect from its being regarded as a hemisphere of $\mathbb{S}^n$. In fact, the two distances are proportional to each other. The natural geodesic distance on projective space is simply the angle between two lines passing through $\{x, -x\}$ and $\{y, -y\}$, with $x, y \in \mathbb{S}^n$, which is just $\theta = \arccos(|x \cdot y|)$, $0 \leq \theta \leq \pi/2$. The distance $d_{\mathbb{RP}^n}$, in which the diameter of $\mathbb{M}$ is π, satisfies $d_{\mathbb{RP}^n}(x, y) = 2\arccos(|x \cdot y|)$. If we use this in (4.2), then $t = |x \cdot y|$ and $\kappa(x, y) = \Phi(|x \cdot y|)$. One can take this farther. In the case of $\mathbb{RP}^n$, the series representation for Φ is

$$\Phi(t) = \sum_{j=0}^\infty \tilde{\kappa}_j c_{2j} P_{2j}^{(\frac{n-2}{2}, \frac{n-2}{2})}(t).$$

Since the Jacobi polynomials $P_n^{(\frac{n-2}{2}, \frac{n-2}{2})}(t)$ are even or odd, depending on whether n is even or odd, and since the series for Φ contains only polynomials with n even, it follows that $\Phi(-t) = \Phi(t)$. As a consequence we have that $\kappa(x, y) = \Phi(x \cdot y)$. Thus, if we regard the variables x and y to be points on $\mathbb{S}^n$, the kernel κ is even in both variables, and is nonnegative definite on $\mathbb{S}^n$.

Our aim now is to lift κ to a polyharmonic kernel κ^* on $\mathbb{S}^n$, with a view toward lifting the whole interpolation problem to $\mathbb{S}^n$. To begin, note that the eignvalues for $-\Delta_{\mathbb{S}^n}$ have the form $\lambda_j^* = j(j + n - 1)$ and so those the $\mathbb{RP}^n$ may be written as $\lambda_j = \lambda_{2j}^*$. Next, let $\pi(x) \in \Pi_m$ be the polynomial associated with the kernel κ in (4.1) and let $\tilde{\kappa}_j^* = \pi(\lambda_j^*)^{-1}$, except where $\pi(\lambda_j^*) \leq 0$. For these we only require that the corresponding $\tilde{\kappa}_j^* > 0$. Define the function

$$\Phi^*(t) = \sum_{j=0}^\infty \tilde{\kappa}_j^* c_j P_j^{(\frac{n-2}{2}, \frac{n-2}{2})}(t),$$

which is associated with the polyharmonic kernel $\kappa^*(x, y) = \Phi^*(x \cdot y)$ on $\mathbb{S}^n$. In constructing Φ^* we have simply added an odd function to Φ. Thus,

$$\Phi(t) = \frac{1}{2}\big(\Phi^*(t) + \Phi^*(-t)\big).$$

Start with the centers X on $\mathbb{RP}^n$. Each center in X corresponds to $\{\xi, -\xi\}$ on $\mathbb{S}^n$, so we may lift X to $X^* = \{\pm\xi \in \mathbb{S}^n : \{\xi, -\xi\} \in X\}$. Following the proof in [16, Theorem 1], we may show that $q_{X'} = \frac{1}{2}q_X$ and $h_{X'} = \frac{1}{2}h_X$, where $d_{\mathbb{RP}^n}$ is used for q and h in X. In addition, we may, and will, identify each $f \in C(\mathbb{RP}^n)$ with an even function in $C(\mathbb{S}^n)$. Now, interpolate an even f on $\mathbb{S}^n$ at the centers in X^*. This gives us

$$I_{X^*}f(x) = \sum_{\zeta \in X^*} a_\zeta^* \kappa^*(x, \zeta) \tag{4.9}$$

Note that $\kappa^*(-x, \zeta) = \Phi^*((-x) \cdot \zeta) = \Phi^*(x \cdot (-\zeta)) = \kappa^*(x, -\zeta)$. Since both ζ and $-\zeta$ are in X^*. it follows that $I_{X^*}f(-x) = \sum_{\zeta \in X^*} a_{-\zeta}^* \kappa^*(x, \zeta)$. Moreover, $I_{X^*}f(-\xi) = f(-\xi) = f(\xi) = I_{X^*}f(\xi)$.

Since interpolation is unique, and the two linear combinations of kernels agree on X^*, they are equal, and so we have $I_{X^*}f(-x) = I_{X^*}f(x)$ and $a_{-\zeta}^* = a_\zeta^*$. Because $I_{X^*}f$ is even, we have, from (4.9), that $I_{X^*}f(x) = \sum_{\zeta \in X^*} a_\zeta^* \frac{1}{2}(\kappa^*(x,\zeta) + \kappa^*(x,-\zeta))$. Since $\kappa^*(x,\zeta) = \Phi^*(x \cdot \zeta)$, we have $\kappa^*(x,\zeta) + \kappa^*(x,-\zeta) = 2\kappa(x,\zeta)$. Consequently,

$$I_{X^*}f(x) = \sum_{\zeta \in X^*} a_\zeta^* \kappa(x,\zeta) = \sum_{\zeta \in X} a_\zeta \kappa(x,\zeta),$$

where $a_\zeta = a_\zeta^* + a_{-\zeta}^* = 2a_\zeta^*$. The sum on the right above is the interpolant to f on $\mathbb{RP}^n$, $I_X f(x)$. Thus, $I_{X^*}f(x) = I_X f(x)$.

Corollary 4.4 (Case of $\mathbb{RP}^n$). *Let κ be a polyhamonic kernel of the form (4.2), with $\deg(\pi(x)) = m$, and with $\tilde{\kappa}_j$, $j \in \mathcal{J}$, chosen to be positive. Assume that the conditions on $X \subset \mathbb{RP}^n$ in Proposition 3.4 are satisfied. If μ is an integer satisfying $m \geq \mu > n/2$ and if $f \in W_2^\mu(\mathbb{RP}^n)$, then, provided h is sufficiently small,*

$$\|I_X f - f\|_{L_2(\mathbb{RP}^n)} \leq Ch^\mu \|f\|_{W_2^\mu(\mathbb{RP}^n)}. \tag{4.10}$$

Proof. The metric $ds_{\mathbb{RP}^n}$ we are using for $\mathbb{RP}^n$ is twice the metric inherited from the sphere; that is, $ds_{\mathbb{RP}^n} = 2ds_{\mathbb{S}^n}$. From the point of view of integration, it is easy to see that $d\mu_{\mathbb{RP}^n} = 2^{n/2}d\mu_{\mathbb{S}^n}$. Thus various integrals and norms are merely changed by d-dependent constant multiples – e.g., $\|I_X f - f\|_{L_2(\mathbb{RP}^n)} = 2^{1-d/2}\|I_X^* f - f\|_{L_2(\mathbb{S}^n)}$. By Proposition 4.3,

$$\|I_X^* f - f\|_{L_2(\mathbb{S}^n)} \leq C_1 h_{X^*}^\mu \|I_{X^*}f - f\|_{W_2^\mu(\mathbb{S}^n)} \leq C_2 h_X^\mu \|I_X f - f\|_{W_2^\mu(\mathbb{RP}^n)}.$$

