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SPHERICAL SPLINES FOR DATA INTERPOLATION AND FITTING*

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Abstract. We study minimal energy interpolation and discrete and penalized least squares approximation problems on the unit sphere using nonhomogeneous spherical splines. Several numerical experiments are conducted to compare approximating properties of homogeneous and nonhomogeneous splines. Our numerical experiments show that nonhomogeneous splines have certain advantages over homogeneous splines.

Key words. spherical splines, data fitting

AMS subject classifications. 65D05, 65D07, 65D17

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1. Introduction.

Contemporary research in atmospheric sciences, geodesy, and geophysics requires the use of global data heterogeneously distributed in space around Earth. For spherical data interpolation/approximation, tensor products of univariate splines are not a good choice, since data locations are not usually spaced over a regular grid. Radial basis functions are not good candidates either, since the data values may have no rotational symmetry.

Spherical Bernstein–Bézier splines (introduced in [1] and studied in [2] and [7]) are well suited for scattered data interpolation/approximation problems. The spherical spline functions have many properties in common with classical polynomial splines over planar triangulations. Moreover, many spline interpolation and approximation methods for planar scattered data problems have analogues in spherical setting [2].

One of the disadvantages of using homogeneous spherical splines is that spline spaces of even and odd degrees have only zero function in common due to homogeneity of the basis. More explicitly, the spline space $S^r_d(\Delta)$ of degree d and smoothness r (defined in [2]) with d odd does not contain constant functions, and the spline space $S^r_d(\Delta)$ with d even does not contain linear functions. Therefore in the homogeneous spline spaces reproduction of polynomials of degree $m \leq d$ is not possible unless $m = d \bmod(2)$.

To overcome this disadvantage we propose a simultaneous employment of two spaces $S^r_d(\Delta)$ and $S^r_{d-1}(\Delta)$, with one degree even and the other odd. A direct sum of two spline spaces forms the larger nonhomogeneous spherical polynomial spline space proposed by [10]. A simple structure of the resulting spline space allows us to use methods developed for homogeneous splines in nonhomogeneous spline spaces. The spline solution obtained via minimization over the larger space has in general higher accuracy. In addition, spherical nonhomogeneous splines reproduce spherical nonhomogeneous polynomials.

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In this paper we establish existence and uniqueness of homogeneous and nonhomogeneous spherical spline approximations. Moreover, we show how the use of a powerful iterative algorithm [4] solving special linear systems leads to efficient computation of spherical splines of arbitrary degree and smoothness.

The paper is organized as follows. In section 2 we discuss homogeneous spherical polynomials and then introduce nonhomogeneous spherical polynomials. We review properties necessary for the implementation of the computational algorithms which are presented in sections 3, 4, 5. In section 3 we describe a minimal energy (ME) interpolation method using both homogeneous and nonhomogeneous splines. We discuss discrete and penalized least squares spline approximation algorithms in sections 4 and 5. In each section we start with a description of the method, follow with a computational algorithm, and end with numerical examples. Some examples are designed to demonstrate advantages of nonhomogeneous splines over homogeneous. In addition, we solve real world data fitting problems and offer visual evaluation of the solutions. One potential application of the development of spherical splines is in the investigation of inverse problems arising in geophysics. Using heterogeneously distributed satellite measurements from new satellite gravity missions such as GRACE (Gravity Recovery and Climate Experiment) [14] we aim to obtain an alternative representation of Earth's gravity field and a more realistic description of the geopotential.

2. Preliminary. In this section we review several basic concepts, outline some properties of spherical splines, explain computational algorithms for scattered data interpolation and fitting, and present a numerical iterative technique for implementation of the algorithms. All the material in this preparatory section can be found either in [1] and [2] or in [4].

Let us define spherical Bernstein–Bézier polynomials first. We begin with a concept of homogeneity. A trivariate function $f(v)$ is homogeneous of degree d if

$$f(\alpha v) = \alpha^d f(v). \tag{2.1}$$

Let $\mathcal{H}_d$ denote the space of trivariate homogeneous polynomials of degree d. That is, $\mathcal{H}_d := \operatorname{span}\{x^i y^j z^k,\ i+j+k=d\}$.

Let $\tau = \langle v_1, v_2, v_3 \rangle$ be a nondegenerate spherical triangle; i.e., assume that the area on the unit sphere bounded by the great circular arcs connecting v_1 and v_2, v_1 and v_3, and v_2 and v_3 is not zero. Let $b_1(v)$, $b_2(v)$, and $b_3(v)$ be the spherical barycentric coordinates of a point $v \in \mathbb{S}^2$, i.e.,

$$v = b_1(v)v_1 + b_2(v)v_2 + b_3(v)v_3.$$

Linear independence of vectors $v_1,\ v_2$, and $v_3 \in \mathbb{R}^3$ imply that the b_i's are uniquely determined. Clearly, the b_i's are linear functions of v. It was shown in [1] that the set

$$B^d_{ijk}(v) = \frac{d!}{i!j!k!} b_1(v)^i b_2(v)^j b_3(v)^k, \qquad i+j+k=d, \tag{2.2}$$

of Bernstein–Bézier basis polynomials of degree d forms a basis for $\mathcal{H}_d$. It is easy to see that $B^d_{ijk}(v)$ is a homogeneous polynomial of degree d. Thus, when restricted to $\mathbb{S}^2$,

$$p(v) = \sum_{i+j+k=d} c_{ijk} B^d_{ijk}(v) \tag{2.3}$$

is called a homogeneous spherical Bernstein–Bézier (SBB)- polynomial of degree d.

Due to this special representation, many properties of SBB polynomials are analogous to those of classical planar Bernstein–Bézier polynomials [1]. However, evaluating integrals of spherical polynomials is considerably more difficult than in the planar setting. All integrals needed for our algorithms have to be evaluated numerically.

Let us now define nonhomogeneous spherical polynomials. It was shown in [10] that $\mathcal{H}_d \oplus \mathcal{H}_{d-1}$ restricted to the unit sphere is identical to the space $\mathcal{P}_d$ of all trivariate polynomials of degree d restricted to the unit sphere. Therefore the set $\{B^d_{ijk},\ i+j+k=d\} \cup \{B^{d-1}_{ijk},\ i+j+k=d-1\}$ on $\mathbb{S}^2$ forms a basis for $\mathcal{P}_d|_{\mathbb{S}^2}$. We can express a nonhomogeneous spherical polynomial p in terms of SBB-basis functions as

$$p = \sum_{i+j+k=d} a_{ijk} B^d_{ijk}(v) + \sum_{i+j+k=d-1} c_{ijk} B^{d-1}_{ijk}(v).$$

With this definition it is easy to see that evaluating (de Casteljau's algorithm), taking derivatives, and computing integrals of homogeneous polynomials can be easily adapted for nonhomogeneous polynomials.

We are now ready to define spherical splines. Given a set $\mathcal{V}$ of points on the unit sphere $\mathbb{S}^2$ we can form a triangulation Δ, which may be a triangulation of a spherical domain on $\mathbb{S}^2$ or of the entire sphere. We will assume that Δ is regular in the sense that any two triangles either do not intersect each other or share their common vertex or their common edge. Let

$$S^r_d(\Delta) := \{s \in C^r(\mathbb{S}^2), s|_\tau \in \mathcal{H}_d, \tau \in \Delta\}$$

be the spherical spline space of degree d and smoothness $r \geq -1$. Here

$$s|_\tau = \sum_{i+j+k=d} c^\tau_{ijk} B^{d,\tau}_{ijk}(v).$$

The space of nonhomogeneous spherical splines is defined as

$$N^r_d(\Delta) := \{s \in C^r(\mathbb{S}^2), s|_\tau \in \mathcal{P}_d, \tau \in \Delta\}$$

with

$$s|_\tau = \sum_{i+j+k=d} a^\tau_{ijk} B^{d,\tau}_{ijk}(v) + \sum_{i+j+k=d-1} c^\tau_{ijk} B^{d-1,\tau}_{ijk}(v).$$

In general, we know neither the dimension of $S^r_d(\Delta)$ nor the construction of locally supported basis functions such as finite elements for arbitrary d and r. However, the lack of understanding of the dimension and construction of locally supported basis functions of general spline spaces does not prevent us from using them for scattered data interpolation and fitting. It is one of the purposes of this paper to show how to use spherical splines of arbitrary d and r with $d > r$ for scattered data interpolation and fitting. The crucial step in the process is to solve a singular linear system arising from the application of the Lagrange multipliers method [2] to the minimization. The linear system has a form which is explained later in detail:

$$\begin{bmatrix} A & L^T \\ L & 0 \end{bmatrix} \begin{bmatrix} \mathbf{c} \\ \lambda \end{bmatrix} = \begin{bmatrix} F \\ G \end{bmatrix}.$$

It is necessary to derive a computational algorithm to efficiently obtain the vector $\mathbf{c}$ containing coefficients of the spline solution. We use the following iterative method [4]:

$$\begin{bmatrix} A & L^T \\ L & -\epsilon I \end{bmatrix} \begin{bmatrix} \mathbf{c}^{(\ell+1)} \\ \lambda^{(\ell+1)} \end{bmatrix} = \begin{bmatrix} F \\ G - \epsilon\lambda^{(\ell)} \end{bmatrix},$$

for $\ell = 0, 1, \ldots,$ where $\epsilon > 0$ is a fixed number, e.g., $\epsilon = 10^{-4}$, $\lambda^{(\ell)}$ is an iterative solution of a Lagrange multiplier coefficient vector with $\lambda^0 = 0$, and I is the identity matrix. The above matrix iterative steps can in fact be rewritten as follows:

$$\left(A + \frac{1}{\epsilon} L^T L\right) \mathbf{c}^{(\ell+1)} = AF\mathbf{c}^{(\ell)} + \frac{1}{\epsilon} L^T G$$

with $\mathbf{c}^{(0)} = 0$. Note that the size of the above linear system is much smaller than the original. The iterations converge very quickly as shown in the following theorem. In our numerical experiments, a few iterations (less than 10) often suffice. A general convergence theorem is proved in [4]. To state the convergence result, we need the following definition.

