Energies, Group Invariant Kernels and Numerical Integration on Compact Manifolds

S. B. Damelin, J. Levesley, D. L. Ragozin and X. Sun

February 10, 2008

AMS(MOS) Classification: Primary 41A05; Secondary 41A15, 41A63

Keywords: Compact Homogeneous Manifold, Discrepancy, Group, Energy, Invariant Kernels, Invariant Polynomial, Numerical Integration, Projection Kernels, Projective Space, Quadature, Reflexive Manifold, Riesz Kernel, Spherical Harmonic, Sphere, Torus, Weight.

Abstract

The purpose of this paper is to derive quadrature estimates on compact, homogenous manifolds embedded in Euclidean spaces, via energy functionals associated with a class of group-invariant kernels which are generalizations of zonal kernels on the spheres or radial kernels in euclidean spaces. Our results apply, in particular, to weighted Riesz kernels defined on spheres and certain projective spaces. Our energy functionals describe both uniform and perturbed uniform distribution of quadrature point sets.

1 Introduction

Let M be a compact d-dimensional manifold ($d \geq 1$) embedded in the Euclidean space $\mathbb{R}^{d+k}$ for some $k \geq 0$. We are interested in obtaining estimates pertaining to numerical integration over M. In the classical setting, the domain of integration is the interval $[-1, 1]$. As is well known, the nodes of the celebrated Gaussian quadrature formula are the zeros of the unique monic polynomial of minimal mean-square deviation on $[-1, 1]$. In other words, the

nodes are the zeros of the unique solution of an extremal problem. In [3], this idea was extended to spheres whereby the authors related numerical integration to an extremal problem using Riesz energy and a class of smooth kernels defined on the spheres which are called *zonal* in what follows. The purpose of this paper is to derive quadrature estimates on compact and homogeneous manifolds M embedded in Euclidean space, via energy functionals associated with a class of group-invariant kernels that are generalizations of zonal kernels on the sphere and radial kernels in euclidean spaces. The quadrature nodes are determined by the criterion that they minimize certain energy functionals defined on M in complete analogy with classical Gauss quadrature. We make, in particular, use of methods of [13, 14] which allow us to demonstrate that certain kernel approximation techniques on spheres may be extended to manifolds which are the orbit of a compact group.

Our investigation in the present article allows us to uncover and identify natural geometric ideas which as we discover, extend past the sphere to a large class of manifolds. Our results are expected to provide a wide range of interdisciplinary applications in areas diverse as meteorology, imaging, financial mathematics, geoscience and material science; see [6, 14] and the references cited therein. Our results apply, in particular to kernels such as weighted Riesz kernels and classes of smooth functions defined on spheres and certain projective spaces. We mention that point sets that minimize discrete Riesz energies enjoy uniform distribution densities on M whereas weighted energies are useful in describing point sets which have density which may not be uniform. The later points, are found for example in computational modeling of surfaces; see for example [6, 7] and the references cited therein.

The remainder of this paper is structured as follows. In Sections 2-4, we outline important ideas we need concerning harmonic analysis on compact manifolds and convolution of group invariant kernels. In Section 5 we state and prove our main result on error estimates of numerical integrations on spheres and projective spaces. The estimate will be established for functions in certain reproducing kernel Hilbert spaces. In Section 6 we extend the estimate obtained in Section 5 to a wider class of smooth functions on spheres and on certain projective spaces.

2 Harmonic analysis on compact homogeneous manifolds

In the sequel we will assume further that M^d is a compact homogeneous C^∞ d-dimensional manifold embedded as the orbit of a compact group G of isometries of $\mathbb{R}^{d+k}$; i.e. there is an $\eta \in M$ (often referred to as the pole) such that $M = \{g\eta : g \in G\}$. In fact, for any $\zeta = g\eta \in M$, since $G = Gg$, $M = G\eta = Gg\eta = G\zeta$. So any point in M can be chosen as the pole. In the special case that for each pair $x, y \in M$, there is a $g_{x,y} \in G$ with $g_{x,y}x = y$ and $g_{x,y}y = x$, M is called a *reflexive* compact homogeneous manifold. Natural reflexive examples to keep in mind are S^d, $d > 1$, the d-dimensional spheres. Each sphere is realized as the subset of $\mathbb{R}^{d+1}$ which is the orbit of any unit vector under the action of $SO(d+1)$, the group of $d+1$ dimensional orthogonal matrices of determinant 1. For $x, y \in S^d$ $g_{x,y} \in SO(d+1)$ can be chosen to be any rotation by π radians about any diameter of a great circle containing x, y which joins the antipodal bisectors of the two arcs between x, y; see [10] for a good description of these later spaces. When $d = 1$, no such rotation of S^1 exists, so the circle realized as the orbit of the rotation group, $SO(2)$, is non-reflexive. Other non-reflexive examples are the flat tori $(S^1)^k$ realized as subsets of $\mathbb{R}^{2k} = (\mathbb{R}^2)^k$ which are the orbits of $([1\ 0]^t)^k$, the k-fold product of the column vector $[1\ 0]^t$ under $G_k = SO(2)^k$. If the G_k are enlarged to be the groups $O(2)^k$, where $O(m)$ is the group of all m dimensional orthogonal matrices, then these homogeneous realizations of the flat tori *are* reflexive, since in the i-th plane, reflection in the bisector of the line-segment $\overline{x_i y_i}$ interchanges x_i, y_i. Henceforth, we will assume that d and k are fixed for a given M.

