Hermite Interpolation with Radial Basis Functions on Spheres

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Abstract. We show how conditionally negative definite functions on spheres coupled with strictly completely monotone functions (or functions whose derivative is strictly completely monotone) can be used for Hermite interpolation. The classes of functions thus obtained have the advantage over the strictly positive definite functions studied in [17] that closed form representations (as opposed to series expansions) are readily available. Furthermore, our functions include the historically significant *spherical multiquadrics*. Numerical results are also presented.

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1. Introduction

In 1975 R. Hardy mentioned the possibility of using multiquadric basis functions for Hermite interpolation (see [10], or the survey paper [11]). This problem, however, was not further investigated until the paper [29] by Wu appeared. Since then, the interest in this topic seems to have increased significantly. In [29] Wu deals with Hermite-Birkhoff interpolation in $\mathbb{R}^m$. His results are limited in the sense that one can have only one interpolation condition per data point (i.e., some linear combination of function value and derivatives). Sun [25] eliminates this restriction. He also deals with the Euclidean setting and gives results analogous to those of Micchelli [15] for ordinary interpolation. Narcowich and Ward [18] and Narcowich [17] develop an even more general theory of Hermite interpolation for conditionally positive definite (matrix-valued) functions in $\mathbb{R}^m$, and positive definite kernels on compact Riemannian manifolds (the sphere being a special case), respectively. Freeden [8, 9] studied a similar problem on the unit sphere in $\mathbb{R}^3$ employing a slightly different type of linear functionals.

As in the Euclidean case, there are functions on spheres which are not positive definite, but only conditionally positive (negative) definite. These functions were characterized by Menegatto [13]. It is the goal of this paper to derive sufficient conditions for which Hermite interpolation based on these functions is well posed. We will see below that using this approach it is possible to obtain many closed form representations of basis functions which can be used in practice.

We introduce the interpolation problem and state our main theorems in Section 2. Section 3 contains some basic definitions needed in the further development. The central part of the paper is Section 4 which contains the proofs of our main results. In the last section we examine two first-order Hermite interpolation problems on the sphere.

2. Formulation of the Problem and Main Results

We will formulate all our results for S^m, the *unit sphere* in $\mathbb{R}^{m+1}$. However, we mention that an extension to S^∞, the unit sphere in ℓ_2, is possible using the functions $\cos^k(t)$ in expansion (2.3) below instead of the normalized Gegenbauer polynomials $p_k^\lambda(\cos t)$ (see e.g. [14, 23]).

We are interested in

Problem 2.1. *Suppose we are given data $d_i = L_i f$, $i = 1, \ldots, n$, generated by a function $f \in C^r(S^m)$ and some linearly independent set $\mathcal{L} = \{L_1, \ldots, L_n\}$ of linear functionals which are either bounded in the supremum norm on $C^r(S^m)$ or can be approximated by such functionals. We want to find an interpolant of the form*

$$s(x) = \sum_{j=1}^{n} c_j L_j^y g\big(\delta(x, y)\big), \qquad x, y \in S^m, \tag{2.1}$$

satisfying

$$L_i s = d_i, \quad i = 1, \ldots, n.$$

Here g is a real-valued function in $C^r[0, \pi]$, and $\delta(x, y)$ is the *geodesic distance* between two points x and y on the unit sphere S^m, i.e.,

$$\delta(x, y) = \arccos(x \cdot y),$$

where $x \cdot y$ stands for the dot product of x and y in $\mathbb{R}^{m+1}$. In analogy to the Euclidean case we will frequently refer to g as a "radial function". This is motivated by the fact that we only consider g in its composition with the geodesic distance, say $G(\xi) = g(\delta(x, \xi))$, and thus for any fixed $x \in S^m$ we have

$$\delta(x, y) = \delta(x, z) \quad \Longrightarrow \quad G(y) = G(z), \quad \text{for all } y, z \in S^m.$$

We write L^y in (2.1) to indicate that the linear functional acts on a function of the variable y. It should also be pointed out that the linear independence of the L_i is equivalent to the absence of redundancies in the given data.

The interpolation problem above will have a unique solution if the *interpolation matrix* A whose entries are given by

$$a_{ij} = L_i^x L_j^y g\big(\delta(x,y)\big), \quad i,j = 1,\ldots,n, \tag{2.2}$$

is nonsingular.

Remark. For standard Hermite interpolation we can think of the L_i either as point evaluation functionals (yielding Lagrange interpolation conditions), or as functionals evaluating certain derivatives of a given function at specified points on the unit sphere S^m. However, we do allow the set $\mathcal{L}$ to contain more general functionals such as, e.g., local integrals. Furthermore, we stress that there is no assumption which requires that – if interpolation to derivative information is being performed – these derivatives must be in consecutive order.

For the case in which $g \circ \delta$ is a C^∞ strictly positive definite kernel on $S^m \times S^m$ Narcowich [17] showed in certain cases the nonsingularity of A by an argument involving the theory of distributions. We will be able to avoid the use of this sophisticated machinery and establish our proofs much in the flavor of those in [15]. The precise definition of strict complete monotonicity used in the following two theorems will be given in the next section.