DEFINITION 2.1. *Let A be a square matrix of size $n \times n$ and L be a rectangular matrix of size $m \times n$. We say a matrix A is positive definite with respect to L if $\mathbf{c}^T A\mathbf{c} \geq 0$, and $A\mathbf{c} = 0$, $L\mathbf{c} = 0$ imply that $\mathbf{c} = 0$.*

THEOREM 2.2. *Suppose that A is symmetric and positive definite with respect to L. Then the matrix $A + \frac{1}{\epsilon} L^T L$ is always invertible for any $\epsilon > 0$. Furthermore, there exists a constant C such that*

$$\|\mathbf{c}^{(\ell+1)} - \mathbf{c}\| \leq C\epsilon \|\mathbf{c}^{(\ell)} - \mathbf{c}\| \quad \textit{for all } \ell \geq 0.$$

3. Minimal energy interpolation.

3.1. Energy functionals. Recall that $\mathcal{V} := \{v \in \mathbb{S}^2\}$ is a set of points on the unit sphere and $\{f(v), v \in \mathcal{V}\}$ is a set of spherical function values given at the locations $\mathcal{V}$. Let Δ be a regular spherical triangulation of $\mathbb{S}^2$ with vertices $\mathcal{V}$. For two integers d and r let $S_d^r(\Delta)$ be the spline space of spherical homogeneous polynomials of degree d and smoothness r.

We need to find a spline function $s \in S_d^r(\Delta)$ interpolating f at $\mathcal{V}$. In general such a spline is not unique. A typical way to use extra degrees of freedom is to minimize a functional $\mathcal{E}(s)$ measuring smoothness of s. In [2] the energy functional

$$\mathcal{E}(s) = \int_{\mathbb{S}^2} (\Delta^* s)^2 d\mu \tag{3.1}$$

was used, where Δ^* is the Laplace–Beltrami operator, μ is the Lebesgue measure on $\mathbb{S}^2$, and the integral in (3.1) is taken over the unit sphere. Note that the Laplace–Beltrami operator annihilates constants only. We propose an alternative functional motivated by Sobolev-type seminorms defined in [12]. Let

$$\mathcal{E}_\delta(s) = \int_{\mathbb{S}^2} \sum_{|\alpha|=2} (D^\alpha s_\delta)^2 d\mu. \tag{3.2}$$

In (3.2) s_δ is the unique homogeneous extension of s of degree δ to $\mathbb{R}^3 \setminus \{0\}$ defined by $s_\delta(v) = |v|^\delta s(\frac{v}{|v|})$. If the degree d of the homogeneous spline space is even, we take $\delta = 0$; if odd, we take $\delta = 1$. After evaluating second order partial derivatives, $D^\alpha s_\delta$ are restricted to $\mathbb{S}^2$ and are then integrated.

To establish existence and uniqueness of a spherical spline in $S_d^r(\Delta)$ interpolating f and minimizing (3.2), we need the following.

LEMMA 3.1. *Let Δ be a spherical triangulation and suppose $f \neq 0$. Then*

(1) *$\mathcal{E}_0(f) = 0$ if and only if f is a constant,*

(2) *$\mathcal{E}_1(f) = 0$ if and only if f is a trivariate homogeneous linear polynomial on $\mathbb{S}^2$.*

Proof. If $\mathcal{E}_\delta(f) = 0$, then by the definition, $D^\alpha f_\delta = 0$ on every triangle $\tau \in \Delta$. Consider $\delta = 1$. Since f_1 is linear homogeneous, $D^\alpha f_1$ is homogeneous of degree -1, and therefore, by the uniqueness of homogeneous extensions, $(D^\alpha f_1|_\tau)_{-1} = D^\alpha f_1$. On the other hand, by the definition, $(D^\alpha f_1|_\tau)_{-1}(v) = |v|^{-1}(D^\alpha f_1|_\tau)(\frac{v}{|v|})$. As we noted above, $D^\alpha f_1|_\tau = 0$, and therefore $D^\alpha f_1 = 0$ as well. Hence f_1 is a polynomial of degree at most 1. Since it is a homogeneous linear function, f_1 must be a homogeneous linear polynomial on $\mathbb{R}^3$. Therefore by the uniqueness of homogeneous extensions, f is a linear homogeneous polynomial on τ. A similar proof works for $\delta = 0$. The other direction follows trivially from definition (3.2). $\square$

Let

$$\Gamma(f) := \{s \in S_d^r(\Delta) : s(v) = f(v) \text{ for all } v \in \mathcal{V}\}$$

be the set of all splines in $S_d^r(\Delta)$ interpolating f at the vertices of triangulation Δ. Let $s_f \in \Gamma(f)$ denote a spherical spline minimizing (3.2) over $\Gamma(f)$.

LEMMA 3.2. *Suppose that $\Gamma(f)$ is not empty. There exists a unique spline $s_f \in S_d^r(\Delta)$ interpolating $f = 0$ and minimizing (3.2) with $\delta = d \bmod(2)$.*

Proof. Since $\mathcal{E}_\delta(s) \geq 0$ for all $s \in S_d^r(\Delta)$, $\mathcal{E}_\delta(s_f) = 0$ is the absolute minimum of $\mathcal{E}_\delta$ achieved at $s_f = 0$. To show the uniqueness, assume there is another $s \in \Gamma(0)$ with $\mathcal{E}_\delta(s) = 0$. We need to prove that $s = s_f$. By our assumption, $\mathcal{E}_\delta(s) = 0$ on every triangle $\tau \in \Delta$. By Lemma 3.1 s is either a linear homogeneous function (if d is odd) or s is a constant (if d is even) on every triangle $\tau \in \Delta$. Since s interpolates 0 at the vertices of each triangle, $s = 0$ on each triangle. Therefore $s = s_f$. $\square$

THEOREM 3.3. *Let Δ be a regular triangulation of $\mathbb{S}^2$ with vertices $\mathcal{V}$ and let $\{f(v),\ v \in \mathcal{V}\}$ be given for some spherical function f. Then for any two positive integers d, r with $d \geq 3r+2$, there exists a unique spline $s_f \in S_d^r(\Delta)$ interpolating the values f and minimizing $\mathcal{E}_\delta$.*

Proof. Since $d \geq 3r + 2$, $\Gamma(f)$ is not empty [3]. There exists an ME spline s_f interpolating f since $\Gamma(f)$ is a nonempty closed convex set. To prove uniqueness suppose there exists $q_f \in \Gamma(f)$ minimizing $\mathcal{E}_\delta$, i.e., $\mathcal{E}_\delta(s_f) = \mathcal{E}_\delta(q_f)$. Since $\mathcal{E}_\delta(s_f + \nu s)$ achieves its minimal value at $\nu = 0$ over $s \in \Gamma(0)$, we have

$$\frac{d}{d\nu}\mathcal{E}_\delta(s_f + \nu s)|_{\nu=0} = 0,$$

which leads to

$$\sum_{|\alpha|=2} \int_{\mathbb{S}^2} (D^\alpha s_{f,\delta})(D^\alpha s_\delta) d\mu = 0$$

for $s \in \Gamma(0)$. In particular for $s = s_f - q_f$ we get

$$\sum_{|\alpha|=2} \int_{\mathbb{S}^2} (D^\alpha s_{f,\delta})^2 d\mu = \sum_{|\alpha|=2} \int_{\mathbb{S}^2} (D^\alpha s_{f,\delta})(D^\alpha q_{f,\delta}) d\mu.$$

Therefore,

$$\mathcal{E}_\delta(s_f - q_f) = 0,$$

and by Lemma 3.2 $s_f - q_f \equiv 0$. This completes the proof. $\square$

To develop ME interpolation using nonhomogeneous splines, we fix integers $d \geq 1$ and $r \geq 0$ and recall that $N_d^r(\Delta) = S_d^r(\Delta) \oplus S_{d-1}^r(\Delta)$. To simplify our notation let us assume that d is odd. We can present a spline function $s \in N_d^r(\Delta)$ as a sum $s_1 + s_0$, where the subscript 1 indicates that $s_1 \in S_d^r(\Delta)$ and that we use its linear extension to compute derivatives. Similarly, the subscript 0 indicates that $s_0 \in S_{d-1}^r(\Delta)$ and that we work with its constant extension.

We define an energy functional which annihilates nonhomogeneous linear polynomials as well as constants and homogeneous linear polynomials

$$\mathcal{E}(s) = \lambda \int_{\mathbb{S}^2} \sum_{|\alpha|=2} (D^\alpha s_1)^2 d\mu + (1-\lambda) \int_{\mathbb{S}^2} \sum_{|\alpha|=2} (D^\alpha s_0)^2 d\mu, \tag{3.3}$$

with $0 < \lambda < 1$.