The inequality (4.10) then follows immediately from this and the remarks above. $\qquad\square$

4.2 Error estimates for interpolation reproducing $\Pi_{\mathcal{J}}$

The interpolation operator associated with κ that reproduces $\Pi_{\mathcal{J}} = \text{span}\{\phi_{j,s} : j \in \mathcal{J}, \ 1 \leq s \leq d_j\}$ is

$$I_{X,\mathcal{J}}f = \sum_{\xi \in X} a_{\xi,\mathcal{J}}\kappa(x,\xi) + p_{\mathcal{J}}, \ p_{\mathcal{J}} \in \Pi_{\mathcal{J}}, \ \text{ and } \ \sum_{\xi \in X} a_{\xi,\mathcal{J}}\phi_{j,s}(\xi) = 0, \ j \in \mathcal{J}.$$

We wish to estimate the L_2-norm of $I_{X,\mathcal{J}}f - f$. To do that, we will need to obtain various equations relating $I_{X,\mathcal{J}}f$, $I_X f$, and $p_{\mathcal{J}}$. (Since the choice of $\tilde{\kappa}_j$, $j \in \mathcal{J}$, obviously has no effect on $I_{X,\mathcal{J}}$, we can and will assume that $\tilde{\kappa}_j > 0$, $j \in \mathcal{J}$.) Let $P_{\mathcal{J}}$ be the L_2 orthogonal projection onto $\Pi_{\mathcal{J}}$. Note that the interpolant $I_{X,\mathcal{J}}f = \sum_{\xi \in X} a_{\xi,\mathcal{J}}\kappa(x,\xi) + p_{\mathcal{J}}$ consists of two terms. It is easy to show that the first term belongs to $(\Pi_{\mathcal{J}})^\perp$ and, of course, $p_{\mathcal{J}} \in \Pi_{\mathcal{J}}$. Consequently,

$$P_{\mathcal{J}}(I_{X,\mathcal{J}}f - f) = p_{\mathcal{J}} - P_{\mathcal{J}}f. \tag{4.11}$$

Next, because both interpolate f, the difference $\sum_{\xi \in X}(a_\xi - a_{\xi,\mathcal{J}})\kappa(x,\xi)$ interpolates $p_{\mathcal{J}}$. This implies that

$$I_X f - I_{X,\mathcal{J}}f = I_X p_{\mathcal{J}} - p_{\mathcal{J}},$$

From this, we have

$$\|I_{X,\mathcal{J}}f - f\|_{L_2(\mathbb{M})} \leq \|I_X f - f\|_{L_2(\mathbb{M})} + \|p_{\mathcal{J}} - I_X p_{\mathcal{J}}\|_{L_2(\mathbb{M})} \tag{4.12}$$

Since $p_{\mathcal{J}} - I_X p_{\mathcal{J}}|_X = 0$, the second term on the right can be estimated via Theorem 3.3, provided h is sufficiently small. Making the estimate yields this bound:

$$\|p_{\mathcal{J}} - I_X p_{\mathcal{J}}\|_{L_2(\mathbb{M})} \leq Ch^m \|p_{\mathcal{J}} - I_X p_{\mathcal{J}}\|_{W_2^m(\mathbb{M})}.$$

17

In addition, by (4.5), the norm induced by κ is equivalent to the $W_2^m(\mathbb{M})$ norm, and thus we have that $\|p_{\mathcal{J}} - I_X p_{\mathcal{J}}\|_{W_2^m(\mathbb{M})} \leq C\|p_{\mathcal{J}} - I_X p_{\mathcal{J}}\|_\kappa \leq C\|p_{\mathcal{J}}\|_\kappa$, where the rightmost inequality follows from the minimization properties of $I_X p_{\mathcal{J}}$ in the norm $\|\cdot\|_\kappa$. From the definition of the κ norm, where we have assumed $\tilde{\kappa}_j = 1$, $j \in \mathcal{J}$, it is easy to see that $\|p_{\mathcal{J}}\|_\kappa = \|p_{\mathcal{J}}\|_{L_2(\mathbb{M})}$. Combining the various inequalities then yields

$$\|p_{\mathcal{J}} - I_X p_{\mathcal{J}}\|_{L_2(\mathbb{M})} \leq Ch^m \|p_{\mathcal{J}}\|_{L_2(\mathbb{M})}.$$

Using this on the right in (4.12) gives us

$$\|I_{X,\mathcal{J}} f - f\|_{L_2(\mathbb{M})} \leq \|I_X f - f\|_{L_2(\mathbb{M})} + Ch^m \|p_{\mathcal{J}}\|_{L_2(\mathbb{M})}. \tag{4.13}$$

Furthermore, employing (4.11) in conjunction with this inequality, we see that

$$\|I_{X,\mathcal{J}} f - f\|_{L_2(\mathbb{M})} \leq \|I_X f - f\|_{L_2(\mathbb{M})} + Ch^m \left(\|I_{X,\mathcal{J}} f - f\|_{L_2(\mathbb{M})} + \|P_{\mathcal{J}} f\|_{L_2(\mathbb{M})}\right)$$

Choosing h so small that $Ch^m < \frac{1}{2}$ and then manipulating the expression above, we obtain this result.

Lemma 4.5. *Let* $f \in L_2(\mathbb{M})$. *For all h sufficiently small, we have*

$$\|I_{X,\mathcal{J}} f - f\|_{L_2(\mathbb{M})} < 2\|I_X f - f\|_{L_2(\mathbb{M})} + Ch^m \|P_{\mathcal{J}} f\|_{L_2(\mathbb{M})}. \tag{4.14}$$

We now arrive at the error estimates we seek.

Theorem 4.6. *Let $\mathbb{M}$ be a two-point homogeneous manifold and let κ be a polyhamonic kernel of the form (4.2), with $\deg(\pi(x)) = m$. Assume that the conditions on $X \subset \mathbb{M}$ in Proposition 3.4 are satisfied. If μ is an integer satisfying $m \geq \mu > n/2$, then, provided h is sufficiently small,*

$$\|I_{X,\mathcal{J}} f - f\|_{L_2(\mathbb{M})} \leq \begin{cases} Ch^m \|f\|_{W_2^m(\mathbb{M})}, & \text{all } \mathbb{M}, \text{ and } f \in W_2^m(\mathbb{M}), \\ Ch^\mu \|f\|_{W_2^\mu(\mathbb{M})}, & \mathbb{M} = \mathbb{S}^n, \mathbb{RP}^n, \text{ and } f \in W_2^\mu(\mathbb{M}). \end{cases} \tag{4.15}$$

Proof. In (4.14), we have $\|P_{\mathcal{J}} f\|_{L_2(\mathbb{M})} \leq \|f\|_{L_2(\mathbb{M})} \leq \|f\|_{W_2^\mu(\mathbb{M})}$; in addition, the various bounds on $\|I_X f - f\|_{L_2(\mathbb{M})}$ follow from (4.7), (4.8), and (4.10). Combining these yields (4.15). $\square$

4.2.1 Optimal convergence rates for interpolation via surface splines

For spheres, the interpolants constructed from the restricted thin-plate splines defined in (4.3) converge at double the rates discussed above – namely, $\mathcal{O}(h^{2m})$ rather than $\mathcal{O}(h^m)$ –, provided f is smooth enough. This also applies in $SO(3)$ for the kernels given in (4.4). The spaces $\Pi_{\mathcal{J}}$ being reproduced here are, for $\mathbb{S}^n$, the spherical harmonics of degree $m-1$ or less; and for $SO(3)$, the Wigner D-functions for representations of the rotation group, again having order $m-1$ or less. The precise result is stated below.