A kernel $\kappa : M \times M \to (0, \infty]$ is termed *zonal* (or G-invariant) if $\kappa(x, y) = \kappa(gx, gy)$ for all $g \in G$ and $x, y \in M$. Since the maps in G are isometries of Euclidean space, they preserve both Euclidean distance and the (arc-length) metric $d(\cdot, \cdot)$ induced on the components of M by the Euclidean metric. Thus the distance kernel $d(x, y)$ on M is zonal, as are all functions $\psi(d(x, y))$, $\psi : \mathbb{R} \to \mathbb{R}$. Moreover, the radial functions, $\phi(\|x - y\|)$, on Euclidean space that depend only on $\|x - y\|$, the Euclidean distance between x, y are also zonal functions; see [5, 13, 15] and the references cited therein. The manifold M carries a Borel *surface* (G-invariant) measure μ such that $\mu(M) = 1$, where G-invariant means

$$g \cdot \mu(B) := \mu(gB), \forall g \in G \text{ and } \forall \text{ Borel sets } B.$$

With this G-invariant measure μ, we define the inner product of real functions $f_1, f_2 : M \to \mathbb{R}$

$$(f_1, f_2) = \int_M f_1 f_2 d\mu.$$

In what follows, we will assume henceforth that a kernel κ always satisfies the following three conditions:

i. The kernel κ is continuous off the "diagonal" of $M \times M$, and is lower semi-continuous on $M \times M$. Here, the "diagonal" of $M \times M$ means the set $\{(x, y) \in M \times M : x = y\}$.

ii. For each fixed $x \in M$, $\kappa(x, \cdot)$ and $\kappa(\cdot, y)$ are integrable with respect to surface measure μ; i.e., $\kappa(x, \cdot)$ and $\kappa(\cdot, y) \in L_1(\mu)$.

iii. For each non-trivial finite signed measure ν on M, we have

$$\int_M \int_M \kappa(x, y) d\nu(x) d\nu(y) > 0,$$

where the iterated integral may be infinite.

We will say that a kernel κ is admissible if κ satisfies all the three conditions above. We note that kernels satisfying (iii) are referred to as "strictly positive definite" in the literature. Examples of admissible kernels are the weighted Riesz kernels

$$\kappa(x, y) = w(x, y)\|x - y\|^{-s}, \quad 0 < s < d, \quad x, y \in M.$$

Here $w : M \times M \to (0, \infty]$ is chosen so that κ is admissible. If, in addition, w is G-invariant, then κ is zonal. Such kernels (in the case $w \equiv 1$), arise naturally in describing uniform distributions of electrons on rectifiable manifolds such as the sphere S^d. The uniformity arises because of the singularity in the kernel which forces points not to stay close to each other. See [6, 7] and the references cited therein for more details. If w is active, then perturbations of the distributions in the electrons are allowed. Perturbations of this type, arise for example in problems in computer modeling. For the sphere S^d, zonal type kernels were introduced into the study of discrepancy first by Damelin and Grabner in [3].

Harmonic analysis on M, in our case, requires the construction of polynomials on M. In this regard, if Π_j is the space of all polynomials of total

degree j on the space $\mathbb{R}^{d+k}$, then $P_j := \Pi_j|_M$ is the space of degree j polynomials on M. When $j < 0$, $\Pi_j = \{0\}$ and so $P_j = \{0\},\ j < 0$. We can also construct the sets $H_j := P_j \bigcap P_{j-1}^{\perp}$, where the orthogonality is with respect to the inner product $(\cdot, \cdot)$. We call H_j the *harmonic* polynomials of degree j.

It is straightforward to show that H_j is G-invariant, in the sense that $g \cdot p_j \in H_j$ for all $p_j \in H_j$ and $g \in G$, where for any function f on M, $g \cdot f$ is defined by

$$g \cdot f(x) := f(g^{-1}x), \forall g \in G \text{ and } \forall x \in M. \tag{1}$$

Moreover, each H_j has an orthogonal decomposition into irreducible G-invariant subspaces (i.e., subspaces with no proper G-invariant subspace)

$$H_j = \oplus_{l=1}^{h_j} \Xi_{j,l}.$$

The machinery above, gives the following easily proved but important fact.

Lemma 2.1 *Let M be a compact homogeneous space embedded in Euclidean space. The harmonic polynomials, $\sum_{i=0}^{\infty} H_i$ are dense in $C(M)$, where "perp", in the definition of H_i is with respect to the inner product $(.)$ induced by the tangential portion of Lebesgue measure(equivalently the measure derived from the Riemannian structure on M which is induced from the embedding).*