Theorem 2.2. *Let*

$$h(t) = a_0 + \sum_{k=1}^{\infty} a_k[1 - p_k^\lambda(\cos t)], \tag{2.3}$$

where $\lambda = (m-1)/2$, all $a_k \geq 0$ (and $a_k > 0$ for some odd k), $\sum_{k=1}^{\infty} a_k < \infty$, $p_k^\lambda(x) = P_k^\lambda(x)/P_k^\lambda(1)$, and $P_k^\lambda(x)$ are the usual Gegenbauer polynomials (see e.g. [26]).

If H is a continuous and nonnegative function on $[0,\infty)$, and H' is strictly completely monotone on $[0,\infty)$, then the matrix A in (2.2) formed by using the function g with $g(t) = H\big(h(t)\big)$ is symmetric. Moreover,

(i) if $\mathcal{L}$ contains at least two point evaluation functionals, then A has one positive and $n-1$ negative eigenvalues.

(ii) if $a_0 > 0$ and $\mathcal{L}$ contains at least one point evaluation functional, then A has one positive and $n-1$ negative eigenvalues.

(iii) if $\mathcal{L}$ consists only of functionals which annihilate constants, then A is negative definite.

Theorem 2.3. *If h is as in (2.3), and if H is strictly completely monotone on $[0,\infty)$, then the matrix A formed by using $g(t) = H(h(t))$ in (2.2) is symmetric and positive definite.*

Remark 1. Since the function H with $H(t) = t^\alpha$, $0 < \alpha < 1$, has a strictly completely monotone derivative, this is a special case of Theorem 2.2. We point out that in the historic treatment of isometric imbeddings (Blumenthal and Schoenberg first studied imbeddings with metric transforms of the form t^α, see e.g. [21]), as well as in the discussion in [5] this function plays an important role.

Remark 2. Note that Theorem 2.2 does not cover the case where the generating set $\mathcal{L}$ consists only of two nonempty subsets; one containing derivative functionals, and the other one containing functionals which do not include point evaluation functionals.

3. Background

In the formulation of Theorems 2.2 and 2.3 we used the notion of a strictly completely monotone function.

Definition 3.1. *A function $F : [0,\infty) \to \mathbb{R}$ which is in $C[0,\infty) \cap C^\infty(0,\infty)$ and which satisfies*

$$(-1)^\ell F^{(\ell)}(t) \geq 0, \quad \ell = 0, 1, 2, \ldots,$$

is called completely monotone on $[0,\infty)$. If the inequality is strict, then F is strictly completely monotone.

The following characterization of a strictly completely monotone function in terms of Laplace-Stieltjes transforms can be found in [25], and is a modification of the well-known Bernstein-Widder theorem (see [28]).

Theorem 3.2. *A function $F : [0,\infty) \to \mathbb{R}$ is strictly completely monotone on $[0,\infty)$ if and only if F is of the form*

$$F(t) = \int_0^\infty e^{-\sigma t} d\mu(\sigma),$$

where μ is a finite nonnegative Borel measure on $[0,\infty)$ which satisfies

$$\int_0^\infty d\mu(\sigma) < \infty \qquad \textit{and} \qquad \int_\epsilon^\infty d\mu(\sigma) > 0$$

for some positive constant ϵ.

Note that a strictly completely monotone function can be characterized as a completely monotone function which is not constant.

Schoenberg [22] gave the following characterization of a function whose derivative is strictly completely monotone.

Theorem 3.3. *In order that $F \in C[0,\infty)$ and F' is strictly completely monotone on $[0,\infty)$ it is necessary and sufficient that*

$$F(t) - F(0) = \int_0^\infty [1 - e^{-\sigma t}] \frac{d\mu(\sigma)}{\sigma},$$

where μ is a finite nonnegative Borel measure on $[0,\infty)$ which satisfies

$$\int_1^\infty \frac{d\mu(\sigma)}{\sigma} < \infty \qquad \text{and} \qquad \int_\epsilon^\infty d\mu(\sigma) > 0$$

for some positive constant ϵ.

In the discussion that follows we will not require the environment of a normed linear space. Usually it will be sufficient to work with the following "relaxed" metric spaces defined e.g. in [22].

Definition 3.4. *A set $\mathcal{S}$ is called a semi-metric space, if $\mathcal{S}$ is provided with a distance function $d : \mathcal{S} \times \mathcal{S} \to [0,\infty)$, such that for arbitrary points $P, Q \in \mathcal{S}$*

(i) $d(P,Q) = d(Q,P)$,

(ii) $d(P,Q) = 0 \iff P = Q$.

The following property (again due to Schoenberg) plays one of the central roles in our discussion and is a generalization of the classical notion of positive definite functions given by Mathias and Bochner (see e.g. [24]).

Definition 3.5. *Let $\mathcal{S}$ be a semi-metric space with distance function d. A function $F \in C[0,\infty)$ is called positive definite in $\mathcal{S}$, if*

$$\sum_{i=1}^n \sum_{j=1}^n F\big(d(x_i,x_j)\big) c_i c_j \geq 0 \tag{3.1}$$

for any n distinct points $x_i \in \mathcal{S}$, $i = 1,\ldots,n$, arbitrary real constants c_i, and all $n = 2,3,\ldots$. The function F is strictly positive definite if equality in (3.1) implies $c_1 = \cdots = c_n = 0$.