Proposition 4.7 ([22, Corollaries 5.9 & 5.10]). *Suppose $m > n/2$ and let $I_{X,\mathcal{J}}$ denote the interpolation operator corresponding to the restricted surface spline defined in (4.3) for $s = m - n/2$. Then, there is a constant C depending on ρ, m and n such that, for a sufficiently dense set $X \subset \mathbb{S}^n$, and for $f \in C^{2m}(\mathbb{S}^n)$, the following holds:*

$$\|I_{X,\mathcal{J}} f - f\|_\infty \leq Ch^{2m} \|f\|_{C^{2m}(\mathbb{S}^n)},$$

Similarly, for the kernels in (4.4), if $f \in C^{2m}(SO(3))$, then $\|I_{X,\mathcal{J}} f - f\|_\infty \leq Ch^{2m} \|f\|_{C^{2m}(SO(3))}$.

4.3 Lagrange functions and Lebesgue constants

If $\chi_\xi(x)$ is the Lagrange function associated with a kernel κ and a space $\Pi_{\mathcal{J}}$, then, by (2.7), the weights in the quadrature formula have the form $c_\xi = \int_{\mathbb{M}} \chi_\xi(x) d\mu(x)$, $\xi \in X$. Our aim is to use properties of χ_ξ to obtain bounds on these weights. Before we do this, we will need the following decay estimates for χ_ξ.

Proposition 4.8 ([22, Theorem 5.5]). *Suppose that $\mathbb{M}$ is an n-dimensional compact, two-point homogeneous manifold and that κ is a polyharmonic kernel, with $\deg(\pi(x)) = m$, where $m > n/2$. There exist positive constants h_0, ν and C, depending only on m, $\mathbb{M}$ and the operator $\mathcal{L}_m = \pi(-\Delta)$ so that if the set of centers X is quasi-uniform with mesh ratio ρ and has mesh norm $h \le h_0$, then the Lagrange functions for interpolation by κ with auxiliary space $\Pi_{\mathcal{J}}$ satisfy*

$$|\chi_\xi(x)| \le C\rho^{m-n/2} \max\left(\exp\left(-\frac{\nu}{h} d(x,\xi) \right), h^{2m} \right). \tag{4.16}$$

There are two results that we want to obtain. First, we want to estimate the size of each weight in terms of the mesh norm h; and second, we want to estimate $\sum_{\xi \in X} |c_\xi|$.

We only need to estimate $\|\chi_\xi\|_{L_1(\mathbb{M})}$, since $|c_\xi| \le \|\chi_\xi\|_{L_1(\mathbb{M})}$. Our approach is to divide the manifold into a ball $B = B_{\xi,R_h}$, having radius R_h and center ξ, and its complement $B^{\complement}$. The radius R_h is the "break-even" distance in (4.16); it is obtained by solving $\exp\left(-\frac{\nu}{h} R_h \right) = h^{2m}$ for R_h. The result is $R_h = \frac{2m}{\nu} h |\log(h)|$. By (4.16), we obtain

$$\int_{B_0^{\complement}} |\chi_\xi(x)| d\mu(x) \le C\rho^{m-n/2} \mu(\mathbb{M}) h^{2m}.$$

Next, again by (4.16), we have that

$$\int_B |\chi_\xi(x)| d\mu(x) \le C'\rho^{m-n/2} \int_0^{R_h} e^{-r\nu/h} r^{n-1} dr < C'\rho^{m-n/2} \underbrace{\int_0^\infty e^{-r\nu/h} r^{n-1} dr}_{(n-1)!(h/\nu)^n}$$

Consequently, $|c_\xi| \le \|\chi_\xi\|_{L_1(\mathbb{M})} \le C\rho^{m-n/2}(h/\nu)^n (1 + h^{2m-n}\nu^n)$. Because $2m > n$, for h small enough, it follows that

$$|c_\xi| \le \|\chi_\xi\|_{L_1(\mathbb{M})} \le C'\rho^{m-n/2} h^n, \tag{4.17}$$

where $C' = C'(\mathbb{M}, \kappa, \mathcal{J})$.

The next result concerns the boundedness of the Lebesgue constant, which played a significant role in section 2.3 in the analysis of the stability of the quadrature operator.

Proposition 4.9 ([22, Theorem 5.6]). *Let the notation be the same as that in Proposition 4.8. If $h \le h_0$, then the Lebesgue constant, $\Lambda_{X,\mathcal{J},\kappa} = \max_{x \in \mathbb{M}} \sum_{\xi \in X} |\chi_\xi(x)|$, associated with X, $\mathcal{J}$, and κ, satisfies the bound $\Lambda_{X,\mathcal{J},\kappa} \le C$, where C depends only on m, ρ, and $\mathbb{M}$.*

4.4 Quadrature via polyharmonic kernels

In this section, we will employ the various properties of polyharmonic kernels, which are of course invariant, to obtain results concerning accuracy and stability of the associated quadrature formulas.

Theorem 4.10. *Suppose that $\mathbb{M}$ is an n-dimensional compact, two-point homogeneous manifold and that κ is a polyharmonic kernel, with $\deg(\pi(x)) = m$, where $m > n/2$. Let $X \subset \mathbb{M}$ be a finite set having mesh ratio $\rho_X \le \rho$, $\Pi_{\mathcal{J}} = \text{span}\{\phi_{j,s} : j \in \mathcal{J}, 1 \le s \le d_j\}$, and Q_{V_X} be*

19

the corresponding quadrature operator given in Definition 2.3 . The norm of Q_{V_X} is bounded, $\|Q_{V_X}\|_{C(\mathbb{M})} \leq \mu(\mathbb{M})\Lambda_{X,\mathcal{J},\kappa} \leq C_{m,\rho,\mathbb{M}}$, and the error satisfies the estimates

$$\left|Q_{V_X}(f) - \int_{\mathbb{M}} f d\mu\right| \leq \begin{cases} Ch^m\|f\|_{W_2^m(\mathbb{M})}, & \text{all } \mathbb{M}, \text{ and } f \in W_2^m(\mathbb{M}), \\ Ch^\mu\|f\|_{W_2^\mu(\mathbb{M})}, & \mathbb{M} = \mathbb{S}^n, \mathbb{RP}^n, \text{and } f \in W_2^\mu(\mathbb{M}), \ n/2 < \mu \leq m. \end{cases} \tag{4.18}$$

Finally, the standard deviation σ_Q from Proposition 2.4 satisfies $\sigma_Q \leq C\sigma_\nu h^{n/2}$, where $C = C(\rho, m, \mathbb{M}, \mathcal{J})$.