3 Group invariant kernels and smooth convolution

The *kernel operator* T_κ associated with a kernel $\kappa(x, y)$ is defined by

$$(T_\kappa f)(x) = \int_M \kappa(x, y) f(y) d\mu(y), \quad x \in M \tag{2}$$

for those Borel measurable f for which the right hand side exists. More generally, $T_\kappa(\nu)(x) := \int_M \kappa(x, y) d\nu(y)$. When κ is zonal, then T_κ is G-equivariant in the sense expressed by the following equation:

$$T_\kappa(g \cdot f) = g \cdot T_\kappa(f), \tag{3}$$

where $g \cdot f$ is defined at (1). We now form the *convolution product* of kernels κ and σ,

$$(\kappa * \sigma)(x, y) = \int_M \kappa(x, z)\sigma(z, y) d\mu(z),\ x, y \in M$$

which is the kernel whose associated operator $T_{\kappa*\sigma}$ is the product of the operators T_κ and T_σ; i.e., $T_{\kappa*\sigma} = T_\kappa T_\sigma$. When κ, σ are zonal, then it is easy to show that $\kappa*\sigma$ is itself zonal, since the product of G-equivariant operators is obviously G-equivariant. However, when κ and σ are merely symmetric, we have

$$\kappa * \sigma(x, y) = \sigma * \kappa(y, x).$$

Thus the convolution product of symmetric kernels, $\kappa*\sigma$, is symmetric when and only when κ and σ commute with respect to the convolution product, just as the product of symmetric(self-adjoint) operators is symmetric exactly when the operators commute. Now in case M is *reflexive*, then

i. Any zonal kernel κ is symmetric, since $\kappa(x, y) = \kappa(g_{x,y}x, g_{x,y}y) = \kappa(y, x)$.

ii. Two zonal kernels commute since $\kappa * \sigma$ is zonal, hence symmetric.

Now let an admissible kernel κ be given. For a signed Borel measure on M, its κ-energy integral is defined by:

$$\mathcal{E}_\kappa(\nu) = \int_M \int_M \kappa(x, y) d\nu(x) d\nu(y).$$

Notice that the κ-energy is unchanged when $\kappa(x, y)$ is replaced by its symmetrized form $\frac{1}{2}(\kappa(x, y) + \kappa(y, x))$, which is also an admissible kernel. Hence, we will assume that κ is *symmetric* when dealing with questions about κ-energy.

We remark that the above integral may be infinite though from our assumptions of positive definiteness and lower semicontinuity on κ, combined with the strict convexity of the κ-energy, we know that either $\mathcal{E}_\kappa(\nu) = +\infty$ for all $\nu \neq 0$ or

$$\min_{\{\nu:\, \nu(1)=1\}} \mathcal{E}_\kappa(\nu)$$

exists and the minimizer is unique. We now show remarkably that for all compact homogeneous C^∞ manifolds M and admissible symmetric zonal kernels κ, the unique finite κ-energy minimizer above exists and is precisely the normalized surface measure μ. That this is true is by no means obvious. For the sphere, this fact was established in [3] for a class of zonal kernels. We have:

Lemma 3.1 *The normalized surface measure μ has finite κ-energy. Moreover, $\mathcal{E}_\kappa(\nu) > \mathcal{E}_\kappa(\nu(1)\mu)$ for all $\nu \neq \nu(1)\mu$. So among all signed ν with $\nu(1) = 1$, the κ-energy is uniquely minimized by the normalized surface measure μ.*

Proof: By the admissibility condition (ii) and the fact that κ is zonal, for any $g \in G$

$$\int \kappa(x,y)d\mu(y) = \int \kappa(gx,y)d\mu(y) < \infty.$$

Since $Gx = M$, integrating the constant right hand side over G yields (with dg the Haar measure on G)

$$\begin{aligned} &= \int_G \int_M \kappa(gx,y)d\mu(y)dg \\ &= \int_M \int_M \kappa(z,y)d\mu(y)d\mu(z) \\ &= \mathcal{E}_\kappa(\mu) < \infty. \end{aligned}$$

Now suppose ν is any finite signed measure. Then either $+\infty = \mathcal{E}_\kappa(\nu) > \mathcal{E}_\kappa(\mu)$. Or, $\mathcal{E}_\kappa(\nu) < \infty$ and this finite energy can be written, using the symmetry of κ, as the sum of three finite summands as follows:

$$\begin{aligned} \mathcal{E}_\kappa(\nu) &= \mathcal{E}_\kappa(\nu(1)\mu \ + (\nu - \nu(1)\mu)) \\ &= \mathcal{E}_\kappa(\nu(1)\mu) + \mathcal{E}_\kappa(\nu - \nu(1)\mu) \\ &\qquad + 2\int\int \kappa(x,y)d(\nu(1)\mu)(x)d(\nu - \nu(1)\mu)(y). \end{aligned}$$

Since κ is zonal, for any $g \in G$ the last summand is

$$\begin{aligned} & 2\int\int \kappa(x,y)d(\nu(1)\mu)(x)d(\nu - \nu(1)\mu)(y) \\ &= \ 2\int\int \kappa(gx,gy)d(\nu(1)\mu)(x)d(\nu - \nu(1)\mu)(y) \\ &= \ 2\int\int \kappa(x,y)d(\nu(1)g\cdot\mu)(x)d(g\cdot\nu - \nu(1)g\cdot\mu)(y) \\ &= \ 2\int\int \kappa(x,y)d(\nu(1)\mu)(x)d(g\cdot\nu - \nu(1)\mu)(y). \end{aligned}$$