Remark 3. This distinction between strictness and nonstrictness is the essential modification of these classical ideas for their application in approximation theory.

4. Proofs

The key ingredients in the proofs of Theorems 2.2 and 2.3 are the following two lemmas.

Lemma 4.1. *The function g given by $g(t) = e^{-\sigma h(t)}$, with h as in (2.3) and $\sigma > 0$, is strictly positive definite on S^m.*

Proof: This proof is based essentially on Schoenberg's discussion of isometric imbeddings of (semi-)metric spaces into the Hilbert space ℓ_2 (for a discussion of isometric imbeddings see e.g., [27]). He considered one semi-metric space $\mathcal{S}$ with distance function d and a new semi-metric space $F(\mathcal{S})$ based on the same set $\mathcal{S}$, but with distance function $F \circ d$. Schoenberg calls the function F the *metric transform*. For isometric imbeddings of $\mathcal{S}$ into ℓ_2 he gave the following characterization (see [22]), where the *simplicial class* $\Pi(\mathcal{S})$ denotes the class of all functions F for which $F(\mathcal{S})$ is isometrically imbeddable in ℓ_2:

> *A function $F(t)$ ($F(0) = 0$) belongs to the simplicial class $\Pi(\mathcal{S})$ of a semi-metric space $\mathcal{S}$ if and only if $e^{-\sigma F^2(t)}$ is positive definite in $\mathcal{S}$ for all $\sigma > 0$.*

In order to facilitate the following arguments, we let $f(t) = h(t) - a_0$. In [23] the isometric imbeddings of S^m into ℓ_2 are characterized as having metric transforms of the form $F^2(t) = f(t)$ with $a_k \geq 0$, $k = 1, 2, \ldots$ (we will make use of the fact that, for our purposes, at least one a_k with odd index must be positive below). Thus, we can immediately conclude that $e^{-\sigma f}$, and therefore also $e^{-\sigma h}$, is positive definite in S^m. It remains to establish strictness.

From Schoenberg's work we know that the functions F with $F^2(t) = f(t)$ are metric transforms associated with imbeddings of S^m into ℓ_2. Therefore, by the geometric interpretation of an isometric imbedding given by Menger and Schoenberg (see [20, 22]), we know that corresponding to the (distinct) data points x_i, $i = 1, \ldots, n$, on S^m there exist (distinct) points y_i in Euclidean space $\mathbb{R}^N$ ($N = n - 1$) such that their Euclidean distances equal the geodesic distances of the x's (the points y_i are the vertices of simplices which motivates the terminology simplicial class above.). We use this characterization to interpret the values $f(\delta(x_i, x_j))$ as Euclidean distances $\|y_i - y_j\|^2$. We can do this if we assume that at least one a_k with odd index in (2.3) is positive. This assumption on the a_k ensures that $f(t) = 0$ does not have two roots $t = 0$, and $t = \pi$ violating property (ii) of Definition 3.4. Thus, for the rest of the proof we can assume that we are dealing with Euclidean distances $\|y_i - y_j\|^2$.

It is now a standard argument in the radial basis function literature dealing with interpolation in Euclidean spaces (see e.g. [15]) to consider the Fourier transform

$$e^{-\|\tau\|^2} = \frac{1}{(\sqrt{\pi})^N} \int_{\mathbb{R}^N} e^{2\sqrt{-1}(\tau \cdot \theta)} e^{-\|\theta\|^2} d\theta,$$

where τ and θ are vectors in $\mathbb{R}^N$. Then one sets $\tau = y_i - y_j$, and shows that after multiplication by $c_i c_j$ and summation over i and j it follows that $c_1 = \cdots c_n = 0$.

Clearly, our arguments also hold for

$$e^{-\sigma h(\delta(x_i, x_j))} = e^{-\sigma a_0} e^{-\sigma f(\delta(x_i, x_j))} = e^{-\sigma a_0} e^{-\sigma \|y_i - y_j\|^2}$$

with $\sigma > 0$, and thus the statement of the lemma follows. ■

Remark 1. We point out that the statement of Lemma 4.1 does not contradict the results of Narcowich (see e.g. [17, Theorems 3.6 and 4.2]) since Narcowich considers a notion of positive definiteness in the sense of distributions which is stronger than that of Definition 3.5.

Lemma 4.2. *If the function g is of the form $g(t) = e^{-\sigma h(t)}$, $\sigma > 0$, with h as in (2.3), then the matrix A defined in (2.2) is positive definite.*

Proof: By Lemma 4.1 we know that g is (strictly) positive definite on S^m. Therefore g can be expressed as (see [17, 23])

$$g(t) = \sum_{k=0}^{\infty} b_k P_{k,m+1}(x \cdot y), \qquad b_k \geq 0, \tag{4.1}$$

where $P_{k,m+1}$ are Legendre polynomials of degree k in $m+1$ dimensions, and $\cos(t) = \cos(\arccos(x \cdot y)) = x \cdot y$. It is known that the series above converges absolutely and uniformly for $t \in [0, \pi]$ (see [23]). We use Legendre polynomials here instead of Gegenbauer polynomials, since they are the same up to a constant factor, and are somewhat easier to handle.