Proof. The norm estimate follows from (2.16) and Proposition 4.9. The error estimate is a consequence of (2.14) and Theorem 4.6. Finally, the bound on σ_Q is a consequence of Proposition 2.4, Proposition 4.9, and the bound on $\|\chi_\xi\|$ in (4.17). $\square$

At present, the most important compact two-point homogeneous manifolds are spheres and projective spaces (especially $\mathbb{S}^2$ and $SO(3)$). As we discussed in section 4.2.1, the restricted thin-plate splines (4.3) on $\mathbb{S}^n$ and similar kernels (4.4) on $SO(3)$ give interpolants with optimal convergence for smooth target functions. This also is reflected in the accuracy of the corresponding quadrature formulas:

Corollary 4.11. *Let X, ρ_X, ρ, m, $\Pi_{\mathcal{J}}$ be as in Theorem 4.10. Take $\mathbb{M} = \mathbb{S}^n$ or $SO(3)$ and Q to be the quadrature operator corresponding to the restricted surface spline defined in (4.3) or to that for the polyharmonic kernel in (4.4). If X is a sufficiently dense in $\mathbb{M}$, then there is a constant $C = C(m, n, \rho)$ such that for a sufficiently dense set $X \subset \mathbb{S}^n$ and for all $f \in C^{2m}(\mathbb{S}^n)$,*

$$\left|Q(f) - \int_{\mathbb{M}} f d\mu\right| \leq Ch^{2m}\|f\|_{C^{2m}(\mathbb{S}^n)}, \ \text{where } C = C(m, n, \rho),$$

in addition to the bounds on $\|Q\|$ and σ_Q from Theorem 4.10 holding.

Because of applications in physical sciences and engineering, $\mathbb{S}^2$ is undoubtedly the most important of the manifolds treated here. In the next section, we give some numerical examples for $\mathbb{S}^2$ and the $m = 2$ surface spline $\Phi(t) = (1 - t)\log(1 - t)$ that validate the above theory.

5 Numerical results for $\mathbb{S}^2$

We begin with a brief overview of how the quadrature weights can be computed in an efficient manner for the $m = 2$ surface spline $\Phi(t) = (1 - t)\log(1 - t)$ defined in (4.3), using the local Lagrange preconditioner developed in [12]. This is followed by a description of the nodes used in the numerical experiments and some properties of the resulting surface spline quadrature weights and their stability. Finally, we give some results validating the error estimates from the previous section.

5.1 Computing the quadrature weights

The $m = 2$ surface spline kernel is conditionally positive definite of order 1 and the finite dimensional subspace Π associated with it consists of all spherical harmonics of degree ≤ 1, i.e. $\Pi := \text{span}\{Y_{0,0}, Y_{1,0}, Y_{1,1}, Y_{1,2}\}$, where $Y_{\ell,k}$ is the degree ℓ and order k spherical harmonic and $0 \leq k \leq 2\ell + 1$. Given a set $X = \{x_j\}_{j=1}^N$ of distinct nodes on $\mathbb{S}^2$, the quadrature weights c for this kernel can be computed by first solving (2.10) for $c_\perp$ and then computing c via (2.11). In these equations, $A_{i,j} = (1 - x_i \cdot x_j)\log(1 - x_i \cdot x_j)$, $i, j = 1, \ldots, N$, and Ψ is the N-by-4 matrix

with columns $\Psi_{i,1} = Y_{0,0}(x_i)$ and $\Psi_{i,k+2} = Y_{1,k}(x_i)$, for $i = 1, \cdots, N$, $k = 0, 1, 2$. Additionally, $J = \begin{bmatrix} 4\pi & 0 & 0 & 0 \end{bmatrix}^T$ and $J_0 = 2\pi(4 \log(2) - 1)$.

Since Ψ only has 4 columns, computing $\Psi(\Psi^T\Psi)^{-1}J$ in (2.10) can be done rapidly using, for example, QR decomposition. Thus, the bulk of the computational effort in computing the quadrature weights is in solving for $c_\perp$ in (2.10). Since the matrix A is dense, direct methods cannot be realistically applied for large N, and one must then resort to iterative methods. However, for iterative methods to be useful, one must apply an effective preconditioner to the system. In [12], we developed a powerful preconditioner for (2.10) based on *local Lagrange functions* and combined it with the generalized minimum residual (GMRES) iterative method [38]. The basic idea of the preconditioner is, for every node $x_j \in X$, to compute the surface spline interpolation weights for a small subset of nodes about x_j consisting its $p = M(\log N)^2$ nearest neighbors, where M is suitably chosen constant. The data for each interpolant is taken to be cardinal about x_j. This is similar to the preconditioner used in [8] for interpolation on a 2-D plane, however, in that study the number of nodes in the local interpolants did not grow with N and it was observed that the preconditioner broke down as N increased. As demonstrated in [12], by allowing the nodes to grow very slowly with N the preconditioner remained effective and the total number of iterations required by GMRES to reach a desired tolerance did not increase with N. We refer the reader to [12] for complete details on the construction of the preconditioner.

In the numerical results that follow, we used the preconditioned GMRES technique from [12] with $p = 2\lceil(\log N)^2\rceil$ and a relative tolerance of 10^{-12} to solve for $c_\perp$ in (2.10). We then used this in (2.11) to find c. Table 2 lists the number of GMRES iterations required to compute $c_\perp$ for three different quasi-uniform node families, which are described in the next section. We see from the table that the number of iterations remains fairly for constant as N grows for all three families of nodes.

Icosahedral		Fibonacci		Min. Energy	
N	Iterations	N	Iterations	N	Iterations
2562	8	2501	9	2500	9
10242	7	10001	8	10000	8
23042	7	22501	11	22500	7
40962	7	40001	8	40000	8
92162	6	62501	10	62500	7
163842	7	90001	10	90000	7
256002	6	160001	8	160000	7
655362	6	250001	10	250000	7

Table 2: Number of GMRES iterations required to compute $c_\perp$ in (2.10) using the preconditioned iterative method developed [12] for determining the $m = 2$ surface spline. The quadrature weights are then computed from (2.11). In all cases, the relative tolerance of the GMRES method was set to 10^{-12}.

We conclude by noting that as part of the iterative method, matrix-vector products involving A must be computed. Since A is dense, this requires $\mathcal{O}(N^2)$ operations per matrix-vector product. In the computations performed for this study, these products were computed directly, making the overall cost of the weight computation $\mathcal{O}(N^2)$. In a follow up study we will explore the use of fast, approximate matrix-vector products using the algorithm described in [30]. By using this algorithm, it may be possible to reduce the total cost of computing the weights (or a surface spline interpolant) to $\mathcal{O}(N \log N)$.

5.2 Nodes, weights, and stability

We consider three quasi-uniform families of nodes for the numerical experiments. The first is the icosahedral nodes, which are obtained from successive refinement of the 20 spherical triangular faces formed from the icosahedron. The second are the Fibonacci (or *phyllotaxis*) nodes, which mimic certain plant behavior in nature (see, for example, [15] and the references therein). The third are the quasi-minimum energy nodes, which are obtained by arranging the nodes so that their Riesz energy is near minimal [25]. In the examples below, a power of 3 was used in the Riesz energy and the nodes were generated using the technique described in [5]. The mesh norm for all three of these families satisfies $h \sim \frac{1}{\sqrt{N}}$, where N is the total number of nodes. The mesh ratio ρ stays roughly constant for the Fibonacci and quasi-minimum energy nodes as N increases. For the icosahedral points ρ grows slowly with N since the spacing of the nodes decreases faster towards the vertices of the triangles of the base icosahedron than at the centers [39]. However, in the numerical examples that follow, this increase seems to be of little concern. All three of these families of nodes are quite popular in applications; see, for example [14, 31, 37, 43] for the icosahedral nodes, [29, 41, 44] for the Fibonacci nodes, and [10, 11, 40, 50] for the quasi-minimum energy nodes. Quadrature over these nodes also plays an important role in applications, for example, for computing the mass of a certain quantity, the energy for a certain process, or the spectral decomposition of some data.