But averaging this constant function of g over G and changing the order of integration twice, the inner integral is, $\int (g\cdot\nu - \nu(1)\mu)dg = \nu(1)\mu - \nu(1)\mu = 0$, so we see the summand is 0. Hence,

$$\mathcal{E}_\kappa(\nu) = \mathcal{E}_\kappa(\nu(1)\mu) + \mathcal{E}_\kappa(\nu - \nu(1)\mu) > \mathcal{E}_\kappa(\nu(1)\mu)$$

since κ is strictly positive definite. ■

4 N-point discrete κ energy

Let $N \geq 1$. Let Z be a finite subset of M with $|Z| = N$. We define the N-point discrete κ-energy associated with Z by

$$E_\kappa(Z) = \frac{1}{N^2} \sum_{\substack{y,z\in Z \\ y\neq z}} \kappa(y,z).$$

Since κ is continuous off the diagonal of $M \times M$, and is lower semi-continuous on $M\times M$, the minimal N-point discrete κ-energy can be attained at some $Z^* \subset M$ with $|Z^*| = N$. That is

$$E_\kappa(Z^*) = \inf_{Z\subset M} E_\kappa(Z),$$

where the infimum is taken over all subsets Z of M with $|Z| = N$. We will simply call such a set Z^* a minimal energy configuration. It is clear that for each $g \in G$, gZ^* is also a minimal energy configuration. Heuristics suggests that probability measures supported on minimal energy configurations provide good approximation to the measure μ in the sense that the integral of a continuous $f : M \to \mathbb{R}$ with respect to μ is approximated well by a discrete sum over the points of Z. This was first shown by Damelin and Grabner in [3] for a class of unweighted Riesz kernels on the sphere S^d, $d \geq 2$, for a class of Lipchitz functions, where μ is the rotation invariant probability measure on S^d. For the circle, S^1, it is easy to see that every minimal energy configuration corresponds to the set of vertices of a regular N-gon and are thus the best points to use for numerical integration for equally weighted quadrature rules.

We find it convenient to work with the full quadratic form

$$\sum_{y,z\in Z} \kappa(y,z).$$

However, the diagonal entries in the above quadratic form, $\kappa(x,x), x \in Z$, may not be finite. As a matter of fact, for Riesz kernels, these diagonal entries are infinity. The lower semi-continuity of the kernel κ allows us to consider approximating κ from below by a sequence of smooth kernels via convolution. To make this precise, let us fix an $\alpha_0 > 0$. Assume that, for each $0 < \alpha < \alpha_0$, σ_α is a zonal kernel such that the convolution kernel $\kappa_\alpha := \kappa * \sigma_\alpha$ is well defined and satisfies the following properties:

a. κ_α is continuous on $M \times M$.

b. κ_α is strictly positive definite.

c. $\kappa_\alpha(x,y) \le \kappa(x,y)$ for all $x, y \in M$.

d. $\lim_{\alpha\downarrow 0} \kappa_\alpha(x,y) = \kappa(x,y)$ for all $x, y \in M$.

If the above construction is possible, we say that κ is *strongly admissible*. The construction details are often delicate and entail case-by-case analysis. We offer two examples in which the criteria are all satisfied.

Example 1. Wagner [18], [19] studied a kind of modified Riesz kernel in the form

$$\kappa_\alpha(x,y) = (1+\alpha-xy)^{-s/2},\ x,y \in S^2,\ 0 < s < 1,\ \alpha > 0,$$

where xy denotes the Euclidean inner product of the vectors x and y. On S^2, this kernel can be written as the convolution of the Riesz kernel $\kappa(x,y) = (1-xy)^{-1/2}$ and the smooth kernel σ_α with the Fourier-Legendre expansion

$$\sigma_\alpha(x,y) = \frac{1}{\sqrt{2\pi}} \sum_{n=0}^{\infty} h^{2n+1} Q_n(xy),$$

in which $h = 2/(\sqrt{\alpha} + \sqrt{4+\alpha})$, and Q_n is the Legendre polynomial normalised so that $\|Q_n\|^2_{2,[-1,1]} = 2n+1$. This expansion can be found in the work of Hubbert and Baxter [11].

Example 2 On the 2-torus embedded in $\mathbb{R}^4$, one may form kernels as products of univariate kernels:

$$\kappa(x,y) = \rho(x_1,y_1)\rho(x_2,y_2), \quad x_1,y_1,x_2,y_2 \in S^1,$$

where

$$\rho(s,t) = |1-st|^{-1/4}.$$

The kernel

$$\rho_\alpha(s,t) = (1+\alpha-st)^{-1/4},\ s,t \in S^1,$$

can be written as a convolution of ρ with the analytic kernel

$$\sigma_\alpha(s,t) = \sum_{n=0}^{\infty} \frac{F(n+1/4,n+1/2;2n+1;\frac{4}{4+\alpha})}{F(n+1/4,n+1/2;2n+1;1)} T_n(st),$$

where T_n is the Chebyshev polynomial and $F(a,b;c;z)$ is the Gauss hypergeometric function ([1, 15.1.1]). Again see [11] for details.