We split the proof into two parts. First we show that the matrix A is positive definite if the functionals in $\mathcal{L}$ are bounded in the supremum norm on $C(S^m)$. Then we establish the validity of the lemma for such functionals which can be approximated by continuous linear functionals (this covers in particular those functionals which correspond to evaluation of derivatives).

If we are dealing with continuous linear functionals on $(C(S^m), \|\cdot\|_\infty)$ we can employ the Riesz representation theorem to regard the linear functionals in $\mathcal{L}$ as integrals of the form

$$L_i f = \int_{S^m} f(x) d\mu_i(x), \qquad i = 1, \ldots, n,$$

where the μ_i are regular signed Borel measures on S^m. With this and (4.1) we can rewrite the entries of the matrix A as

$$L_i^x L_j^y e^{-\sigma h(\delta(x,y))} = \int_{S^m} \int_{S^m} \sum_{k=0}^{\infty} b_k P_{k,m+1}(x \cdot y) d\mu_i(x) d\mu_j(y), \quad i, j = 1, \ldots, n. \tag{4.2}$$

The other ingredient we use is the addition theorem for spherical harmonics which states that

$$\sum_{l=1}^{N(m,k)} Y_{k,l}(x) Y_{k,l}(y) = \frac{N(m,k)}{\omega_m} P_{k,m+1}(x \cdot y), \tag{4.3}$$

where $Y_{k,l}$, $l = 1, \ldots, N(m,k)$, are the spherical harmonics of order k on S^m, $N(m,k) = \frac{(2k+m-1)\Gamma(k+m-1)}{\Gamma(k+1)\Gamma(m)}$ is the dimension of the space of these functions, and $\omega_m = \frac{2\pi^{(m+1)/2}}{\Gamma((m+1)/2)}$ is the surface area of S^m (see e.g. [16]).

Replacing $P_{k,m+1}$ in (4.2) via (4.3) we arrive at

$$L_i^x L_j^y e^{-\sigma h(\delta(x,y))} = \int_{S^m} \int_{S^m} \sum_{k=0}^{\infty} b_k \frac{\omega_m}{N(m,k)} \sum_{l=1}^{N(m,k)} Y_{k,l}(x) Y_{k,l}(y) d\mu_i(x) d\mu_j(y).$$

Since the infinite series is absolutely and uniformly convergent as noted earlier we can interchange the infinite summation with the integration which yields

$$\begin{aligned} L_i^x L_j^y e^{-\sigma h(\delta(x,y))} &= \sum_{k=0}^{\infty} b_k \frac{\omega_m}{N(m,k)} \int_{S^m} \int_{S^m} \sum_{l=1}^{N(m,k)} Y_{k,l}(x) Y_{k,l}(y) d\mu_i(x) d\mu_j(y) \\ &= \sum_{k=0}^{\infty} b_k \frac{\omega_m}{N(m,k)} \sum_{l=1}^{N(m,k)} \int_{S^m} Y_{k,l}(x) d\mu_i(x) \int_{S^m} Y_{k,l}(y) d\mu_j(y). \end{aligned}$$

Now, multiplying by $c_i c_j$ and summing over i and j, we obtain

$$\begin{aligned} c^T A c &= \sum_{i=1}^{n} \sum_{j=1}^{n} c_i c_j \sum_{k=0}^{\infty} b_k \frac{\omega_m}{N(m,k)} \sum_{l=1}^{N(m,k)} \int_{S^m} Y_{k,l}(x) d\mu_i(x) \int_{S^m} Y_{k,l}(y) d\mu_j(y) \\ &= \sum_{k=0}^{\infty} b_k \frac{\omega_m}{N(m,k)} \sum_{l=1}^{N(m,k)} \sum_{i=1}^{n} \sum_{j=1}^{n} c_i c_j \int_{S^m} Y_{k,l}(x) d\mu_i(x) \int_{S^m} Y_{k,l}(y) d\mu_j(y) \\ &= \sum_{k=0}^{\infty} b_k \frac{\omega_m}{N(m,k)} \sum_{l=1}^{N(m,k)} \left[\sum_{i=1}^{n} c_i \int_{S^m} Y_{k,l}(x) d\mu_i(x) \right]^2, \end{aligned}$$

which is obviously nonnegative. Since certainly not all of the b_k are zero, we see that the only possibility for $c^T A c = 0$ is

$$\sum_{i=1}^{n} c_i \int_{S^m} Y_{k,l}(x) d\mu_i(x) = 0$$

for $l = 1, \ldots, N(m,k)$, and all k such that $b_k > 0$. Remembering that this is the same as

$$\sum_{i=1}^{n} c_i L_i Y_{k,l} = 0,$$

and making use of the fact that $\mathcal{L}$ is a linearly independent set, it follows that $c_1 = \cdots = c_n = 0$. This establishes the claim of the lemma for the case of continuous linear functionals.