It should be noted that previous studies have been devoted to developing quadrature formulas and error estimates for icosahedral [1, Ch. 5] and Fibonacci [24] nodes. However, these results rely on the specific construction of the node sets and cannot be applied to more general quasi-uniformly distributed nodes such as the quasi-minimum energy nodes.

Figures 1 (a)–(c) show examples of the different families of nodes and provide a visualization of the values of the corresponding quadrature weights for the $m = 2$ surface spline. The geometric pattern of the icosahedral nodes in part (a) of this figure are clearly reflected in the values of the corresponding quadrature weights. This is also true of the Fibonacci nodes in part (b), which have a slight clustering near their seed value (in this case the north pole), but then are quasi-uniformly distributed. There are no clear patterns for the minimum energy nodes in part (c) of Figure 1, as these are not distributed in a discernible pattern. Looking at the color bars in each of the plots we see that the range of values of the weights is similar between the different node families and comparable to $1/N$, and are also positive.

To estimate σ_Q in (2.17), and hence the stability of the quadrature weights in the presence of noise, we performed the following experiments. For each family of nodes, a value of N was selected and then a sample set was generated consisting of 500 values of the N-point quadrature of different independent, identically, distributed, zero mean (quasi) random data. The standard deviation of the sample sets was then computed to estimate σ_Q. The results are plotted in Figure 2 as a function of N for each of the three families of nodes. Comparing the results to the dashed line on the plot, we see that the estimated σ_Q decreases like $\mathcal{O}(N^{-1/2})$, or like $\mathcal{O}(h)$ since $h \sim N^{-1/2}$ for these families of nodes. This is in perfect agreement with the rate predicted by the last part of Theorem 4.10 for the surface splines.

5.3 Convergence results

Two target functions of different smoothness were used to test the error estimates of Theorem 4.10 and Corollary 4.11. The target functions were chosen so that the Funk-Hecke formula (see, for example, [1, §2.5]) could be used to determine their exact integral over $\mathbb{S}^2$. Letting $x, x_c \in \mathbb{S}^2$ and g be a zonal kernel, i.e. $g(x, x_c) = g(x \cdot x_c)$, such that $g \in L^1[-1, 1]$, the Funk-Hecke formula gives
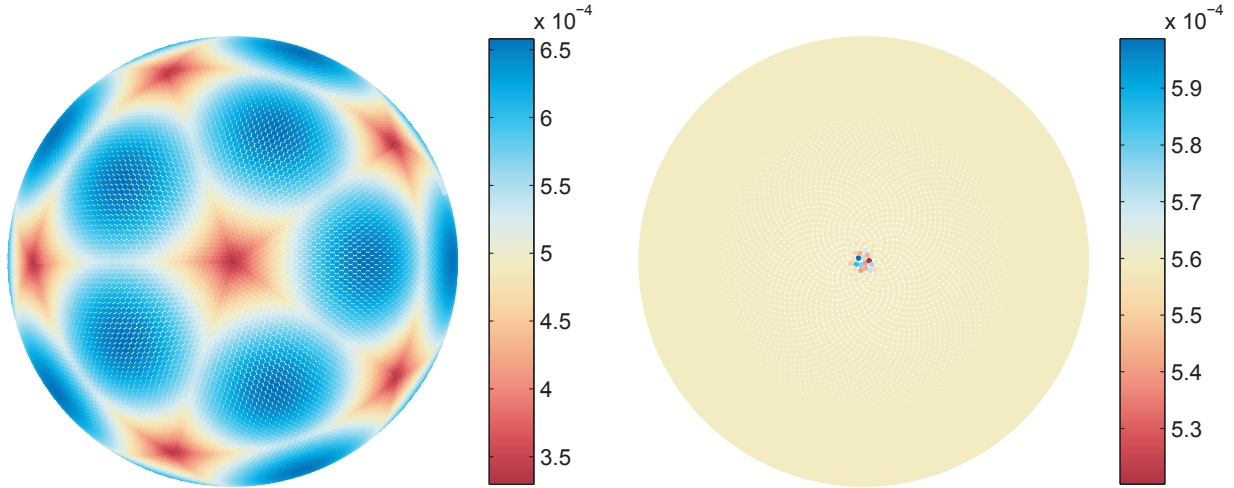
(a) Icosahedral nodes and weights, $N = 23042$ (b) Fibonacci nodes and weights, $N = 22501$
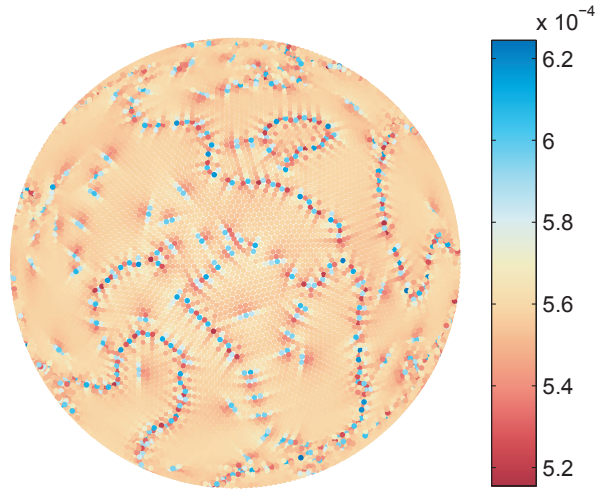
(c) Quasi-minimum energy nodes and weights, $N = 22500$

Figure 1: Visualization of the different families of nodes used in the numerical experiments and the corresponding quadrature weights for the $m = 2$ spherical spline. The nodes are plotted on $\mathbb{S}^2$ using an orthographic projection about the north pole. Each node has been given a color corresponding to the value of the quadrature weight for that node.

the following result:

$$\int_{\mathbb{S}^2} g(x \cdot x_c) Y_{\ell,k}(x) d\mu(x) = \frac{4\pi a_\ell}{2\ell + 1} Y_{\ell,k}(x_c), \tag{5.1}$$

where $Y_{\ell,k}$ is any degree ℓ, order k spherical harmonic, and a_ℓ is the ℓth coefficient in the Legendre expansion of $g(t)$.