Lemma 3.4. *Choose degree d and smoothness r for a spline space $N_d^r(\Delta)$ as above. Given a spherical function f let*

$$\widetilde{\Gamma}(f) := \{s \in N_d^r(\Delta) : s(v) = f(v) \;\; \textit{for all } v \in \mathcal{V}\}$$

be the set of all splines in $N_d^r(\Delta)$ interpolating f at the vertices of triangulation Δ. The spline $s_f = 0 \in N_d^r(\Delta)$ is the unique spline interpolating $f = 0$ and minimizing (3.3).

Proof. By the definition, $0 = s_f = s_1 + s_0$, where $s_1|_\tau$ is a homogeneous polynomial of degree d and $s_0|_\tau$ is a homogeneous polynomial of degree $d-1$. Since $S_d^r(\Delta) \cap S_{d-1}^r(\Delta) = 0$, $s_1 = 0$ and $s_0 = 0$. By definition (3.3), $\mathcal{E}(s_f) = 0$. Since $\mathcal{E}(s) \geq 0$ for all $s \in N_d^r(\Delta)$, $\mathcal{E}(0) = 0$ is the absolute minimum of $\mathcal{E}$. To show the uniqueness, assume there is $q_f \in \Gamma(0)$ with $\mathcal{E}(q_f) = 0$. We need to show that $q_f = s_f = 0$. As above, we know $q_f = q_1 + q_0$ for some $q_1 \in S_d^r(\Delta)$ and $q_0 \in S_{d-1}^r(\Delta)$. Then $\mathcal{E}_1(q_1) = 0$ and $\mathcal{E}_0(q_0) = 0$ on every triangle $\tau \in \Delta$. By Lemma 3.1 q_1 is a linear homogeneous polynomial and q_0 is a constant on $\mathbb{S}^2$. Therefore $q_1 + q_0$ is a trivariate linear polynomial satisfying zero interpolation conditions over points $v \in \mathcal{V}$, none of which is the origin. By the linear independence of x, y, z, and 1, $q_f = 0$ on every triangle. Therefore $q_f = s_f$. □

Theorem 3.5. *Let Δ be a regular triangulation of $\mathbb{S}^2$ with vertices $\mathcal{V}$. Let $\{f(v), v \in \mathcal{V}\}$ be the given set of data values. Then for any integers $d \geq 1$, $r \geq 0$ such that $d \geq 3r+2$, there exists a unique spline $s_f \in N_d^r(\Delta)$ interpolating values of f and minimizing $\mathcal{E}$.*

Proof. The proof follows from Lemma 3.4 as in the proof of Theorem 3.3. □

3.2. Computational algorithms. In this section we explain how to compute ME spherical interpolating splines. We use a coefficient vector $\mathbf{c} := (c_{ijk}^\tau, i+j+k = d, \tau \in \Delta)$ to represent each spline function in $S_d^r(\Delta)$. To simplify the data management we linearize the triple indices of SBB-coefficients c_{ijk} and correspondingly the indices of SBB-basis functions B_{ijk}^d. From the properties of SBB-polynomials, we have

$$c_{d00} = f(v_1), \quad c_{0d0} = f(v_2), \quad c_{00d} = f(v_3)$$

for the vertices of each triangle $\tau \in \Delta$. We assemble interpolation conditions into a matrix $\mathbf{K}$, according to the order of the coefficient vector $\mathbf{c}$. Then $\mathbf{Kc} = \mathbf{F}$ is the linear system of equations such that the coefficient vector $\mathbf{c}$ corresponds to a spline s interpolating f at the data sites $\mathcal{V}$.

To ensure the C^r continuity across each edge of Δ, we impose smoothness conditions which can be found in [1]. Let $\mathbf{M}$ denote the smoothness matrix such that $\mathbf{Mc} = 0$ if and only if $s \in S_d^r(\Delta)$.

Next fix $\delta = d \bmod(2)$. Define the energy matrix $\mathbf{E}$ by $\mathbf{E} = \mathrm{diag}(\mathbf{E}_\tau,\ \tau \in \Delta)$. Each block $\mathbf{E}_\tau$ is associated with a triangle τ and contains the entries

$$\mathbf{E}_{ij} := \int_\tau \sum_{|\alpha|=2} D^\alpha (B_i)_\delta D^\alpha (B_j)_\delta d\mu, \tag{3.4}$$

where B_i denotes a SBB-polynomial basis function (2.2) of degree d corresponding to the order of the linearized triple indices (i,j,k), $i+j+k=d$.

The problem of minimizing (3.2) over $S_d^r(\Delta)$ can be formulated as follows:

$$\text{Minimize } \mathbf{c}^T\mathbf{E}\mathbf{c} \text{ subject to } \mathbf{M}\mathbf{c} = 0 \text{ and } \mathbf{K}\mathbf{c} = \mathbf{F}.$$

Using the method of Lagrange multipliers, we must solve the linear system

$$\begin{bmatrix} \mathbf{E} & \mathbf{K}^T & \mathbf{M}^T \\ \mathbf{K} & 0 & 0 \\ \mathbf{M} & 0 & 0 \end{bmatrix} \begin{bmatrix} \mathbf{c} \\ \eta \\ \gamma \end{bmatrix} = \begin{bmatrix} 0 \\ \mathbf{F} \\ 0 \end{bmatrix}.$$

Here γ and η are vectors of Lagrange multiplier coefficients. We obtain the least square solution to the singular linear system above using the iterative method discussed in section 2. Lemma 3.2 implies that $\mathbf{E}$ is symmetric and positive definite with respect to

$$\begin{bmatrix} \mathbf{K} \\ \mathbf{M} \end{bmatrix}.$$

By Theorem 2.2, the iterative method converges to the vector $\mathbf{c}$, which is the coefficient vector of the unique interpolating spline minimizing (3.2). This furnishes a computational algorithm.

To solve the interpolation problem over $N_d^r(\Delta)$, we proceed similarly. Consider $s = s_1 + s_0$ with splines s_1 and s_0 of degrees d and $d-1$, respectively. Order the coefficients over each triangle τ as above and denote them by $\mathbf{c}_1^\tau$ and $\mathbf{c}_0^\tau$. Let $\tilde{\mathbf{c}} = (\mathbf{c}_1, \mathbf{c}_0)$, with $\mathbf{c}_1 := (\mathbf{c}_1^\tau,\ \tau \in \Delta)$ and $\mathbf{c}_0 := (\mathbf{c}_0^\tau,\ \tau \in \Delta)$. We denote interpolation, smoothness and energy matrices by $\mathbf{K}_1$, $\mathbf{K}_0$, $\mathbf{M}_1$, $\mathbf{M}_0$, $\mathbf{E}_1$, $\mathbf{E}_0$ correspondingly. Therefore interpolation conditions for s are

$$\tilde{\mathbf{K}}\tilde{\mathbf{c}} := \begin{bmatrix} \mathbf{K}_1 & \mathbf{K}_0 \end{bmatrix} \begin{bmatrix} \mathbf{c}_1 \\ \mathbf{c}_0 \end{bmatrix} = \mathbf{F}.$$

For s to be smooth we require both s_1 and s_0 to be smooth. The C^r smoothness conditions for s are

$$\tilde{\mathbf{M}}\tilde{\mathbf{c}} := \begin{bmatrix} \mathbf{M}_1 & 0 \\ 0 & \mathbf{M}_0 \end{bmatrix} \begin{bmatrix} \mathbf{c}_1 \\ \mathbf{c}_0 \end{bmatrix} = 0.$$

With definition (3.3) it is clear that the energy matrix in this case is defined by

$$\tilde{\mathbf{E}} = \begin{bmatrix} \lambda\mathbf{E}_1 & 0 \\ 0 & (1-\lambda)\mathbf{E}_0 \end{bmatrix}.$$

Therefore $s \in N_d^r(\Delta)$ minimizes (3.3), interpolates f at the vertices of Δ, and is C^r continuous if and only if the vector $\tilde{\mathbf{c}}$ of its coefficients satisfies the system of linear equations

$$\begin{bmatrix} \tilde{\mathbf{E}} & \tilde{\mathbf{K}}^T & \tilde{\mathbf{M}}^T \\ \tilde{\mathbf{K}} & 0 & 0 \\ \tilde{\mathbf{M}} & 0 & 0 \end{bmatrix} \begin{bmatrix} \tilde{\mathbf{c}} \\ \gamma \\ \eta \end{bmatrix} = \begin{bmatrix} 0 \\ \mathbf{F} \\ 0 \end{bmatrix}.$$

TABLE 3.1
Linear and constant polynomial reproduction on eight triangles.