We illustrate the second part of the proof by assuming all functionals in $\mathcal{L}$ to be derivative functionals which can be written as $L_i = \lim_{\epsilon\to 0} L_i^\epsilon$. The L_i^ϵ are defined by considering a regular parametric curve C in the neighborhood $N_i \cap S^m$ of x_im, parametrized such that $C(0) = x_i$. The approximating functionals are then defined as

$$L_i^\epsilon f = \frac{f(x_i+\epsilon) - f(x_i)}{\epsilon},$$

where $x_i + \epsilon$ is used as symbolic notation for the point $C(\epsilon)$ in the neighborhood of x_i. The "direction" of the derivative is thus defined by the choice of C. In the last section of the paper a special choice of C (leading to partial derivatives with respect to the spherical coordinates on S^2) is employed.

For any fixed value of ϵ the same argumentation as above will yield

$$c^T A^\epsilon c = \sum_{k=0}^{\infty} b_k \frac{\omega_m}{N(m,k)} \sum_{l=1}^{N(m,k)} \left[\sum_{i=1}^{n} c_i L_i^\epsilon Y_{k,l} \right]^2 \geq 0.$$

Here A^ϵ denotes the matrix corresponding to the use of the linear functionals L_i^ϵ. Now it is also clear that

$$c^T A c = \lim_{\epsilon\to 0} c^T A^\epsilon c \geq 0.$$

As mentioned above, the infinite series (4.1) converges absolutely and uniformly for $t \in [0, \pi]$, and therefore we can interchange the summation and the limit and arrive at

$$c^T A c = \sum_{k=0}^{\infty} b_k \frac{\omega_m}{N(m,k)} \sum_{l=1}^{N(m,k)} \left[\sum_{i=1}^{n} c_i \lim_{\epsilon\to 0} L_i^\epsilon Y_{k,l} \right]^2 \geq 0. \tag{4.4}$$

Finally, as in the first part of the proof, it follows that the quadratic form (4.4) is positive since the functionals $L_i = \lim_{\epsilon\to 0} L_i^\epsilon$ were assumed to form a linearly independent set. Any other derivative functionals can be approximated in an analogous way, and thus the proof is complete. ■

Remark 2. Lemma 4.2 by itself gives a class of radial basis functions suitable for Hermite interpolation on S^m. In analogy to the Euclidean setting we refer to the functions $e^{-\sigma h}$ as *spherical Gaussians.* We point out that this allows for closed form representations of basis functions (since only one coefficient in the series (2.3) needs to be positive) which can be manipulated much more easily in practice than the long series expansions required for strictly positive definite functions. The same is true for the basis functions covered by Theorems 2.2 and 2.3.

Proof of Theorem 2.2. We will split the proof into three parts. First we show that the interpolation matrix A is symmetric, then we prove it is negative definite on a subspace of dimension $n-1$, and finally we give an argument for the eigenvalue structure of A and thus its nonsingularity.

a) Note that g is a continuous function of the geodesic distance, which itself is a function of the dot product, i.e., $G(x,y) = \tilde{g}(x\cdot y) = g(\arccos(x\cdot y))$ is continuous on $S^m \times S^m$. Furthermore, by using the same approximation argument combined with the Riesz representation theorem as in the proof of Lemma 4.2 along with a version of Fubini's theorem for finite measures (see e.g. [4, p. 193]) we can interchange the order in which we apply L^x and L^y, i.e.,

$$a_{ij} = L_i^x L_j^y \tilde{g}(x\cdot y) = L_j^y L_i^x \tilde{g}(x\cdot y).$$

Finally, we switch x and y, so that by the symmetry of the dot product we have

$$L_j^y L_i^x \tilde{g}(x\cdot y) = L_j^x L_i^y \tilde{g}(y\cdot x) = L_j^x L_i^y \tilde{g}(x\cdot y) = a_{ji}.$$

b) We will now show that A is negative definite whenever

$$\sum_{i=1}^{n} c_i L_i[1] = 0, \tag{4.5}$$

where $c(\neq 0) \in \mathbb{R}^n$.

If we apply Theorem 3.3 to the function H and substitute $h(\delta(x,y))$ for t in the integral representation given there, the associated quadratic form is

$$\sum_{i=1}^{n}\sum_{j=1}^{n} c_i c_j L_i^x L_j^y H(h(\delta(x,y))) - \sum_{i=1}^{n}\sum_{j=1}^{n} c_i c_j L_i^x L_j^y H(0) =$$
$$\int_0^\infty \sum_{i=1}^{n}\sum_{j=1}^{n} c_i c_j L_i^x L_j^y [1 - e^{-\sigma h(\delta(x,y))}] \frac{d\mu(\sigma)}{\sigma}.$$

Here the interchange of the functionals with the integral is permitted by the ideas used in the proof of Lemma 4.2 (Riesz representation theorem, and approximation), Fubini's theorem for finite measures, and the condition on the measure μ stated in Theorem 3.3 which guarantees the convergence of the integral.

We can now use condition (4.5) to get

$$\sum_{i=1}^{n}\sum_{j=1}^{n} c_i c_j L_i^x L_j^y H(h(\delta(x,y))) = -\int_0^\infty \sum_{i=1}^{n}\sum_{j=1}^{n} c_i c_j L_i^x L_j^y e^{-\sigma h(\delta(x,y))} \frac{d\mu(\sigma)}{\sigma}. \tag{4.6}$$

Finally, Lemma 4.2 tells us that the integrand is positive, and the only possibility for (4.6) to be zero is that the measure μ has all its mass concentrated at the origin, which would contradict the assumption of *strict* complete monotonicity of the function H'.

c) To complete the proof we need to discuss four cases:

(i) $\mathcal{L}$ contains only point evaluation functionals,

(ii) $\mathcal{L}$ contains at least two point evaluation functionals,

(iii) $\mathcal{L}$ contains one point evaluation functional, and $a_0 > 0$,

(iv) $\mathcal{L}$ contains only functionals of the form $L_i[1] = 0$.