The following two kernels were used in constructing the target functions:

$$g_1(t) = -(2 - 2t)^{1/4}, \tag{5.2}$$

$$g_2(t) = \frac{1 - \varepsilon^2}{(1 + \varepsilon^2 - 2\varepsilon t)^{\frac{3}{2}}} \quad (0 < \varepsilon < 1), \tag{5.3}$$
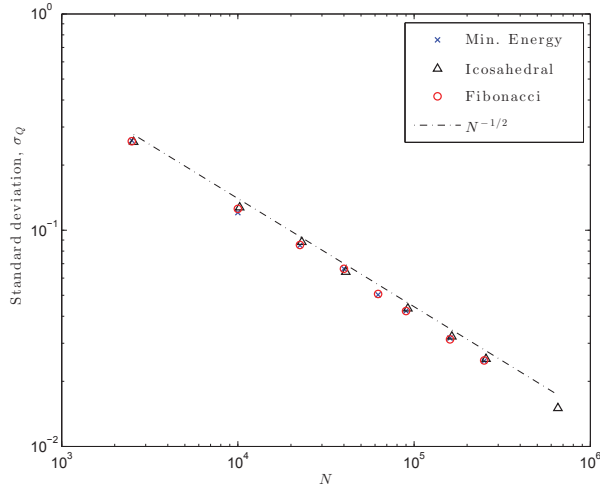
23

Figure 2: Estimate of the standard deviation σ_Q in (2.17) for the different families of nodes. The estimate is based on sample sets of 500 N-point quadratures of different independent, identically, distributed, zero mean (quasi) random data with a standard deviation of 1. The dashed line corresponds to taking all weights equal in (2.17), which gives $\sigma_Q = 4\pi\sigma_\nu N^{-1/2}$. This confirms the stability estimate in the last part of Theorem 4.10.

which are known as the *potential spline* kernel of order $1/4$ and the *Poisson* kernel, respectively. The Legendre expansion coefficients for these kernels are given as follows (see [3]):

$$g_1 : \quad a_\ell = \frac{(-1)^{\ell+1}\sqrt{2}(\Gamma\left(\frac{5}{4}\right))^2(2\ell+1)}{\Gamma\left(\frac{5}{4}-\ell\right)\Gamma\left(\frac{9}{4}+\ell\right)}, \tag{5.4}$$

$$g_2 : \quad a_\ell = (2\ell+1)\varepsilon^\ell. \tag{5.5}$$

The smoothness of these kernels is of course determined by the decay rate of the Legendre coefficients a_ℓ. For g_1, we have $a_\ell \sim \ell^{-3/2}$, which means g_1 belongs to every Sobolev space $W_2^\mu(\mathbb{S}^2)$ with $\mu < \frac{5}{2}$. While for g_2 the Legendre coefficients decay exponentially fast, which means $g_2 \in C^\infty(\mathbb{S}^2)$, analytic in fact.

Using the above results, we define the following two target integrands:

$$f_1(x) = \sum_{k=1}^{41} \text{sign}(Y_{20,k}(x_c))Y_{20,k}(x)g_1(x \cdot x_c), \tag{5.6}$$

$$f_2(x) = \sum_{k=1}^{41} \text{sign}(Y_{20,k}(x_c))Y_{20,k}(x)g_2(x \cdot x_c), \tag{5.7}$$

where $x_c = (\cos(-2.0281)\sin(0.76102), \sin(-2.0281)\cos(0.76102), \sin(0.76102))$ and $\varepsilon = 2/3$ for g_2; see Figure 3 (a) and (b) for plots of these respective functions. Integrating these functions over $\mathbb{S}^2$ and applying the Funk-Hecke formula (5.1) gives

$$\int_{\mathbb{S}^2} f_1(x)d\mu(x) = 0.014830900415995, \tag{5.8}$$

$$\int_{\mathbb{S}^2} f_2(x)d\mu(x) = 0.032409262543520. \tag{5.9}$$
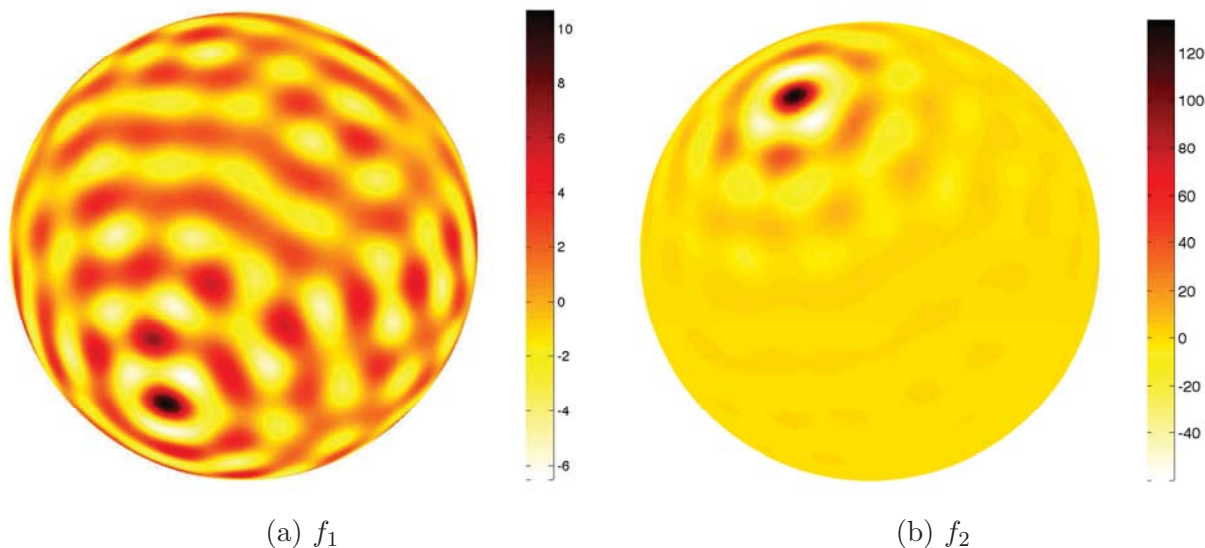
24

(a) f_1 (b) f_2

Figure 3: Target integrands used to test the error estimates. (a) $f_1(x)$ from (5.6) and (b) $f_2(x)$ from (5.7).

Both f_1 and f_2 inherit their smoothness directly from g_1 and g_2, respectively. Thus, f_1 belongs to every Sobolev space $W_2^\mu(\mathbb{S}^2)$ with $\mu < \frac{5}{2}$ and $f_2 \in C^\infty(\mathbb{S}^2)$.

Tables 3 and 4 display the relative errors in the N-point quadrature of f_1 and f_2, respectively, for the different family of nodes, while Figures 4(a) and (b) display these respective results graphically on a $\log-\log$ scale. Focusing first on the results for f_1 in Figure 4(a) and comparing the results to the included dashed line, it is clear that for all three families the error is decreasing approximately like $\mathcal{O}(N^{-1.25})$. Since $h \sim N^{-1/2}$ for these families of nodes, this observed rate of decrease in the error is approximately $\mathcal{O}(h^{2.5})$, which is precisely the rate predicted by the estimates in Theorem 4.10 for functions with f_1's smoothness. Doing a similar comparison of the results for f_2 in Figure 4(b), we see that the errors associated with the icosahedral nodes very clearly decrease like $\mathcal{O}(N^{-2})$. The results for the other two nodes are not as clear, but for larger values of N the errors do appear to be decreasing approximately like $\mathcal{O}(N^{-2})$. Again, because of the relationship between h and N for these nodes, the errors for f_2 are thus decreasing approximately like $\mathcal{O}(h^4)$. This is the expected rate from Corollary 4.11 since f_2 is infinitely smooth and we have used the $m = 2$ surface spline.