5 Quadrature for polynomials on compact, reflexive homogeneous manifolds

In this section and henceforth, we will need to assume that M is reflexive. In this case, we need some more machinery on reflexive spaces. Firstly, if $d_{j,l} = \dim \Xi_{j,l}$ and $\{Y_{j,l}^1, \ldots, Y_{j,l}^{d_{j,l}}\}$ is any orthonormal basis for $\Xi_{j,l}$, then

$$P_{j,l}(x,y) := \sum_{m=1}^{d_{j,l}} Y_{j,l}^m(x) Y_{j,l}^m(y), \quad x,y \in M,$$

is the unique G-invariant reproducing kernel for $\Xi_{j,l}$. In other words, if $T_{j,l}$ is the orthogonal projector onto $\Xi_{j,l}$,

$$T_{j,l}f(x) := \int_M P_{j,l}(x,y) f(y) d\mu(y), \quad x \in M. \tag{4}$$

In particular,

$$T_{j,l}f(x) := (T_{j,l}f, P_{j,l}(\cdot,x)), \quad x \in M. \tag{5}$$

Moreover, for any $g \in G$, $\{g \cdot Y_{j,l}^1, \ldots, g \cdot Y_{j,l}^{d_{j,l}}\}$ is another orthonormal basis for $\Xi_{j,l}$. So the uniqueness of a reproducing kernel shows $P_{j,l}(g^{-1}x, g^{-1}y) = P_{j,l}(x,y)$; i.e., $P_{j,l}$ is zonal. From its definition, it is obvious that each $P_{j,l}$ is symmetric. Observe that the self-adjoint projectors $T_{j,l}$ associated with the G-invariant kernels $P_{j,l}$ are *kernel operators* $T_{P_{j,l}}$ defined by Equation (2). By reflexivity, we conclude that for any zonal κ T_κ commutes with each projector $T_{j,l}$ and hence $T_\kappa T_{j,l}$ is a G-equivariant self-adjoint linear transformation of $\Xi_{j,l}$. Since $\Xi_{j,l}$ is an irreducible G-invariant subspace, $T_\kappa T_{j,l} = a_{j,l} T_{j,l}$ for some scalar $a_{j,l}$, i.e. the subspace $\Xi_{j,l}$ of degree j harmonic polynomials is also a subspace of the T_κ eigenspace associated to the eigenvalue $a_{j,l}$. Moreover, if κ is admissible, so strictly positive definite, and $0 \neq p \in \Xi_{j,l}$, we have $\mathcal{E}_\kappa(p\mu) = a_{j,l}\|p\|^2_{L_2(\mu)} > 0$; i.e., all $a_{j,l} > 0$. Thus, on reflexive spaces, by the density of harmonic polynomials, each admissible zonal kernel κ has an expansion with positive coefficients (convergent in an appropriate operator norm)

$$\kappa(x,y) = \sum_{j=0}^{\infty} \sum_{l=1}^{h_j} a_{j,l}(\kappa) P_{j,l}(x,y),\ x,y \in M.$$

Let us define the *native space* $\mathcal{N}_\kappa$ for an admissible κ via the kernels defined by Equation (2) and coefficients $a_{j,l}$ defined by Equation (6).

Let

$$\mathcal{N}_\kappa := \left\{ f : \|f\|^2_{\mathcal{N}_\kappa} := \sum_{j=0}^{\infty} \sum_{l=1}^{h_j} \frac{\|T_{j,l} f\|^2}{a_{j,l}(\kappa)} < \infty \right\}.$$

In this paper, we are interested in the error of integration for a class of smooth real valued functions f on M, when f is given on a point set $Z \subset M$ of finite cardinality $N \geq 1$. The error in integration is defined by

$$R(f,Z) := \int_M f(y) d\mu(y) - \frac{1}{N} \sum_{z \in Z} f(z).$$

We may now state the main result of this section.

Theorem 5.1 *Let κ be strongly admissible on M and $Z \subset M$ be a point subset of cardinality $N \geq 1$. Fix $x \in Z$. Then, for $0 < \alpha < \alpha_0$, the following estimate holds true for every $f \in \mathcal{N}_{\kappa_\alpha}$:*

$$|R(f,Z)| \ \leq \ \|f\|_{\mathcal{N}_{\kappa_\alpha}} \left(E_\kappa(Z) + \frac{1}{N} \kappa_\alpha(x,x) - a_{0,1}(\kappa_\alpha) \right)^{1/2}.$$

Remark The special case of a sphere S^d and a class of G invariant kernels on S^d, the above theorem was established first in [3]. A further elaboration on the estimate of Theorem 5.1 is also appropriate. Notice that the right hand side of the estimate depends on both the function and the point set Z. One way to obtain tighter upper bounds in Theorem 5.1, is to link the kernel studied with the function space with a different measure of energy. This is done in [4] but at the price of smaller classes of functions. Another way, is to replace the energy function in the right hand side by a potential. This is done in [2]. Again there are trade-offs with the generality of Theorem 5.1. Future research clearly demands the study of tight estimates that simultaneously incorporate different discrepancy factors and different levels of smoothness of kernels.