(i) In this case condition (4.5) simply becomes $\sum_{i=1}^{n} c_i = 0$, and thus A is conditionally (or almost) negative definite in the classical sense (see e.g. [3]). To determine the eigenvalue structure of A we recall that a matrix which is negative definite on a subspace of dimension $n-1$ has at least $n-1$ negative eigenvalues by the Courant-Fischer theorem (see e.g. [12]). If $n \geq 2$ we can show that A must have also at least one positive eigenvalue by concluding from the definition of g that $\operatorname{trace}(A) \geq 0$. For the special case $n = 1$ it is necessary to have $a_0 > 0$. Then $g(0) > 0$ and therefore A is nonsingular for $n = 1$ also (the only entry of A is positive).

(ii) From part b) of the proof we already know that A is negative definite on a subspace of dimension $n-1$ and therefore has at least $n-1$ negative eigenvalues. To show that A must have at least one positive eigenvalue in this case, we reorganize the matrix A into the following symmetric block form

$$A = \begin{pmatrix} A_{11} & A_{12} \\ A_{12}^T & A_{22} \end{pmatrix}, \tag{4.7}$$

where A_{11} is a block (of size at least 2×2) which corresponds to Lagrange interpolation. Using the symmetry of A and the fact that A_{11} is invertible as shown in (i), we can perform a congruence transformation with the transformation matrix

$$P = \begin{pmatrix} I & -A_{11}^{-1} A_{12} \\ 0 & I \end{pmatrix},$$

and we then obtain

$$\widetilde{A} = P^T A P = \begin{pmatrix} A_{11} & 0 \\ 0 & A_{22} - A_{12}^T A_{11}^{-1} A_{12} \end{pmatrix}.$$

Since it is well known from linear algebra (see e.g. [12]) that congruent symmetric matrices have the same inertia (an integer triple $\operatorname{In}(M) = (p, n, z)$ representing the number of positive, negative and zero eigenvalues of the symmetric matrix M), and it is also easily seen that the inertia of a block-diagonal matrix is the sum of the inertias of those diagonal blocks, it follows that $\operatorname{In}(\widetilde{A}) \geq \operatorname{In}(A_{11})$. Finally, since we just showed in (i) that A_{11} must have at least one positive eigenvalue, the same must be true for $\widetilde{A}$, and by congruence for the Hermite matrix A.

(iii) The case $n = 1$ and $a_0 > 0$ will work analogously based on the argumentation at the end of (i).

(iv) If all functionals in $\mathcal{L}$ annihilate constants, i.e., $L_i[1] = 0$, for all $i = 1, \ldots, n$, then condition (4.5) is void and it follows that A is negative definite. ■

Remark 3. If the elements of the interpolation matrix A are arranged as in (4.7), then efficient block decomposition algorithms can be used to invert A. In particular, the inertia argument above shows that the Schur complement, $A_{22} - A_{12}^T A_{11}^{-1} A_{12}$, is not only symmetric, but also negative definite.

Proof of Theorem 2.3. The symmetry of the interpolation matrix follows as in the proof of Theorem 2.2. We will now show that A is positive definite. Recall that the radial functions g are of the form $g(t) = H(h(t))$, where H is strictly completely monotone on $[0, \infty)$. Consider the quadratic form

$$c^T Ac = \sum_{i=1}^{n} \sum_{j=1}^{n} c_i c_j L_i^x L_j^y H(h(\delta(x, y)).$$

Using the Bernstein-Widder characterization of completely monotone functions (see Theorem 3.2), this becomes

$$c^T Ac = \int_0^\infty \sum_{i=1}^{n} \sum_{j=1}^{n} c_i c_j L_i^x L_j^y e^{-\sigma h(\delta(x,y))} d\mu(\sigma),$$

where an argument analogous to that used in the proof of Theorem 2.2 permits the change of the L's with the integral. Now it follows directly from Lemma 4.2 and the fact that the *strict* complete monotonicity of H implies that the measure μ does not have all of its mass at the origin that A is positive definite. ■

5. An Example

In this section we discuss an example of first-order Hermite interpolation on the sphere S^2. We will consider the following situation:

Example 5.1. *Assume we are given ν distinct points x_i, $i = 1, \ldots, \nu$, on the unit sphere S^2 in $\mathbb{R}^3$ represented in spherical coordinates*

$$x = \cos\theta \cos\phi$$
$$y = \sin\theta \cos\phi$$
$$z = \sin\phi$$

with $\theta \in [0, 2\pi)$ and $\phi \in [-\pi/2, \pi/2]$, and a function $f \in C^1(S^2)$, as well as associated data of the form

$$d_i = \begin{cases} f(x_i) & i = 1, \ldots, \nu, \\ \dfrac{\partial f}{\partial \phi}(x_{i-\nu}) & i = \nu + 1, \ldots, 2\nu, \\ \dfrac{\partial f}{\partial \theta}(x_{i-2\nu}) & i = 2\nu + 1, \ldots, 3\nu. \end{cases}$$

To be specific, we could imagine using *spherical multiquadrics* (see e.g. [11]), i.e., basis functions of the form

$$g(t) = \sqrt{1 + R^2 - 2R\cos t},$$

where $R(\neq 1)$ is a user-selectable parameter, to interpolate to this set of data.