Icosahedral		Fibonacci		Min. Energy	
N	Rel. Error	N	Rel. Error	N	Rel. Error
2562	1.926×10^{-1}	2501	5.112×10^{-3}	2500	3.048×10^{-2}
10242	3.533×10^{-2}	10001	5.549×10^{-3}	10000	6.848×10^{-2}
23042	1.286×10^{-2}	22501	1.770×10^{-3}	22500	2.480×10^{-2}
40962	6.268×10^{-3}	40001	1.040×10^{-3}	40000	1.217×10^{-2}
92162	2.273×10^{-3}	62501	6.460×10^{-4}	62500	6.989×10^{-3}
163842	1.107×10^{-3}	90001	4.068×10^{-4}	90000	4.393×10^{-3}
256002	6.330×10^{-4}	160001	1.844×10^{-4}	160000	2.083×10^{-3}
655362	1.957×10^{-4}	250001	1.085×10^{-4}	250000	1.228×10^{-3}

Table 3: Relative error in the N-point quadrature of the "rough" target function f_1 in (5.6) for the different families of nodes.

Icosahedral		Fibonacci		Min. Energy	
N	Rel. Error	N	Rel. Error	N	Rel. Error
2562	3.358×10^{-2}	2501	1.045×10^{-4}	2500	6.951×10^{-2}
10242	1.888×10^{-3}	10001	4.690×10^{-5}	10000	5.932×10^{-4}
23042	3.642×10^{-4}	22501	3.189×10^{-6}	22500	1.077×10^{-4}
40962	1.143×10^{-4}	40001	7.437×10^{-6}	40000	2.730×10^{-5}
92162	2.245×10^{-5}	62501	1.805×10^{-6}	62500	8.276×10^{-6}
163842	7.098×10^{-6}	90001	9.204×10^{-7}	90000	6.944×10^{-6}
256002	2.897×10^{-6}	160001	3.009×10^{-7}	160000	1.250×10^{-6}
655362	4.433×10^{-7}	250001	1.411×10^{-7}	250000	5.414×10^{-7}

Table 4: Relative error in the N-point quadrature of the "smooth" target function f_2 in (5.7) for the different families of nodes.

(a) Rough target, f_1.
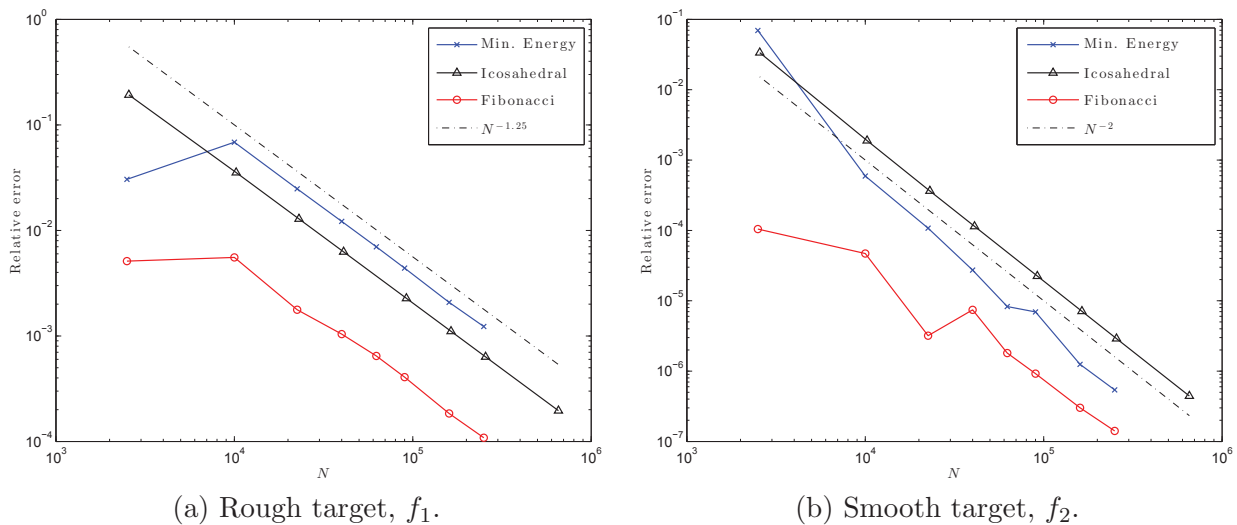

(b) Smooth target, f_2.

Figure 4: Relative errors in the N-point quadratures of (a) f_1 and (b) f_2 for the three different families of nodes. The mesh-norm for all three families of nodes satisfies $h \sim N^{-1/2}$, so that the dashed lines in the figures indicate convergence like (a) $\mathcal{O}(h^{2.5})$ and (b) $\mathcal{O}(h^4)$. These are the predicted convergence rates from Theorem 4.10 and Corollary 4.11, respectively.

We conclude by noting that the nodes and quadrature weights used in the numerical experiments above are available for download from [49].

6 Quadrature on Manifolds Diffeomorphic to Homogeneous Spaces

Numerical integration of functions defined on smooth surfaces that are diffeomorphic to $\mathbb{S}^2$ arise in a number of applications. For example, the shape of the earth, as well as the other planets, is a "flattened sphere" – i.e., an oblate spheroid, which is diffeomorphic to a sphere. To numerically compute integrals over the earth's surface then requires quadrature formulas over oblate spheroids. In addition, the need for numerical integration over various surfaces also arises in boundary element formulations of continuum problems in $\mathbb{R}^3$ [1, Ch. 6]. In this section, we discuss quadrature in a more general context. We will show how to use quadrature weights for a homogeneous manifold $\mathbb{M}$ to obtain an invariant, coordinate independent quadrature formula for a smooth Riemannian

26

manifold $\mathbb{L}$ diffeomorphic to $\mathbb{M}$. Of course, the case in which $\mathbb{L}$ is an oblate spheroid and $\mathbb{M} = \mathbb{S}^2$ is of special interest.

Recall that a C^∞ manifold $\mathbb{L}$ is diffeomorphic to $\mathbb{M}$ if there is a C^∞ bijection $F : \mathbb{M} \to \mathbb{L}$. Let g_{ij} be the Riemannian metric for $\mathbb{M}$. Suppose that $\mathbb{L}$ has the metric h_{ij}. Consider a local chart $(U, \phi : U \to \mathbb{R}^n)$ near $p_0 \in \mathbb{M}$. Using this chart we have coordinates $x = (x^1, \ldots, x^n) = \phi(p)$ and a parametrization $p = \phi^{-1}(x)$.

