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WELL CONDITIONED SPHERICAL DESIGNS FOR INTEGRATION AND INTERPOLATION ON THE TWO-SPHERE*

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Abstract. A set $\mathcal{X}_N$ of N points on the unit sphere is a spherical t-design if the average value of any polynomial of degree at most t over $\mathcal{X}_N$ is equal to the average value of the polynomial over the sphere. This paper considers the characterization and computation of spherical t-designs on the unit sphere $\mathbb{S}^2 \subset \mathbb{R}^3$ when $N \geq (t+1)^2$, the dimension of the space $\mathbb{P}_t$ of spherical polynomials of degree at most t. We show how to construct well conditioned spherical designs with $N \geq (t+1)^2$ points by maximizing the determinant of a matrix while satisfying a system of nonlinear constraints. Interval methods are then used to prove the existence of a true spherical t-design very close to the calculated points and to provide a guaranteed interval containing the determinant. The resulting spherical designs have good geometrical properties (separation and mesh norm). We discuss the usefulness of the points for both equal weight numerical integration and polynomial interpolation on the sphere and give an example.

Key words. spherical design, fundamental system, mesh norm, maximum determinant, Lebesgue constant, numerical integration, interpolation, interval method

AMS subject classifications. 65D32, 65H10

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1. Introduction.

Let $\mathcal{X}_N = \{\mathbf{x}_1, \ldots, \mathbf{x}_N\}$ be a set of N points on the unit sphere $\mathbb{S}^d = \{\mathbf{x} \mid \|\mathbf{x}\|_2 = 1\} \subset \mathbb{R}^{d+1}$, and let $\mathbb{P}_t = \mathbb{P}_t(\mathbb{S}^d)$ be the linear space of restrictions of polynomials of degree at most t in $d+1$ variables to $\mathbb{S}^d$. The set $\mathcal{X}_N$ is a *spherical t-design* if

$$\frac{1}{N}\sum_{j=1}^{N} p\left(\mathbf{x}_j\right) = \frac{1}{|\mathbb{S}^d|}\int_{\mathbb{S}^d} p(\mathbf{x})d\omega(\mathbf{x}) \tag{1.1}$$

holds for all spherical polynomials $p \in \mathbb{P}_t(\mathbb{S}^d)$, where $d\omega(\mathbf{x})$ denotes the surface measure on $\mathbb{S}^d$ and $|\mathbb{S}^d|$ is the surface area of the unit sphere $\mathbb{S}^d$. In other words, we see that $\mathcal{X}_N$ is a spherical t-design if the average value over $\mathcal{X}_N$ of any polynomial of degree at most t is equal to the average value of the polynomial over the sphere.

The concept of spherical t-designs was introduced by Delsarte, Goethals, and Seidel [9] in 1977. Since then, spherical t-designs have been studied extensively [2, 3, 6, 7, 13, 17, 29, 30, 32]. In 2009, Bannai and Bannai gave a comprehensive survey of research on spherical t-designs in the last three decades [4].

In this paper we focus our attention on $\mathbb{S}^2$. The study of distribution of points on $\mathbb{S}^2$ has many applications, including climate modeling and global approximation in geophysics and virus modeling in bioengineering, as the earth and cell are approximate

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spheres. We look at spherical t-designs on $\mathbb{S}^2$ that are good for numerical integration and also (if the number of points N is right) for polynomial interpolation.

It is well known that, for $d = 2$, the dimension of $\mathbb{P}_t$ is $(t+1)^2$. For $N \geq (t+1)^2$, we introduce a new concept of *extremal spherical t-designs*. These are spherical t-designs for which the determinant of a certain $(t+1)^2 \times (t+1)^2$ Gram matrix (see (3.5a)), or equivalently the product of the singular values of a basis matrix, takes its maximum value. This extends the definition of extremal spherical design introduced in [7] for the case $N = (t+1)^2$.