$S^r_d(\Delta_1) \setminus f$	1	$x+z$	$z+1$
$S^1_3(\Delta_1)$	$4.2265e-01$	$1.1016e-15$	$2.1144e-01$
$S^1_4(\Delta_1)$	$4.6629e-15$	$2.5398e-01$	$9.1140e-02$
$N^1_4(\Delta_1)$	$6.4389e-15$	$1.4950e-15$	$1.5551e-15$

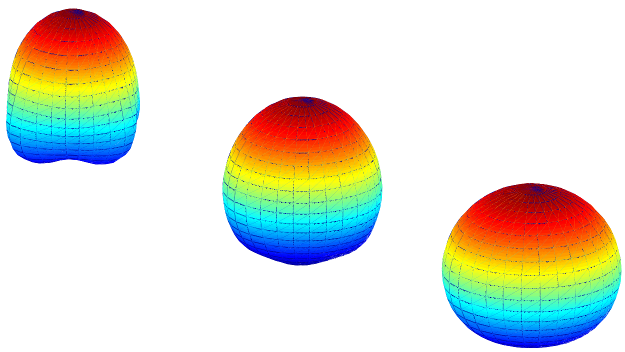

FIG. 3.1. *Interpolation of $z+1$ in S^1_3, S^1_4, and N^1_4 from left to right.*

As in the case of homogeneous splines, the linear system is singular. However, by Lemma 3.4 we have the following.

COROLLARY 3.6. $\tilde{\mathbf{E}}$ *is symmetric and positive definite with respect to*

$$\begin{bmatrix} \tilde{\mathbf{K}} \\ \tilde{\mathbf{M}} \end{bmatrix}.$$

Proof. Since $\mathcal{E}(s) = \tilde{\mathbf{c}}^T\tilde{\mathbf{E}}\tilde{\mathbf{c}} \geq 0$, $\tilde{\mathbf{c}}^T\tilde{\mathbf{E}}\tilde{\mathbf{c}} = 0$ implies that s is a linear polynomial. Zero side conditions force $s = 0$. By the linear independence of the basis functions, $\tilde{\mathbf{c}} = 0$. $\square$

Thus by Theorem 2.2, the application of the iterative scheme allows us to successfully obtain its numerical solution.

3.3. Numerical experiments with ME splines. In this section we present several examples on scattered data interpolation using the ME method.

Example 3.1. Let Δ_1 be the triangulation of the entire sphere based on six vertices $(1,0,0)$, $(0,1,0)$, $(0,0,1)$, $(-1,0,0)$, $(0,-1,0)$, and $(0,0,-1)$ and consisting of eight triangles. We sample 1, $x+z$ and $z+1$ at the six vertices, and compute ME spline interpolants in spherical spline spaces $S^1_3(\Delta)$, $S^1_4(\Delta)$, and $N^1_4(\Delta)$.

The maximal relative errors

$$\frac{\|s(w) - f(w)\|_\infty}{\|f(w)\|_\infty}$$

are computed based on the errors at 5120 points w almost evenly spaced over $\mathbb{S}^2$ and reported in Table 3.1. Note that not only linear and constant homogeneous polynomials are reproduced in $N^1_4(\Delta)$, but a nonhomogeneous polynomial $z+1$ is reproduced as well. In Figure 3.1 we present a visualization of the results of the last column of Table 3.1. It was shown in [1] that spherical linear functions are spheres through the origin. As expected from the table, the first two surfaces are not spheres.

TABLE 3.2
Dependence of ME splines on weights in $\mathcal{E}$.

$\lambda \ \backslash \ e(\Delta)$	$e(\Delta_1)$	$e(\Delta_2)$	$e(\Delta_3)$	$e(\Delta_4)$
0.1	$9.4421e-02$	$2.3349e-02$	$2.2270e-03$	$2.1254e-04$
0.2	$9.4363e-02$	$2.2691e-02$	$1.7986e-03$	$2.0737e-04$
0.3	$9.4292e-02$	$2.2085e-02$	$1.7570e-03$	$2.1420e-04$
0.4	$9.4222e-02$	$2.1608e-02$	$1.9870e-03$	$2.2644e-04$
0.5	$9.4141e-02$	$2.1168e-02$	$2.1526e-03$	$2.4197e-04$
0.6	$9.4053e-02$	$2.0780e-02$	$2.4118e-03$	$2.5990e-04$
0.7	$9.3948e-02$	$2.0461e-02$	$2.7717e-03$	$2.7978e-04$
0.8	$9.3833e-02$	$2.0265e-02$	$3.1331e-03$	$3.1210e-04$
0.9	$9.3701e-02$	$2.0109e-02$	$3.5004e-03$	$3.6150e-04$

TABLE 3.3
Convergence of various splines interpolating f.

$S^r_d(\Delta) \ \backslash \ e(\Delta)$	$e(\Delta_1)$	$e(\Delta_2)$	$e(\Delta_3)$	$e(\Delta_4)$
$S^1_3(\Delta)$	$3.7879e-01$	$6.5860e-02$	$3.7846e-03$	$2.9833e-04$
$S^1_4(\Delta)$	$8.2341e-02$	$1.9801e-02$	$3.8708e-03$	$4.1190e-04$
$N^1_4(\Delta)$	$9.3702e-02$	$2.0109e-02$	$1.7570e-03$	$2.0737e-04$

Example 3.2. Next we investigate how the choice of λ affects the error in minimization over $N^r_d(\Delta)$. We interpolate $f(x,y,z) = 1 + 0.3x^8 + e^{0.2y^3}$ in $N^1_4(\Delta_i)$, $i = 1,\ldots,4$. The initial triangulation is Δ_1. The triangulation Δ_2 is obtained by bisecting the edges of Δ_1 and splitting each triangle into four subtriangles. Similarly we obtain uniform refinements Δ_3 and Δ_4. Each time, we evaluate the spline interpolant at 5120 almost evenly spaced points w and list maximal relative errors

$$e(\Delta_i) := \frac{\|s(w) - f(w)\|_\infty}{\|f(w)\|_\infty}$$

in Table 3.2. The results suggest that the errors on each Δ_i are almost the same for all the values of λ.

Example 3.3. We compare the interpolation results for the function $f(x,y,z) = 1 + 0.3x^8 + e^{0.2y^3}$ in nonhomogeneous and homogeneous spaces. We use Table 3.2 as a guide for the choice of λ. The results in Table 3.3 demonstrate that on finer triangulations nonhomogeneous splines approximate the original function f better than homogeneous splines.

Example 3.4. This is an example of scattered data spline interpolation. We are given 868 points in $\mathbb{R}^3$ (courtesy of Thomas Grandine at Boeing). We translate the point cloud so that its center coincides with the origin and project translated points onto the unit sphere. The projections give us locations on the sphere surface and the distances between the origin and translated points give us corresponding experimental function values. The locations on the sphere are triangulated, and the ME homogeneous cubic and quartic splines are computed as well as nonhomogeneous quartic splines. In Figure 3.2 we present one of the solutions together with the translated point cloud.

Example 3.5. We present an example of scattered data interpolation over the Earth. We are given a satellite data set of simulated geopotential values (in m^2/s^2) observed by the gravity mission satellite, CHAMP [13], along its orbit for two days. The data collected amount to 5760 values. The CHAllenging Mini-satellite Payload (CHAMP) is a German geoscience satellite, launched on July 15, 2000, with a cir-

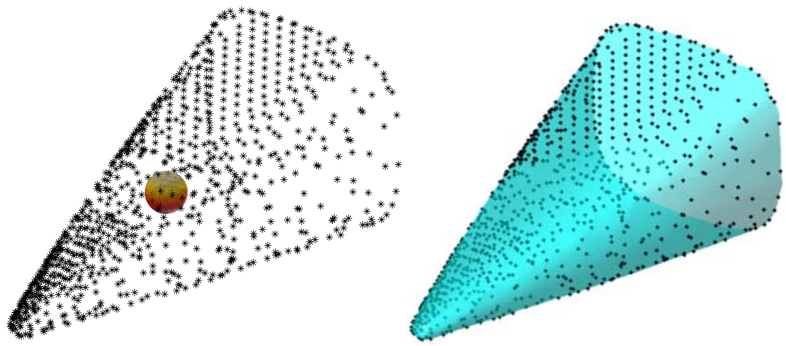

FIG. 3.2. *ME spherical spline interpolant of the point cloud.*

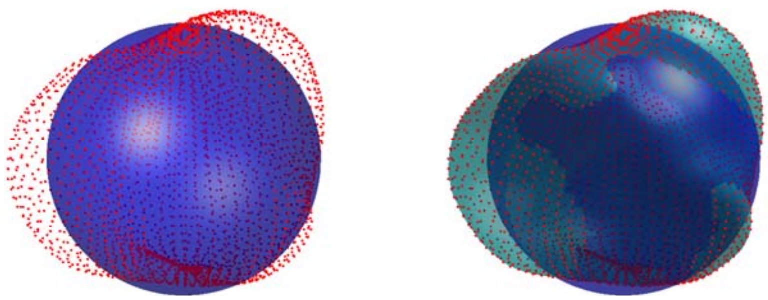

FIG. 3.3. *CHAMP geopotential data and ME spherical spline interpolant.*

cular orbit at an altitude of 450 km and orbital inclination of 87°. The simulated geopotential values are computed using a global geopotential model, EGM96 [11]. In Figure 3.3 we show the set of CHAMP scattered potential values which are normalized by the radius of the Earth and plotted over the unit sphere. The minimal energy homogeneous spherical interpolatory spline surface is shown in Figure 3.3 (right). It is clear that the spherical spline interpolates the given data and produces a reasonable fitting of the given geopotential values.