The proof of Theorem 5.1 uses two Lemmas. The first is:

Lemma 5.2 *Let $Z \subset M$ be a point set of cardinality $N \geq 1$, and let κ be a strongly admissible kernel. Then, for $0 < \alpha < \alpha_0$, we have*

$$\frac{1}{N^2} \sum_{y,z \in Z} \kappa_\alpha(y,z) \leq E_\kappa(Z) + \frac{1}{N} \kappa_\alpha(x,x).$$

Proof: Since $\kappa_\alpha(x,y) \leq \kappa(x,y)$ for all $\alpha < \alpha_0$ we see that

$$\frac{1}{N^2} \sum_{y,z \in Z} \kappa_\alpha(y,z) = \frac{1}{N^2} \sum_{\substack{y,z \in Z \\ y \neq z}} \kappa_\alpha(y,z) + \frac{1}{N} \kappa_\alpha(x,x)$$

$$\leq E_\kappa(Z) + \frac{1}{N} \kappa_\alpha(x,x). \quad \blacksquare$$

Next, we have the analogue of the well known Funk-Hecke formula:

Lemma 5.3 *For any $x, z \in M$,*

$$(P_{j,l} * P_{j,l})(x,z) = \int_M P_{j,l}(x,y) P_{j,l}(y,z) d\mu(y) = P_{j,l}(x,z).$$

Proof: This is an immediate consequence of the fact that $T_{P_{j,l}}$ is the orthogonal projector onto $\Xi_{j,l}$, so

$$T_{P_{j,l} * P_{j,l}} = T_{P_{j,l}} T_{P_{j,l}} = T_{P_{j,l}}. \quad \blacksquare$$

We now proceed with the proof of Theorem 5.1:

Proof Theorem 5.1: We first write

$$f = \sum_{j=0}^{\infty} \sum_{l=1}^{h_j} T_{j,l} f.$$

Then

$$\begin{aligned} -R(f,Z) &= \frac{1}{N} \sum_{z \in Z} f(z) - \int_M f(y) d\mu(y) \\ &= \frac{1}{N} \sum_{j=1}^{\infty} \sum_{l=1}^{h_j} T_{j,l} f(z). \end{aligned}$$

However,

$$T_{j,l} f(z) = \int_M P_{j,l}(z,y) T_{j,l} f(y) d\mu(y),$$

so that

$$R(f,Z) = \sum_{j=1}^{\infty} \sum_{l=1}^{h_j} \int_M T_{j,l} f(y) Q_{j,l}(y,Z) d\mu(y), \tag{6}$$

where

$$Q_{j,l}(y,Z) = \frac{1}{N} \sum_{z \in Z} P_{j,l}(y,z).$$

Using the fact that

$$\|Q_{j,l}(y,Z)\|^2 = \frac{1}{N^2} \sum_{y,z \in Z} P_{j,l}(y,z),$$

we can apply the Cauchy-Schwarz inequality to (6) to obtain

$$\begin{aligned} |R(q,Z)|^2 &\leq \left(\sum_{j=1}^{\infty} \sum_{l=1}^{h_j} \frac{1}{a_{j,l}(\kappa_\alpha)} \|T_{j,l} f\|^2 \right) \left(\sum_{j=1}^{\infty} \sum_{l=1}^{h_j} a_{j,l}(\kappa_\alpha) \|Q_{j,l}(y,Z)\|^2 \right) \\ &\leq \|f\|^2_{\mathcal{N}_{\kappa_\alpha}} \left(\frac{1}{N^2} \sum_{y,z \in Z} \kappa_\alpha(y,z) - a_{0,1}(\kappa_\alpha) \right), \end{aligned}$$

where the last line follows by the positivity of the coefficients $a_{j,l}(\kappa_\alpha)$, and the positive definiteness of the kernels $P_{j,l}$ on $\Xi_{j,l}$. Using Lemma 4.2, we arrive at the required result. ■

Since for a polynomial q of degree n we have the following inequality

$$\|q\|_{\mathcal{N}_\alpha} \leq \max_{1\leq j,1\leq \nu_n} \frac{\|q\|_2}{a_{j,l}(\kappa_\alpha)},$$

we immediately have the following corollary.

Corollary 5.4 *Let κ be strongly admissible on M and $Z \subset M$ be a point subset of cardinality $N \geq 1$. Fix $x \in Z$. If $q \in P_n$, then, for $0 < \alpha < \alpha_0$,*

$$|R(q,Z)| \quad \leq \quad \max_{j\leq n,\, l\leq \nu_n} \frac{1}{(a_{j,l}(\kappa_\alpha))^{1/2}} \|q\|_2 \left(E_\kappa(Z) + \frac{1}{N}\kappa_\alpha(x,x) - a_{0,1}(\kappa_\alpha) \right)^{1/2}.$$

6 Quadrature for smooth functions on the sphere and projective spaces

In this last section, we extend Theorem 5.1 to a class of smooth functions on projective spaces and sphere, which are examples of so-called 2-point homogeneous manifolds (see below for a definition). Let F be one of the following fields: $Q = \{r_0 + r_1 i + r_2 j + r_3 k : r_i \in \mathbb{R}\}$ (quaternions), $C = \{q \in Q : r_2 = r_3 = 0\}$ (complex) or $\mathbb{R}$. Let F have dimension m ($= 4, 2, 1$ respectively) over the reals. The length squared of an element $f \in F$ is $|f|^2 = r_0^2 + r_1^2 + r_2^2 + r_3^2$. Writing a vector $f \in F^{m+1}$ in the form $f = (f_1, f_2, \cdots, f_{m+1})$, the sphere $S(F^{m+1}) = \{f \in F^{m+1} : \sum_{i=1}^{m+1} |f_i|^2 = 1\}$. The standard definition of the projective space $P^{dm}(F)$ is the set of points on the sphere $S(F^{m+1})$, where points x and y are identified if $x = \alpha y$ for some $\alpha \in F$ with $|\alpha| = 1$.