We can use (U, ϕ) to produce a local chart $(V, \psi : V \to \mathbb{R}^n)$ near $q_0 = F(p_0) \in \mathbb{L}$. Simply let $V = F(U) \subset \mathbb{L}$ and $\psi = \phi \circ F^{-1}$. The coordinates for V are thus $x = \psi(q)$, and so the two metrics g_{ij} and h_{ij} can be expressed in terms of the same set of coordinates. In these coordinates, the volume elements are given by

$$d\mu_{\mathbb{M}}(x) = \sqrt{\det(g_{ij}(x))}\, dx^1 \cdots dx^n \text{ and } d\mu_{\mathbb{L}}(x) = \sqrt{\det(h_{ij}(x))}\, dx^1 \cdots dx^n.$$

It follows that

$$d\mu_{\mathbb{L}}(x) = \underbrace{\sqrt{\frac{\det(h_{ij}(x))}{\det(g_{ij}(x))}}}_{w(x)}\, d\mu_{\mathbb{M}}(x). \tag{6.1}$$

Suppose that we now make a change of coordinates, from $x = \phi(p)$ to new coordinates $y = \varphi(p)$, or $x = x(y)$. Let $x'(y)$ be the Jacobian matrix for the transformation, and let $J(y) = \det(x'(y))$. In y coordinates, the metrics are $\tilde{g}(y) = (x'(y))^T g(x(y)) x'(y)$ and $\tilde{h}(y) = (x'(y))^T h(x(y)) x'(y)$. Consequently, we have that

$$\det(\tilde{g}_{ij}(y)) = J(y)^2 \det(g_{ij}(x(y))) \text{ and } \det(\tilde{h}_{ij}(y)) = J(y)^2 \det(h_{ij}(x(y))),$$

and, furthermore, that

$$w(x(y)) = \sqrt{\frac{\det(h_{ij}(x(y)))}{\det(g_{ij}(x(y)))}} = \sqrt{\frac{\det(h'_{ij}(y))}{\det(g'_{ij}(y))}} = \tilde{w}(y).$$

This means that $w \circ \phi(p) = \tilde{w} \circ \psi(p) =: W(p)$ is thus a scalar invariant that is independent of the choice of coordinates. In terms of integrals, we have

$$\int_{\mathbb{L}} f(q) d\mu_{\mathbb{L}}(q) = \int_{\mathbb{M}} f \circ F(p) W(p) d\mu_{\mathbb{M}}(p). \tag{6.2}$$

An invariant, coordinate independent quadrature formula for $\mathbb{L}$ can be obtained from the one for $\mathbb{M}$. We have the following result.

Proposition 6.1. *Let X denote the set of centers on $\mathbb{L}$ and let $X' = F^{-1}(X)$ be the corresponding set on $\mathbb{M}$. Suppose that we have a quadrature formula for $\mathbb{M}$ with weights $\{C_{\xi'}\}_{\xi' \in X'}$. Then we have the following quadrature formula for $\mathbb{L}$,*

$$Q_{\mathbb{L}}(f) := \sum_{\xi \in X} f(\xi) c_\xi, \text{ where } c_\xi := W(F^{-1}(\xi)) C_{F^{-1}(\xi)}. \tag{6.3}$$

Proof. Applying the quadrature formula for the homogeneous manifold $\mathbb{M}$ to the integral on the right-hand side of (6.2) yields

$$Q_{\mathbb{M}}\big(f \circ F(p) W(p)\big) = \sum_{\xi' \in X'} f \circ F(\xi') W(\xi') C_{\xi'}.$$

Since $\xi' = F^{-1}(\xi)$, we have $f \circ F(\xi') = f(\xi)$ and $W(\xi') = W(F^{-1}(\xi))$. Taking $c_\xi = W(F^{-1}(\xi)) C_{F^{-1}(\xi)}$ we obtain (6.3). $\qquad \square$

Oblate spheroid Consider the oblate spheroid $\mathbb{L}$, $x^2 + y^2 + z^2/a^2 = 1$, where $0 < a < 1$, and the 2-sphere $\mathbb{S}^2 (= \mathbb{M})$, $X^2 + Y^2 + Z^2 = 1$. The diffeormorphism between the two manifolds is $F(X,Y,Z) := (X, Y, aZ)$; that is, $(x, y, z) = (X, Y, aZ)$. Our aim is to find the scale factor W. Since the end result will be coordinate independent, we choose to work in spherical coordinates (θ, ϕ), where θ is the longitude and ϕ is the latitude on $\mathbb{S}^2$. (The north pole is $(0, 0, 1)$.) Obviously, for $\mathbb{L}$ we have $x = \sin\theta \cos\phi$, $y = \sin\theta \sin\phi$, $z = a\cos\theta$. The metric for the sphere is $dS^2 = d\theta^2 + \sin^2(\theta)d\phi^2$. The metric for $\mathbb{L}$ is the Euclidean metric $dx^2 + dy^2 + dz^2$ on $\mathbb{R}^3$ restricted to $\mathbb{L}$. Making a straightforward calculation, one can show that the metric for $\mathbb{L}$ is

$$ds^2 = (\cos^2\theta + a^2\sin^2\theta)d\theta^2 + \sin^2\theta d\phi^2 = \left(a^2 + (1-a^2)\cos^2\theta\right)d\theta^2 + \sin^2\theta d\phi^2.$$

Consequently, the volume element for $\mathbb{L}$ is

$$d\mu_{\mathbb{L}} = \sqrt{a^2 + (1-a^2)\cos^2\theta}\,\sin\theta\,d\theta d\phi = \underbrace{\sqrt{a^2 + (1-a^2)\cos^2\theta}}_{w(\theta,\phi)}\,d\mu_{\mathbb{S}^2}.$$

To put this in invariant form on $\mathbb{S}^2$, we use $Z = \cos\theta$ to obtain $W(X, Y, Z) = \sqrt{a^2 + (1-a^2)Z^2}$. Pulling this back to $\mathbb{L}$, we have $W \circ F^{-1}(x, y, z) = \sqrt{a^2 + (a^{-2} - 1)z^2}$. The weights for $Q_{\mathbb{L}}$ are thus

$$c_\xi = \sqrt{a^2 + (a^{-2} - 1)\xi_z^2}\,C_{(\xi_x, \xi_y, \xi_z/a)}.$$

As we mentioned above, the earth is approximately an oblate spheroid. The parameter a is the ratio of the polar radius to the equatorial radius. The *flattening* of the earth is $f = 1 - a$, and has the approximate value $f \approx 1/300$ (cf. Earth Fact Sheet [48]). From this, we get that $a \approx 299/300$, and so $W \circ F^{-1}(x, y, z) \approx \sqrt{0.993 + 0.007z^2}$. This factor varies between 0.9967 and 1, about 0.3%. Even so, it could affect the accuracy of the quadrature formula for functions with large values near the equator. As an aside, Jupiter has $f \approx 1/15$ (cf. Jupiter Fact Sheet (ellipticity) [48]), and for it the change in $W \circ F^{-1}$ would be a hefty 7%.

7   Concluding Remarks and Acknowledgments

In this paper we provide a general method for generating accurate and stable quadrature rules for scattered nodes on homogeneous spaces. This extends an approach to kernel quadrature on spheres in two important directions. First, it provides an easy tool for obtaining quadrature weights on general manifolds (homogeneous spaces) with more general kernels (conditionally positive definite kernels) whereby weights are calculated by solving a single kernel interpolation problem. Second, for problems on the sphere (and oblate spheroids) a number of recent breakthroughs in kernel interpolation with certain conditionally positive definite kernels permits us to compute quadrature weights in a stable and computationally efficient manner, and in such a way that quadrature error decays at a nearly optimal rate.

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