4. Discrete least squares fitting.

4.1. Existence and uniqueness. When the given data set is extremely large, e.g., $n \geq 10{,}000$, and highly redundant, it is suitable to find a discrete least squares (DLS) fitting to the given data instead of computing an interpolating spherical spline. The DLS approximation problem in $S_d^r(\Delta)$ can be described as follows. Let $\mathcal{V} = \{v_\ell, \ell = 1, \ldots, n\}$ be the given data sites over $\mathbb{S}^2$ and Δ be a triangulation whose vertices may not relate to the data locations. For a given degree d, we assume that the data sites are rich enough in the following sense.

DEFINITION 4.1. *The data sites v_ℓ, $\ell = 1, \ldots, n$, are said to be evenly distributed over the triangulation Δ with respect to d if the matrix*

$$\left[B_{ijk}^{d,\tau}(v_\ell)\right]_{i+j+k=d, v_\ell \in \tau}$$

is of full rank for each $\tau \in \Delta$.

Suppose that the given data values are from a function f, i.e., $f(v_\ell) =: f_\ell$, $\ell = 1, \dots, n$ are given. The least squares functional is defined by

$$\mathcal{L}(s) = \sum_{\ell=1}^{n} (s(v_\ell) - f_\ell)^2. \tag{4.1}$$

A DLS spherical spline $s_f \in S_d^r(\Delta)$ is the function minimizing $\mathcal{L}(s)$ over $S_d^r(\Delta)$, i.e.,

$$\mathcal{L}(s_f) = \min\{\mathcal{L}(s),\ s \in S_d^r(\Delta)\}.$$

THEOREM 4.2. *Suppose that the given data sites v_ℓ, $\ell = 1, \dots, n$, are evenly distributed over Δ with respect to d. There exists a unique spline s_f of degree d and smoothness r minimizing* (4.1).

Proof. Recall that any $s \in S_d^r(\Delta)$ can be written as

$$s(v)|_\tau = \sum_{i+j+k=d} c_{ijk}^\tau B_{ijk}^{d,\tau}(v)$$

on a spherical triangle $\tau \in \Delta$. Let $\mathbf{c} = (c_{ijk}^\tau,\ i+j+k = d,\ \tau \in \Delta)$ be the coefficient vector of s. Note that

$$L(\mathbf{c}) := \mathcal{L}(s) = \sum_{\ell=1}^{n} |s(v_\ell) - f_\ell|^2 = \sum_{\tau\in\Delta} \sum_{v_\ell \in \tau} \left(\sum_{i+j+k=d} c_{ijk}^\tau B_{ijk}^{d,\tau}(v_\ell) - f_\ell \right)^2$$

is a continuous convex function of $\mathbf{c}$, $L(0) = \|\mathbf{f}\|_2^2$ with $\mathbf{f} = (f_\ell,\ \ell = 1, \dots, n)$ the data value vector and $\|\mathbf{f}\|_2 := (\sum_{\ell=1}^n |f_\ell|^2)^{1/2}$ denoting the standard ℓ_2 norm of the vector $\mathbf{f}$. Consider $A = \{\mathbf{c},\ L(\mathbf{c}) \le \|\mathbf{f}\|_2^2\}$ and let us show that A is a bounded and closed set.

Fix any triangle $\tau \in \Delta$. For any $\mathbf{c} \in A$ we have

$$\left| \sum_{i+j+k=d} c_{ijk}^\tau B_{ijk}^{d,\tau}(v_\ell) - f_\ell \right|^2 \le \|\mathbf{f}\|_2^2 \quad \text{for all } v_\ell \in \tau.$$

It follows that

$$\left| \sum_{i+j+k=d} c_{ijk}^\tau B_{ijk}^{d,\tau}(v_\ell) \right| \le 2\|\mathbf{f}\|_2 \quad \text{for all } v_\ell \in \tau.$$

Since the data sites are evenly distributed with respect to d, the matrix

$$\left[B_{ijk}^{d,\tau}(v_\ell) \right]_{i+j+k=d, v_\ell \in \tau}$$

is of full rank and hence, there exists an index set $I_\tau \subset \{1, \dots, n\}$ such that the square matrix $B^\tau = [B_{ijk}^{d,\tau}(v_\ell)]_{i+j+k=d, \ell \in I_\tau}$ is invertible. Therefore $\|(c_{ijk, i+j+k=d}^\tau)\|_2 \le C_\tau$, with C_τ a positive constant depending only on $\|\mathbf{f}\|_2$ and the norm of the inverse matrix of B^τ. Hence $\|\mathbf{c}\|_2$ is bounded above and A is bounded. It is easy to see that A is closed and that $A_s := \{\mathbf{c} : \mathbf{M}\mathbf{c} = 0\}$ is also closed. Here $\mathbf{M}\mathbf{c} = 0$ is the linear system representing the smoothness conditions for $S_d^r(\Delta)$. Hence, the set $A \cap A_s$ is compact, and there exists a $\mathbf{c}_f \in A \cap A_s$ minimizing $L(\mathbf{c})$.

To show uniqueness of the solution $\mathbf{c}_f$, we assume that there exist two solutions $\mathbf{c}_f$ and $\widehat{\mathbf{c}}_f$. The convexity of L implies that for any $0 \le \nu \le 1$ a convex combination $\mathbf{c}_f + \nu(\widehat{\mathbf{c}}_f - \mathbf{c}_f)$ also minimizes L. Thus

$$\begin{aligned}
&\frac{d}{d\nu} L(\mathbf{c}_f + \nu(\widehat{\mathbf{c}}_f - \mathbf{c}_f)) \\
&= \sum_{\tau\in\Delta}\sum_{v_\ell\in\tau}\left(\sum_{i+j+k=d} (\mathbf{c}^\tau_{ijk} + \nu(\widehat{\mathbf{c}}^\tau_{ijk} - \mathbf{c}^\tau_{ijk}))B^\tau_{ijk}(v_\ell) - f_\ell)(\widehat{\mathbf{c}}^\tau_{ijk} - \mathbf{c}^\tau_{ijk})B^\tau_{ijk}(v_\ell)\right) \\
&= \nu \sum_{\tau\in\Delta}\sum_{v_\ell\in\tau}\left(\sum_{i+j+k=d} (\widehat{\mathbf{c}}^\tau_{ijk} - \mathbf{c}^\tau_{ijk})^2 B^\tau_{ijk}(v_\ell)^2\right) \\
&+ \sum_{\tau\in\Delta}\sum_{v_\ell\in\tau}\left(\sum_{i+j+k=d} \mathbf{c}^\tau_{ijk}(\widehat{\mathbf{c}}^\tau_{ijk} - \mathbf{c}^\tau_{ijk})B^\tau_{ijk}(v_\ell)\right)^2 \\
&- \sum_{\tau\in\Delta}\sum_{v_\ell\in\tau}\left(\sum_{i+j+k=d} f_\ell(\widehat{\mathbf{c}}^\tau_{ijk} - \mathbf{c}^\tau_{ijk})B^\tau_{ijk}(v_\ell)\right) = 0
\end{aligned}$$

for any $0 \le \nu \le 1$. Since this expression is independent of ν, we have

$$\sum_{\tau\in\Delta}\sum_{v_\ell\in\tau}\left(\sum_{i+j+k=d} (\widehat{\mathbf{c}}^\tau_{ijk} - \mathbf{c}^\tau_{ijk})^2 B^\tau_{ijk}(v_\ell)\right)^2 = 0.$$

Since the data sites are evenly distributed over Δ, $\mathbf{c}_f = \widehat{\mathbf{c}}_f$. □

For nonhomogeneous spherical splines DLS approximation can be treated similarly. We seek a function $s = s_1 + s_0 \in N^r_d(\Delta)$ minimizing $\mathcal{L}(s)$.

For the nonhomogeneous case, Definition 4.1 has to be modified to take into account that the basis functions in $N^r_d(\Delta)$ consist of homogeneous SBB-basis polynomials of degrees d and $d-1$.

DEFINITION 4.3. *The given data sites v_ℓ, $\ell = 1, \ldots, n$, are said to be evenly distributed over the triangulation Δ with respect to d if the matrix*

$$\begin{bmatrix} B^{d,\tau}_{ijk}(v_\ell) \\ B^{d-1,\tau}_{i'j'k'}(v_\ell) \end{bmatrix}_{i+j+k=d,\, i'+j'+k'=d-1,\, v_\ell\in\tau}$$

is of full rank for every $\tau \in \Delta$.

THEOREM 4.4. *Suppose that the given data locations v_ℓ, $\ell = 1, \ldots, n$ are evenly distributed with respect to d. There exists a unique spline $s_f \in N^r_d(\Delta)$ minimizing (4.1).*

Proof. The proof is similar to the proof of Theorem 4.2. □

4.2. Computational algorithms. We first explain a computational algorithm for the DLS fit in $S^r_d(\Delta)$. The Lagrange multipliers method leads to the linear system

$$\begin{bmatrix} \mathbf{L}^T\mathbf{L} & \mathbf{M}^T \\ \mathbf{M} & 0 \end{bmatrix} \begin{bmatrix} \mathbf{c} \\ \eta \end{bmatrix} = \begin{bmatrix} \mathbf{L}^T\mathbf{F} \\ 0 \end{bmatrix},$$

where $\mathbf{L}$ is the observation matrix with entries $\mathbf{L}_{ij} = B_j(v_i)$, $i = 1, \ldots, n$, and j runs from 1 to $\#\tau(d+1)(d+2)/2$, where $\#\tau$ denotes the number of triangles in Δ.