This description of the projective spaces does not give us a homogeneous manifold, but, as shown in [17] and described in [16], one can provide an equivalent definition of the projective spaces as orbits of a compact subgroup of an orthogonal group acting in $\mathbb{R}^{d+k}$ for some d and k. This construction is given explicitly in [16].

To extend our result we require some additional machinery which we now state; see [16]. We denote by $C^k(M)$, the space of k times, continuously

differentiable functions $f : M \to \mathbb{R}$. It is well known that M carries an inner product and the action of G on M translates this inner product to the tangent spaces at each point in M so that M has a well defined Riemannian metric which in turn induces a well defined arc-length metric ρ on $M \times M$. To define suitable moduli of smoothness, let $\mathbf{g}$ be the natural Lie algebra on M formed by taking the set of all skew-symmetric operators D on $\mathbb{R}^{d+k}$ such that $\exp tD \in G$, $\forall t \in G$. Let G act on $C(M)$ as in (1). Then we define the space $C^1(M)$ as the space of functions $f \in C(M)$, such that for each $D \in \mathbf{g}$, there exists $D(f) \in C(M)$ such that

$$\lim_{t \to 0} ||t^{-1}(\exp tD \cdot f - f) - D(f)||_\infty = 0.$$

The space C^k, $k \in \mathbb{N}$, $k \geq 2$ is then defined inductively.

We define a *first modulus of continuity* on $C(M)$ by

$$\omega_1(f, h) := \sup \{|f(x) - f(y)| : \rho(x, y) \leq h\}$$

Similarly, if x_+, x, x_- denote equaly spaced points along a geodesic in M, then the *second modulus of continuity* on $C(M)$ is defined by way of

$$\omega_2(f, h) := \sup \{|f(x_+) - 2f(x) + f(x_-)| : \rho(x_+, x) \leq h\}.$$

Now choose an orthonormal basis $D_1, ...D_j$ for $\mathbf{g}$ for some $j \geq 1$. Then define inductively for $f \in C^{k+1}$, $k \geq 0$:

$$\omega_r(f^{k+1}; h) := \sum_{i=1}^{j} \omega_r \left((D_i(f))^{(k)}; h \right), \ r = 1, 2,$$

where $f^{(0)} = f$.

A two-point homogeneous space is one for which, given two pairs of points, x_1, y_1 and x_2, y_2 on M, with $\rho(x_1, y_1) = \rho(x_2, y_2)$, there exists a $g \in G$ such that $gx_1 = x_2$ and $gy_1 = y_2$. If this is the case then, for $\rho(x_1, y_1) = \rho(x_2, y_2)$ and a zonal kernel κ,

$$\kappa(x_2, y_2) = \kappa(gx_1, gy_1) = \kappa(x_1, y_1),$$

so that κ is a function only of the distance between the points. In this case we have a simple representation of the reproducing kernels as a univariate polynomial of an inner product. This is exploited in [16].

Also, it is straightforward to see that such spaces are reflexive. Indeed, choose two points x and y in M and let $d(x,y) = \rho = d(y,x)$ where the metric $d(\cdot,\cdot)$ is induced on the components of M by the Euclidean metric. Now, using the 2 point homogeneous condition applied to the two pair $(x_1,x_2) = (x,y)$ and $(y_1,y_2) = (y,x)$, there is a $g \in G$ such that $gx = y$ and $gy = x$. Hence g switches x and y.

In order to prove our extension, we use the following result given in Theorems 3.3 and 4.6 of [16].

Proposition 6.1 *Let M be a sphere or a projective space. Then there are positive constants $A(s,r)$, $r = 1,2$, such that for each $f \in C^s(M)$, there exist polynomials q_n, of degree n for which*

$$\|f - q_n\|_\infty \;\leq\; A(s,r) n^{-s} \omega_r(f^{(s)}; 1/n).$$

Note that for $r = 1$, for the sphere case, the construction used by Ragozin to produce q_n was introduced first by Newman and Shapiro and was used by Damelin and Grabner to prove Theorem 6.2 for $r = 1, s = 1$. As alluded to above, on projective spaces, the construction for the sphere can be followed (as in [16, Prop 4.2]) as the reproducing kernels are essentially univariate. The univariate nature of κ also can be used to show that each H_j is irreducible, so for each j there is only one l and only one eigenvalue a_j for T_κ acting on H_j.