It can easily be seen that the spherical multiquadrics satisfy the conditions of Theorem 2.2 if we let $H(t) = t^{1/2}$, $a_0 = (1 - R)^2$, and $a_1 = 2R$. Note that the condition $R \neq 1$ (or equivalently $a_0 \neq 0$) ensures differentiability of g. The formulation of Example 5.1 means that in Problem 2.1 we would have $n = 3\nu$ functionals L_i, the first ν corresponding to point evaluations at the data points, and the others corresponding to evaluation of the partial derivatives with respect to the spherical coordinates at the same points.

Proposition 5.2. *If the data points x_i, $i = 1, \ldots, \nu$, contain either the North or the South Pole, the interpolation matrix A for Example 5.1 is singular.*

Proof: We can interpret the partial derivative $\frac{\partial f}{\partial \theta}$ as an inner product of the form $\nabla f \cdot \vartheta$ where ∇f is the gradient of f (in Cartesian coordinates), and $\vartheta = (-\sin\theta\cos\phi, \cos\theta\cos\phi, 0)^T$. At the North Pole we have $\phi = \pi/2$ and thus ϑ is the zero vector. Therefore, it is easily seen that a complete row (column) in the matrix A will be zero. The same holds for the South Pole with $\phi = -\pi/2$. ■

Remark 1. It is immediate to see that the linear functionals chosen in the example above are linearly dependent if one of the poles is among the data points, since the functional corresponding to $\frac{\partial f}{\partial \theta}$ is the zero functional at the poles.

Remark 2. It is clear that the real trouble here is caused by the singularity in the parametrization chosen for the sphere. Thus, the above difficulties could be avoided using a combination of parametrizations which are regular at the poles. Another possibility would be the use of *covariant derivatives.*

Remark 3. Even though the interpolation matrix is singular for the situation described in Proposition 5.2, one can still solve the interpolation problem since the singularity of the matrix is consistent with zero data on the right-hand side (see the numerical experiment at the end of the paper).

If this approach does not seem appealing, it is possible to give a positive result concerning a slightly modified version of Example 5.1.

Proposition 5.3. *If the data points x_i, $i = 1, \ldots, \nu$, are distinct, and if α_i and β_i are two linearly independent directions in the tangent plane to the sphere at x_i, then interpolation to data of the form*

$$d_i = \begin{cases} f(x_i) & i = 1, \ldots, \nu, \\ D_{\alpha_{i-\nu}} f(x_{i-\nu}) & i = \nu + 1, \ldots, 2\nu, \\ D_{\beta_{i-2\nu}} f(x_{i-2\nu}) & i = 2\nu + 1, \ldots, 3\nu, \end{cases}$$

using any of the functions g classified in Theorems 2.2 and 2.3 is well posed. Here D_{α_i} and D_{β_i} are the usual directional derivatives in $\mathbb{R}^3$.

Proof: The hypotheses imply the linear independence of the functionals in $\mathcal{L}$. ■

Remark 4. If we compare

$$\varphi = (-\cos\theta \sin\phi, -\sin\theta \sin\phi, \cos\phi)^T, \qquad \vartheta = (-\sin\theta\cos\phi, \cos\theta\cos\phi, 0)^T$$

with

$$\alpha_i = (-\cos\theta_i \sin\phi_i, -\sin\theta_i \sin\phi_i, \cos\phi_i)^T, \qquad \beta_i = (-\sin\theta_i, \cos\theta_i, 0)^T,$$

we see that Proposition 5.3 can be interpreted as a "scaled" version of Example 5.1. Note that in this case α_i and β_i are even orthonormal directions.

Remark 5. If one would like to use the Hermite basis functions introduced in this paper, but certain derivative data is not available, it is possible to use any of the well established methods for derivative generation. For a survey of these methods see e.g. [1].

We close by illustrating Example 5.1 numerically. To this end we use spherical multiquadrics with parameter $R = 0.4$, and choose the test function f as

$$f(x, y, z) = \frac{1 + 10xyz + x^8 + e^{2y^3} + e^{2z^2}}{14}, \qquad (x, y, z) \in S^2.$$

We take 18 nearly equally spaced points on the sphere (obtained by subdividing a regular tetrahedron) and evaluate the Hermite interpolant on a finer grid of 3846

	Hermite (part.)	Hermite (dir.)	Lagrange (18)	Lagrange (54)
max. error	1.218017e-02	1.218017e-02	1.493461e-01	1.335387e-02
rms. error	1.233846e-05	1.233846e-05	4.226617e-03	1.251992e-05
cond(A)	2.970847e+19	3.508120e+03	1.443921e+03	1.438680e+10

Table 1. Numerical comparison.

points. The table below contains maximum and root-mean-square errors on this grid, as well as the approximate condition number of the interpolation matrices. In order to provide some insight into the advantages of Hermite basis functions we include the results for Hermite interpolation according to Proposition 5.3, as well as those for Lagrange interpolation at the 18 points and at 54 points which were generated by clustering 3 points at each of the 18 original locations.