Here, $\mathbf{F}$ is a vector of function values ordered as the spherical points v_ℓ, $\ell = 1, \ldots, n$, $\mathbf{M}$ is the C^r smoothness matrix, and η is a vector of Lagrange multipliers. The least squares solution of this system is a vector $\mathbf{c}$ of coefficients of a homogeneous spline s of degree d and smoothness r defined with respect to the spherical triangulation Δ minimizing (4.1).

To find the DLS spline in $N_d^r(\Delta)$ we construct the observation matrix

$$\tilde{\mathbf{L}} = \begin{bmatrix} \mathbf{L}_1 & \mathbf{L}_0 \end{bmatrix}$$

and smoothness conditions $\tilde{\mathbf{M}}\tilde{\mathbf{c}} = 0$ as in the previous section. Here $\mathbf{L}_1$ and $\mathbf{L}_0$ are the observation matrices containing values of SBB-basis polynomials at the data sites for the spaces $S_d^{-1}(\Delta)$ and $S_{d-1}^{-1}(\Delta)$. We therefore solve the linear system

$$\begin{bmatrix} \tilde{\mathbf{L}}^T\tilde{\mathbf{L}} & \tilde{\mathbf{M}}^T \\ \tilde{\mathbf{M}} & 0 \end{bmatrix} \begin{bmatrix} c \\ \eta \end{bmatrix} = \begin{bmatrix} \tilde{\mathbf{L}}^T\mathbf{F} \\ 0 \end{bmatrix},$$

where $\mathbf{F}$ contains given data values and η is a vector of Lagrange multiplier coefficients.

THEOREM 4.5. *Suppose that the given data sites v_ℓ, $\ell = 1, \ldots, n$, are evenly distributed over Δ with respect to d. The matrix $\tilde{\mathbf{L}}^T\tilde{\mathbf{L}}$ is positive definite with respect to $\tilde{\mathbf{M}}\tilde{\mathbf{c}} = 0$.*

Proof. If $\tilde{\mathbf{c}}^T\tilde{\mathbf{L}}^T\tilde{\mathbf{L}}\tilde{\mathbf{c}} = 0$, then $\tilde{\mathbf{L}}\tilde{\mathbf{c}} = 0$. Then $\tilde{\mathbf{L}}\tilde{\mathbf{c}}|_\tau = 0$ for every $\tau \in \Delta$, where $\tilde{\mathbf{L}}|_\tau$ is of full rank and therefore $\tilde{\mathbf{c}} = 0$. ☐

Note that similar considerations apply to the homogeneous case; i.e. it is easy to see that the matrix $\mathbf{L}^T\mathbf{L}$ is positive definite with respect to $\mathbf{Mc} = 0$.

Hence Theorem 2.2 can be applied to find the DLS fittings in both homogeneous and nonhomogeneous spherical spline spaces.

4.3. Numerical experiments with DLS splines. The following are examples of DLS approximation on the sphere.

Example 4.1. First we conduct experiments similar to the ones for ME splines in $S_3^1(\Delta_1)$, $S_4^1(\Delta_1)$, and $N_4^1(\Delta_1)$. The total number of scattered data points is 1006. Evaluation points and computation of errors are the same as in section 3.3. In addition we test higher degree polynomials to demonstrate the ability of $N_d^r(\Delta)$ to reproduce nonhomogeneous polynomials of degree d. Results are shown in Table 4.1.

Example 4.2. We illustrate the convergence of DLS splines approximating $f(x, y, z) = 1 + 0.3x^8 + e^{0.2y^3}$ in Table 4.2.

Example 4.3. We continue working with the data in Example 3.5. Recall Δ_1 is a triangulation based on six vertices and eight triangles as in Examples 3.1, 3.2, and 4.1.

TABLE 4.1
Polynomial reproduction over the unit sphere.

$S_d^r(\Delta_1)\ \backslash\ f$	1	$x+z$	$z+1$
$S_3^1(\Delta_1)$	$4.1063e-01$	$5.3912e-10$	$2.0543e-01$
$S_4^1(\Delta_1)$	$2.4365e-09$	$6.3255e-02$	$2.8532e-02$
$N_4^1(\Delta_1)$	$9.4194e-14$	$3.3859e-12$	$9.9751e-14$
$S_d^r(\Delta_1)\ \backslash\ f$	y^2+z	y^3+z+1	x^4+z+1
$S_3^1(\Delta_1)$	$1.5315e-01$	$1.8931e-01$	$1.7120e-01$
$S_4^1(\Delta_1)$	$4.5673e-02$	$2.8735e-02$	$2.6810e-02$
$N_4^1(\Delta_1)$	$1.1709e-13$	$1.2950e-13$	$1.5834e-13$

TABLE 4.2
Relative errors for splines approximating f.

$S_d^r(\Delta) \ \backslash \ e(\Delta)$	$e(\Delta_1)$	$e(\Delta_2)$	$e(\Delta_3)$
$S_3^1(\Delta)$	$3.4124e-01$	$4.1755e-02$	$3.6864e-03$
$S_4^1(\Delta)$	$2.3321e-02$	$1.8815e-03$	$7.4771e-04$
$N_4^1(\Delta)$	$1.0102e-02$	$1.8007e-03$	$3.6840e-04$

TABLE 4.3
The relative errors for geodata approximating splines.

$S_d^r(\Delta) \ \backslash \ e(\Delta)$	$e(\Delta_1)$	$e(\Delta_2)$	$e(\Delta_3)$
$S_3^1(\Delta)$	$3.7228e-01$	$2.0086e-01$	$8.6921e-02$
$S_4^1(\Delta)$	$2.9349e-01$	$9.6814e-02$	$4.5916e-02$
$N_4^1(\Delta)$	$2.0711e-01$	$9.5309e-02$	$3.1303e-02$

TABLE 4.4
The relative standard deviations for geodata approximating splines.

$S_d^r(\Delta) \ \backslash \ \mathrm{s}(\Delta)$	$\mathrm{s}(\Delta_1)$	$\mathrm{s}(\Delta_2)$	$\mathrm{s}(\Delta_3)$
$S_3^1(\Delta)$	$7.020e-02$	$3.5489e-02$	$1.3247e-02$
$S_4^1(\Delta)$	$4.7324e-02$	$1.4640e-02$	$4.4683e-03$
$N_4^1(\Delta)$	$3.5713e-02$	$1.1194e-02$	$3.2933e-03$

Then Δ_1 is refined uniformly twice to obtain Δ_2 and Δ_3. For each triangulation we compute DLS spline solutions in the spaces $S_3^1(\Delta_i)$, $S_4^1(\Delta_i)$, and $N_4^1(\Delta_i)$, $i = 1, 2, 3$. In Table 4.3 we list errors of

$$e(\Delta_i) := \frac{\max_{v\in\mathcal{V}}|s(v) - f(v)|}{\max_{v\in\mathcal{V}}|f(v)|}$$

for each of the computed splines over triangulation Δ_i. In Table 4.4 we list their relative standard deviation values

$$\mathrm{s}(\Delta_i) := \frac{\mathrm{std}|s(v) - f(v)|}{\max_{v\in\mathcal{V}}|f(v)|}.$$

5. Penalized least squares approximation.

5.1. Existence and uniqueness. Again we let $\mathcal{V} := \{v_\ell, \ell = 1, \ldots, n\}$ be a set of sites on $\mathbb{S}^2$ and $\{f_\ell, \ell = 1, \ldots, n\}$ be the corresponding values for some function f. We need to find a smooth surface resembling f. Another commonly used method in this situation is called a penalized least squares (PLS) fit.

Let Δ be a regular triangulation of $\mathbb{S}^2$ whose vertices $\mathcal{W}$ form a subset of the data sites $\mathcal{V}$. Consider the spline space $S_d^r(\Delta)$ of degree d and smoothness r. We look for a spline solution $s_f \in S_d^r(\Delta)$ satisfying

$$\mathcal{P}_\lambda(s_f) = \min\{\mathcal{P}_\lambda(s) : s \in S_d^r(\Delta)\}, \tag{5.1}$$

where λ is a positive weight and

$$\mathcal{P}_\lambda(s) := \mathcal{L}(s) + \lambda\mathcal{E}_\delta(s). \tag{5.2}$$

Here the DLS and ME functionals are as defined in (4.1) and (3.2), respectively. It is clear that for large $\lambda \gg 1$, s_f is close to ME splines, and for small $\lambda \ll 1$ the solution s_f is close to the DLS spline. One way to choose λ is by the cross validation method [15]. We choose a small value for λ to get a good approximation, such as that of the DLS fitting which in the planar setting has high approximation power [9].

THEOREM 5.1. *Fix* $\lambda > 0$. *Suppose the vertices* $\mathcal{W}$ *of* Δ *are part of the data sites* $\mathcal{V}$ *and each triangle can be inscribed into a spherical cap of radius* $\leq 1/2$*; i.e., the size of every triangle* $|\tau|$ *is bounded above by* 1. *There exists a unique spline* $s_f \in S_d^r(\Delta)$ *minimizing* (5.2).