Theorem 6.2 *Let κ be admissible on M and $Z \subset M$ be a point subset of cardinality $N \geq 1$. There exists positive constants C, C' dependent only on d, r, s, M, such that for any $s \geq 0$, any $f \in C^s(M)$, any $n \geq 1$ and any $0 < \alpha < \alpha_0$,*

$$\begin{aligned} |R(f,Z)| \;\leq\; & C n^{-s} \omega_r\left(f^{(s)}; \frac{1}{n}\right) + \\ & C' \max_{j \leq n} \frac{1}{(a_j(\kappa_\alpha))^{1/2}} \|f\|_\infty \left(E_\kappa(Z) + \frac{1}{N}\kappa_\alpha(x,x) - a_0(\kappa_\alpha)\right)^{1/2}. \end{aligned}$$

Proof: Let q_n be the polynomial from Proposition 6.1. From the

definition of $R(f,Z)$, we see that,

$$\begin{aligned} |R(f,Z)| &= |R(f-q_n,Z)+R(q_n,Z)| \\ &\leq \|f-q_n\|_\infty + |R(q_n,Z)| \\ &\leq Cn^{-s}\omega_r(f^{(s)};1/n) \\ &\quad + \max_{j\leq n,}\frac{1}{(a_j(\kappa_\alpha))^{1/2}}\|q_n\|_2\left(E_\kappa(Z)+\frac{1}{N}\kappa_\alpha(x,x)-a_0(\kappa_\alpha)\right)^{1/2}, \end{aligned}$$

and the result follows. ■

Acknowledgements S. B. Damelin was supported, in part, by EP/C000285, NSF-DMS-0439734 and NSF-DMS-0555839. D. L. Ragozin was supported by NSF-DMS-0555839 and X. Sun was supported by EPSRC grant GR/S35400. We acknowledge hospitality from Georgia Southern University and the University of Leicester for research visits.

References

[1] M. Abramowitz and I. A. Stegun, *Handbook of mathematical functions*, National Bureau of Standards, Dover (1964).

[2] S. B. Damelin and D. Ragozin, *Discrepancy via potentials on compact manifolds*, in preparation.

[3] S. B. Damelin and P. Grabner, *Numerical integration, energy and asymptotic equidistributon on the sphere*, *Journal of Complexity*, **19** (2003), pp 231-246.

[4] S. B. Damelin and F. Hickernell, *Discrepancy is equivalent to energy*, submitted to Journal of Complexity.

[5] S. B. Damelin, J. Levesley and X. Sun, *Energy estimates and the Weyl criterion on compact homogeneous manifolds*, Algorithms for Approximation V, Springer, A. Iske and J. Levesley (eds.), Springer-Verlag, Heidelberg, pp 359-368.

[6] S. B. Damelin and V. Maymeskul, *On Point Energies, Separation Radius and Mesh Norm for s-Extremal Configurations on Compact Sets in* $\mathbb{R}^n$, Journal of Complexity, Volume 21(6)(2005), pp 845-863.

[7] S. B. Damelin and V. Maymeskul, *Minimal discrete energy problems and numerical integration on compact sets in Euclidean spaces*, Algorithms for Approximation V, A. Iske and J. Levesley (eds.), Springer-Verlag, Heidelberg, pp 369-378.

[8] S. B. Damelin and V. Maymeskul, *On Dislocation and Mesh Norm Properties of s-Extremal Configurations on Compact Sets in* $\mathbb{R}^n$, submitted to Acta Math Hungarica.

[9] W. Freeden, T. Gervens and M. Schreiner, *Constructive approximation on the sphere with applications to geomathematics*, Clarendon Press, Oxford, 1998.

[10] S. Helgason, *Differential Geometry, Lie Groups, and Symmetric Spaces (Graduate Studies in Mathematics) (Hardcover)*, American Mathematical Society (July 2001).

[11] S. Hubbert and B. Baxter, *Radial basis functions for the sphere*, Recent progress in multivariate approximation, pp 33-47, Internat. Ser. Numer. Math., 137, Birkhäuser, Basel, 2001.

[12] L. Kuipers and H. Niederreiter, *Uniform distribution of sequences*, Wiley-Interscience, New York, 1974.

[13] J. Levesley and D. L. Ragozin, *The density of translates of zonal kernels on compact homogeneous spaces*, J. Approx Theory, **103** (2000), pp 252-268.

[14] J. Levesley and D. L. Ragozin, *Positive definite kernel interpolation on manifolds: Convergence rates*, Approximation Theory X, L. L. Schumaker and J. Stockler (eds), Vanderbilt Univ. Press (2002), pp 277-285.

[15] G. D Mostow, *Equivariant embeddings in Euclidean space*, Ann. Math, **65** (1957), pp 432-446.

[16] D. Ragozin, *Constructive polynomial approximation on spheres and projective spaces*, TAMS, **162**(1971), pp 157-170.

[17] S. S. Tai, *Minimum embeddings of compact symmetric spaces of rank one*, J. Diff. Geom. **2** (1968), pp 55-66.

[18] G. Wagner, On the means of distances on the surface of a sphere (lower bounds), Pacific J. Math. **144** (1990), pp 389-398.

[19] G. Wagner, On the means of distances on the surface of a sphere (upper bounds), Pacific J. Math. **153** (1992), pp 381-396.

S. B. Damelin, Department of Mathematical Sciences, Georgia Southern University, Postoffice Box 8093, Statesboro, GA 30460-8093, U.S.A. damelin@georgiasouthern.edu

J. Levesley, Department of Mathematics, University of Leicester, Leicester LE1 7RH, UK. jl1@mcs.le.ac.uk

D. L. Ragozin, Department of Mathematics, University of Washington, Box 354350, Seattle, WA 98195-4350, U.S.A. rag@math.washington.edu

X. Sun, Department of Mathematics, 10M Cheek Hall, Missouri State University Springfield, MO 65897, U.S.A. XSun@MissouriState.edu