As noted above, the interpolation matrix for Hermite interpolation based on the use of partial derivatives with respect to the spherical coordinates results in a singular matrix. Nevertheless, the errors for both Hermite interpolants are the same. The condition number observed for the Lagrange interpolant with clustered points shows that it is highly recommended to replace such clusters by one representative point, and to use Hermite basis functions there instead of the usual (Lagrange) radial basis functions. This idea was incorporated in an adaptive least squares fitting method in [6]. The basic algorithm (without the Hermite functions) is also described in [7].

References

1. Alfeld, P., Scattered data interpolation in three or more variables, in *Mathematical Methods in Computer Aided Geometric Design,* T. Lyche and L. Schumaker (eds), Academic Press, New York, 1989, 1–33.
2. Alfeld, P., M. Neamtu, and L. L. Schumaker, Fitting scattered data on sphere-like surfaces using spherical splines, J. Comp. Appl. Math. **73** (1996), 5–43.
3. Donoghue, W. F., *Monotone Matrix Functions and Analytic Continuation,* Springer, New York, 1974.
4. Dunford, N. and J. T. Schwartz, *Linear Operators Part I: General Theory,* Interscience Publishers, New York, 1966.
5. Dyn, N., T. Goodman, and C. A. Micchelli, Positive powers of certain conditionally negative definite matrices, Indaga. Math. Proc. Ser.A. **89** (1986), 163–178.
6. Fasshauer, G. E., Radial Basis Functions on Spheres, dissertation, Vanderbilt University, 1995.

7. Fasshauer, G. E., Adaptive least squares fitting with radial basis functions on the sphere, in *Mathematical Methods for Curves and Surfaces,* M. Dæhlen, T. Lyche, and L. Schumaker (eds), Vanderbilt University Press, Nashville & London, 1995, 141–150.

8. Freeden, W., Spline methods in geodetic approximation problems, Math. Meth. Appl. Sci. **4** (1982), 382–396.

9. Freeden, W., A spline interpolation method for solving boundary value problems of potential theory from discretely given data, Num. Meth. Part. Diff. Eq. **3** (1987), 375–398.

10. Hardy, R. L., Research results in the application of multiquadric equations to surveying and mapping problems, Survg. Mapp. **35** (1975), 321–332.

11. Hardy, R. L., Theory and applications of the multiquadric-biharmonic method, Comput. Math. Appl. **19** (1990), 163–208.

12. Horn, R. A. and C. R. Johnson, *Matrix Analysis,* Cambridge University Press, Cambridge, 1985.

13. Menegatto, V. A., Interpolation on spherical domains, dissertation, University of Texas Austin, 1992.

14. Menegatto, V. A., Strictly positive definite kernels on the Hilbert sphere, Appl. Anal. **55** (1994), 91–101.

15. Micchelli, C. A., Interpolation of scattered data: distance matrices and conditionally positive definite functions, Constr. Approx. **2** (1986), 11–22.

16. Müller, C., *Spherical Harmonics,* Springer Lecture Notes in Mathematics, Vol. 17, 1966.

17. Narcowich, F. J., Generalized Hermite interpolation and positive definite kernels on a Riemannian manifold, J. Math. Anal. Appl. **190** (1995), 165–193.

18. Narcowich, F. J. and J. D. Ward, Generalized Hermite interpolation via matrix-valued conditionally positive definite functions, Math. Comp. **63** (1994), 661–687.

19. Powell, M. J. D., The theory of radial basis functions in 1990, in *Advances in Numerical Analysis II: Wavelets, Subdivision, and Radial Basis Functions,* W. Light (ed), Oxford University Press, Oxford, 1992, 105–210.

20. Schoenberg, I. J., On certain metric spaces arising from euclidean spaces by a change of metric and their imbedding in Hilbert space, Ann. of Math. **38** (1937), 787–793.

21. Schoenberg, I. J., Metric spaces and positive definite functions, Trans. Amer. Math. Soc. **44** (1938), 522–536.

22. Schoenberg, I. J., Metric spaces and completely monotone functions, Ann. of Math. **39** (1938), 811–841.

23. Schoenberg, I. J., Positive definite functions on spheres, Duke Math. J. **9** (1942), 96–108.

24. Stewart, J., Positive definite functions and generalizations, an historical survey, Rocky Mountain J. Math. **6** (1976), 409–434.

25. Sun, X., Scattered Hermite interpolation using radial basis functions, Linear Algebra Appl. **207** (1994), 135–146.

26. Szegő, G., *Orthogonal Polynomials,* Amer. Math. Soc. Coll. Publ., Vol. XXIII, 1959.

27. Wells, J. H. and R. L. Williams, *Embeddings and Extensions in Analysis,* Springer, New York, (1975).

28. Widder, D. V., *The Laplace Transform,* Princeton University Press, Princeton, 1941.

29. Wu, Z., Hermite-Birkhoff interpolation of scattered data by radial basis functions, Approx. Theory Appl. **8** (1992), 1–10.

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