Proof. Recall that any $s \in S_d^r(\Delta)$ can be written as

$$s(v)|_\tau = \sum_{i+j+k=d} c_{ijk}^\tau B_{ijk}^{d,\tau}(v)$$

on a spherical triangle $\tau \in \Delta$. Let $\mathbf{c} = (c_{ijk}^\tau,\ i+j+k=d,\ \tau \in \Delta)$ be the coefficient vector of s. Recall that the energy functional $\mathcal{E}(s)$ can be expressed in terms of $\mathbf{c}$ as

$$\mathcal{E}(s) = \mathbf{c}^T \mathbf{E} \mathbf{c}$$

with the entries of $\mathbf{E}$ defined in (3.4). The DLS functional $\mathcal{L}(s)$ is expressed as

$$\begin{aligned}\mathcal{L}(s) = \sum_{\ell=1}^{n} |s(v_\ell) - f_\ell|^2 &= \sum_{\tau\in\Delta} \sum_{v_\ell \in \tau} \left(\sum_{i+j+k=d} c_{ijk}^\tau B_{ijk}^\tau(v_\ell) - f_\ell \right)^2 \\ &= \mathbf{c}^T \mathbf{L}^T \mathbf{L} \mathbf{c} - 2\mathbf{f}^T \mathbf{L} \mathbf{c} + \|\mathbf{f}\|_2^2,\end{aligned}$$

with $\mathbf{f} = (f_\ell,\ \ell = 1, \ldots, n)$ being the vector of data values. Thus

$$\mathcal{P}_\lambda(s) = \lambda \mathbf{c}^T \mathbf{E} \mathbf{c} + \mathbf{c}^T \mathbf{L}^T \mathbf{L} \mathbf{c} - 2\mathbf{f}^T \mathbf{L} \mathbf{c} + \|\mathbf{f}\|_2^2.$$

Note that $\mathcal{P}_\lambda(0) = \|\mathbf{f}\|_2^2$. Consider $A = \{\mathbf{c}, \mathcal{P}_\lambda(s) \leq \|\mathbf{f}\|_2^2\}$. Let us show that A is a bounded and closed set so that the continuous function $\mathcal{P}_\lambda(s)$ has a minimum in A.

Fix $\mathbf{c} \in A$ and let s be the corresponding spline. Then $\mathcal{P}_\lambda(s) \leq \|\mathbf{f}\|_2^2$. By the definition of $\mathcal{P}_\lambda$ we must have $\lambda \mathcal{E}_\delta(s) \leq \|\mathbf{f}\|_2^2$. By Lemma 10 in [6] and Lemma 3.9 in [5] the energy of a spline is equivalent to the square of its second order Sobolev seminorm on every triangle of Δ and all norms of a spline on each triangle are equivalent; i.e., we have

$$|s|_{2,\infty,\tau} \leq \frac{C_1}{\sqrt{\lambda}} \|\mathbf{f}\|_2 \text{ and } |s|'_{2,\infty,\tau} \leq \frac{C_2}{\sqrt{\lambda}} \|\mathbf{f}\|_2$$

with C_1, C_2 depending on degree d of the spline space and the smallest angle in τ. Let r_τ denote the center of the smallest spherical cap containing τ. Let $\mathbf{T}_\tau$ be a plane tangent to τ at r_τ. Define $\bar{\tau}$ in this plane as a set of points $\{w : \frac{w}{|w|} \in \tau\}$. Define $s_\delta(w) = |w|^\delta s(\frac{w}{|w|})$ to be a homogeneous extension of s of degree δ and $\bar{s}_\delta$ to be its restriction to $\bar{\tau}$. Similarly define f_δ and $\bar{f}_\delta$. By Proposition 2.26 in [5]

$$|\bar{s}_1|_{2,\infty,\bar{\tau}} \leq C_3 |s|_{2,\infty,\tau} \text{ and } |\bar{s}_0|_{2,\infty,\bar{\tau}} \leq C_4 |s|'_{2,\infty,\tau}.$$

Therefore

$$|\bar{s}_\delta|_{2,\infty,\bar{\tau}} \leq \frac{C_5}{\sqrt{\lambda}} \|\mathbf{f}\|_2. \tag{5.3}$$

Since the vertices, say v_1, v_2, v_3, of τ belong to $\mathcal{W}$,

$$\begin{aligned}|\bar{s}_\delta(\bar{v}_i)| &\leq |\bar{s}_\delta(\bar{v}_i) - \bar{f}_\delta(\bar{v}_i)| + |\bar{f}_\delta(\bar{v}_i)| \\ &\leq |v_i|^\delta(|s(v_i) - f(v_i)| + |f(v_i)|) \\ &\leq C_6((\mathcal{P}_\lambda(s))^{1/2} + \|\mathbf{f}\|_2) \leq 2C_6\|\mathbf{f}\|_2,\end{aligned}$$

for $C_6 = \max\{|v_\ell|^\delta : v_\ell \in \tau\} \leq 1/\cos(1/2)$ and $i = 1, 2, 3$. For any point $\bar{v}$ in $\bar{\tau}$ we need to show that $\bar{s}_\delta(\bar{v})$ is bounded. Use Taylor expansion to get

$$\bar{s}_\delta(\bar{v}_1) = \bar{s}_\delta(\bar{v}) + \nabla\bar{s}_\delta(\bar{v}) \cdot (\bar{v}_1 - \bar{v}) + O(|\bar{s}_\delta|_{2,\infty,\bar{\tau}}|\bar{\tau}|^2). \tag{5.4}$$

Using similar expressions for $\bar{v}_2$ and $\bar{v_3}$ we get

$$\begin{aligned}\bar{s}_\delta(\bar{v}_1) - \bar{s}_\delta(\bar{v}_2) = \nabla\bar{s}_\delta(\bar{v}) \cdot (\bar{v}_1 - \bar{v}_2) + O(|\bar{s}_\delta|_{2,\infty,\bar{\tau}}|\bar{\tau}|^2), \\ \bar{s}_\delta(\bar{v}_2) - \bar{s}_\delta(\bar{v_3}) = \nabla\bar{s}_\delta(\bar{v}) \cdot (\bar{v}_2 - \bar{v_3}) + O(|\bar{s}_\delta|_{2,\infty,\bar{\tau}}|\bar{\tau}|^2).\end{aligned}$$

Solving this linear system for $\nabla\bar{s}_\delta$, we get

$$\begin{aligned}D_x\bar{s}_\delta(\bar{v}) = O(|\bar{\tau}|^3|\bar{s}_\delta|_{2,\infty,\bar{\tau}}/A_{\bar{\tau}}) + |\bar{s}_\delta(\bar{v}_1)| + |\bar{s}_\delta(\bar{v}_2)||\bar{\tau}|/A_{\bar{\tau}}, \\ D_y\bar{s}_\delta(\bar{v}) = O(|\bar{\tau}|^3|\bar{s}_\delta|_{2,\infty,\bar{\tau}}/A_{\bar{\tau}}) + |\bar{s}_\delta(\bar{v}_1)| + |\bar{s}_\delta(\bar{v}_2)||\bar{\tau}|/A_{\bar{\tau}},\end{aligned}$$

where $A_{\bar{\tau}}$ denotes the area of $\bar{\tau}$. Using these estimates for $\nabla\bar{s}_\delta$ we get

$$|\bar{s}_\delta(\bar{v})| \leq C_7((1 + |\bar{\tau}| + |\bar{\tau}|^2/A_{\bar{\tau}})\|\mathbf{f}\|_2 + |\bar{\tau}|^4|\bar{s}_\delta|_{2,\infty,\bar{\tau}}/A_{\bar{\tau}}).$$

Hence we use (5.3) and (5.4) to get

$$|\bar{s}_\delta(\bar{v})| \leq C_8\|\mathbf{f}\|_2$$

with C_8 depending on the size of τ. By the definition,

$$|s(v)| = |\bar{v}|^{-\delta}|\bar{s}_\delta(\bar{v})| \leq C_{\bar{\tau}}\|\mathbf{f}\|_2$$

is bounded since $|\bar{v}| \geq 1$ and $|\bar{\tau}|$ is bounded. By the stability of SBB-basis [12], $\mathbf{c}$ is bounded, and hence A is a bounded set. Since A is closed, it is compact. By the definition, $\mathcal{P}_\lambda(s)$ is a continuous function of $\mathbf{c}$ and therefore $\mathcal{P}_\lambda$ attains its minimum in A.

To show uniqueness of the minimizer s_f suppose there exists $\hat{s}_f$ with $\mathcal{P}_\lambda(s_f) = \mathcal{P}_\lambda(\hat{s}_f)$. Since $\mathcal{P}_\lambda$ is a convex functional for any $0 \leq \nu \leq 1$,

$$\mathcal{P}_\lambda(\nu s_f + (1-\nu)\hat{s}_f) \leq \nu\mathcal{P}_\lambda(s_f) + (1-\nu)\mathcal{P}_\lambda(\hat{s}_f) = \mathcal{P}_\lambda(s_f).$$

On the other hand, since $\mathcal{P}_\lambda$ achieves minimum value at s_f,

$$\mathcal{P}_\lambda(s_f) \leq \mathcal{P}_\lambda(\nu s_f + (1-\nu)\hat{s}_f).$$

Therefore $\mathcal{P}_\lambda(\hat{s}_f + \nu(s_f - \hat{s}_f))$ is a constant function of ν on $[0, 1]$. It follows that $\frac{d}{d\nu}\mathcal{P}_\lambda(\hat{s}_f + \nu(s_f - \hat{s}_f)) = 0$ for all $0 \leq \nu \leq 1$, i.e.,

$$\begin{aligned}0 &= \frac{d}{d\nu}\mathcal{P}_\lambda(\hat{s}_f + \nu(s_f - \hat{s}_f)) \\ &= 2\lambda(\hat{\mathbf{c}}_f + \nu(\mathbf{c}_f - \hat{\mathbf{c}}_f))^T\mathbf{E}(\mathbf{c}_f - \hat{\mathbf{c}}_f) \\ &\quad + 2(\hat{\mathbf{c}}_f + \nu(\mathbf{c}_f - \hat{\mathbf{c}}_f))^T\mathbf{L}^T\mathbf{L}(\mathbf{c}_f - \hat{\mathbf{c}}_f) - 2\mathbf{f}^T\mathbf{L}(\mathbf{c}_f - \hat{\mathbf{c}}_f).\end{aligned}$$

The above holds for any ν in $[0,1]$. It follows, as in Theorem 4.2, that

$$0 = 2\lambda(\mathbf{c}_f - \hat{\mathbf{c}}_f)^T \mathbf{E}(\mathbf{c}_f - \hat{\mathbf{c}}_f) + 2(\mathbf{c}_f - \hat{\mathbf{c}}_f)^T \mathbf{L}^T \mathbf{L}(\mathbf{c}_f - \hat{\mathbf{c}}_f).$$

Hence, we must have $(\mathbf{c}_f - \hat{\mathbf{c}}_f)^T \mathbf{E}(\mathbf{c}_f - \hat{\mathbf{c}}_f) = 0$ and $(\mathbf{c}_f - \hat{\mathbf{c}}_f)^T \mathbf{L}^T \mathbf{L}(\mathbf{c}_f - \hat{\mathbf{c}}_f) = 0$ since both $\mathbf{E}$ and $\mathbf{L}^T\mathbf{L}$ are nonnegative definite. Then $\mathcal{E}(s_f - \hat{s}_f) = 0$ and therefore $s_f - \hat{s}_f$ is a linear homogeneous polynomial, and $s_f(v_\ell) - \hat{s}_f(v_\ell) = 0$ at every vertex v_ℓ of Δ. Therefore $s_f = \hat{s}_f$. ◻

To solve the PLS problem using nonhomogeneous splines we work in $N_d^r(\Delta)$. We have to replace the energy functional (3.2) in (5.2) by (3.3). For a spherical spline function $s = s_1 + s_0$ define

$$\mathcal{P}_\lambda(s) = \mathcal{L}(s_1 + s_0) + \lambda_1 \int_{\mathbb{S}^2} \sum_{|\alpha|=2} (D^\alpha s_1)^2 d\mu + \lambda_0 \int_{\mathbb{S}^2} \sum_{|\alpha|=2} (D^\alpha s_0)^2 d\mu, \tag{5.5}$$

with $\lambda_1 > 0$, $\lambda_0 > 0$.

THEOREM 5.2. *Fix $\lambda_1 > 0$ and $\lambda_0 > 0$. Suppose all vertices $\mathcal{W}$ of Δ are part of the data sites $\mathcal{V}$ and* $\max\{|\tau|,\ \tau \in \Delta\} =: |\Delta| \le 1$. *There exists a unique spline $s_f \in N_d^r(\Delta)$ minimizing* (5.5).

Proof. The proof is similar to the proof of Theorem 5.1. ◻

5.2. Computational algorithms. We first consider PLS fitting in $S_d^r(\Delta)$. By the method of Lagrange multipliers, minimization of (5.2) over $S_d^{-1}(\Delta)$ subject to the smoothness C^r conditions in the matrix form $\mathbf{Mc} = 0$ results in a system of linear equations

$$\begin{bmatrix} \mathbf{P} & \mathbf{M}^T \\ \mathbf{M} & 0 \end{bmatrix} \begin{bmatrix} \mathbf{c} \\ \eta \end{bmatrix} = \begin{bmatrix} \mathbf{L}^T\mathbf{F} \\ 0 \end{bmatrix}.$$

Here $\mathbf{P} = \mathbf{L}^T\mathbf{L} + \lambda\mathbf{E}$ and $\mathbf{f}$ is a vector of function values ordered as the spherical points v_ℓ, $\ell = 1, \ldots, n$, $\mathbf{M}$ is a smoothness matrix, and η is a vector of Lagrange multiplier coefficients. The solution of this system is a vector $\mathbf{c}$ of coefficients of a homogeneous spline s of degree d and smoothness r defined over the spherical triangulation Δ minimizing (5.2). Note that the linear system is of the same form as the one in section 2. We use the iterative scheme to compute an approximation of $\mathbf{c}$.

To find the PLS spline in $N_d^r(\Delta)$ we construct the observation matrix $\tilde{\mathbf{L}}$ and smoothness conditions $\tilde{\mathbf{M}}\tilde{\mathbf{c}} = 0$ as in the setting of DLS splines. We also assemble the energy matrices $\mathbf{E}_1$ and $\mathbf{E}_0$ and solve the linear system

$$\begin{bmatrix} \tilde{\mathbf{P}} & \tilde{\mathbf{M}}^T \\ \tilde{\mathbf{M}} & 0 \end{bmatrix} \begin{bmatrix} \tilde{\mathbf{c}} \\ \eta \end{bmatrix} = \begin{bmatrix} \tilde{\mathbf{L}}^T\mathbf{f} \\ 0 \end{bmatrix},$$

where $\tilde{\mathbf{P}}$ in this case is

$$\tilde{\mathbf{L}}^T\tilde{\mathbf{L}} + \begin{bmatrix} \lambda_1\mathbf{E}_1 & 0 \\ 0 & \lambda_0\mathbf{E}_0 \end{bmatrix}.$$

COROLLARY 5.3. *The matrix $\tilde{\mathbf{P}}$ is positive definite with respect to* $\tilde{\mathbf{M}}\tilde{\mathbf{c}} = 0$.

Proof. $\tilde{\mathbf{c}}^T\tilde{\mathbf{P}}\tilde{\mathbf{c}} = 0$ implies that $\tilde{\mathbf{c}}^T\tilde{\mathbf{E}}\tilde{\mathbf{c}} = 0$. Therefore $\mathcal{P}_\lambda(s) = 0$ implies that s is a linear polynomial. $\mathcal{L}(s) = 0$ as well, and therefore s interpolates $f = 0$ at every vertex of Δ. Hence $s = 0$ and so is $\tilde{\mathbf{c}} = 0$. ◻

Note that considerations of Corollary 5.3 apply to the homogeneous case, and therefore we can efficiently obtain homogeneous PLS spline solutions as well.

TABLE 5.1
The relative errors for PLS splines.

$S^r_d(\Delta) \ \backslash \ e(\Delta)$	$e(\bar{\Delta}_1)$	$e(\bar{\Delta}_2)$	$e(\bar{\Delta}_3)$
$S^1_3(\Delta)$	$7.3001e-01$	$2.5346e-01$	$1.0829e-01$
$S^1_4(\Delta)$	$3.2211e-01$	$1.1959e-01$	$4.4371e-02$
$N^1_4(\Delta)$	$2.5707e-01$	$9.4001e-02$	$4.2157e-02$

TABLE 5.2
The relative standard deviations for PLS splines.

$S^r_d(\Delta) \ \backslash \ \mathrm{s}(\Delta)$	$\mathrm{s}(\bar{\Delta}_1)$	$\mathrm{s}(\bar{\Delta}_2)$	$\mathrm{s}(\bar{\Delta}_3)$
$S^1_3(\Delta)$	$1.3024e-01$	$4.4337e-02$	$1.4585e-02$
$S^1_4(\Delta)$	$5.5051e-02$	$1.7656e-02$	$4.5250e-03$
$N^1_4(\Delta)$	$3.9482e-02$	$1.3479e-02$	$4.1267e-03$

5.3. Numerical experiments with PLS splines. In this section we present an example of a PLS fitting similar to Example 4.3.

Example 5.1. Note that for PLS fit we require the data at the vertices of a triangulation to be given. To deal with this requirement we modify the triangulation Δ_1 by replacing its vertices by points in $\mathcal{V}$ closest to them. Denote the new triangulation by $\bar{\Delta}_1$. After refining $\bar{\Delta}_1$ we again may not have the values of geopotential values available at the vertices of the refined triangulation. We replace these vertices by the points in $\mathcal{V}$ closest to them where values of geopotential are available. We call this new triangulation $\bar{\Delta}_2$. Similarly we obtain $\bar{\Delta}_3$. That is, $\bar{\Delta}_{i+1}$ is not exactly a uniform refinement of $\bar{\Delta}_i$. For each triangulation we compute PLS spline solutions in the spaces $S^1_3(\bar{\Delta}_i)$, $S^1_4(\bar{\Delta}_i)$, and $N^1_4(\bar{\Delta}_i)$, $i = 1, 2, 3$, with $\lambda = \lambda_1 = \lambda_2 = 10^{-6}$. In Table 5.1 we list relative error values

$$e(\bar{\Delta}_i) := \frac{\max_{v\in\mathcal{V}}|s(v) - f(v)|}{\max_{v\in\mathcal{V}}|f(v)|}$$

for each of the computed splines over triangulation Δ_i. In Table 5.2 we list their relative standard deviation values

$$\mathrm{s}(\bar{\Delta}_i) := \frac{\mathrm{std}|s(v) - f(v)|}{\max_{v\in\mathcal{V}}|f(v)|}.$$

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