As is well known, there is no proof that spherical t-designs (and hence extremal spherical t-designs) exist with $N = (t+1)^2$ points (or even with $N = O\,(t+1)^2$ points) for all degrees t. The above definition is empty if spherical t-designs do not exist. However, from the work of [6] we know that, for $d = 2$, spherical t-designs with $(t+1)^2$ points do exist for all degrees t up to 100, so extremal spherical t-designs are well defined up to at least $t = 100$, but until now no attempt has been made to compute them. This range of t values is large enough to persuade us of the usefulness of the definition. Moreover, Seymour and Zaslavsky [26] showed that a spherical t-design exists for any t if N is sufficiently large. This is one of our motivations for considering $N \geq (t+1)^2$.

In this paper we construct approximate extremal spherical t-designs for $d = 2$ for all t up to 60 and then use interval methods to prove that a well conditioned true spherical t-design exists in a small neighborhood of the numerically computed point set. We also compute a relatively narrow interval containing the determinant of the matrix for the true spherical design. This is a new kind of problem in interval analysis and introduces a preconditioned matrix interval technique. In practice the computation is extremely stable because of the maximizing (subject to the constraint) of the determinant.

Our claim is that the constructed well conditioned spherical t-designs with $N \geq (t+1)^2$ are valuable for numerical integration (where (1.1) provides an equal weight integration rule) and if $N = (t+1)^2$ also for polynomial interpolation. When $N = (t+1)^2$, the quadrature rule and the interpolant are consistent, in that the quadrature rule for a given function f is the exact integral of the interpolant of f.

The constructed point sets also have very good geometrical properties, as we discuss in section 5. One might be tempted to believe that every spherical t-design is a well distributed point set, but this is not the case. First the tensor product construction of Korevaar and Meyers [17], as well as Bajnok [2], has $O\left(t^3\right)$ points (compared to $(t+1)^2$ points for the current construction) and very bad geometrical properties. Second Hesse and Leopardi [14] have pointed out that any nonoverlapping union of spherical t-designs is also a spherical t-design. This makes it possible to construct a spherical t-design with an arbitrarily small minimum distance between points.

In the next section we summarize the required background on spherical t-designs. In section 3 we give several variational characterizations of spherical t-designs based on fundamental systems and also present a new variational characterization that extends the existing result in [29]. We also introduce the concept of extremal spherical t-designs and generalize the nonlinear system approach of Chen and Womersley [7] to provide the foundation for the later computations in the present paper. In section 4 we describe the computational construction and the interval analysis used to overcome numerical uncertainties from rounding error. In section 5 we consider the geometry of well conditioned spherical t-designs and describe what is known and what is conjectured about their geometry. In section 6, for $N = (t+1)^2$, we present numerical evidence on the quality of the resulting well conditioned spherical t-designs on $\mathbb{S}^2$ for interpolation by computing the resulting Lebesgue constant and comparing it with the best known Lebesgue constant. Finally in section 7 we give an example of both integration and interpolation with these well conditioned spherical t-designs.

2. Background. Lower bounds for the number of points N needed to construct a spherical t-design are [9]

$$N \geq N_* = \begin{cases} \frac{(t+1)(t+3)}{4}, & t \quad \text{is odd,} \\ \frac{(t+2)^2}{4}, & t \quad \text{is even.} \end{cases}$$

A catalogue of known spherical t-designs on $\mathbb{S}^2$ with small values of N is given by Hardin and Sloane [13]. These authors also suggested a sequence of putative spherical t-designs with $N = \frac{1}{2}t^2 + o(t^2)$, but there is no proof that the construction is valid for all values of t. Results in [29, 32] also provide strong numerical evidence that there exist spherical t-designs with close to $(t+1)^2/2$ points.

In this paper we are interested in finding well conditioned spherical t-designs with $N \geq (t+1)^2$. Rather than minimizing the number of points, the extra degrees of freedom are used to ensure well conditioning, in a sense to be made clear later in the paper.

Let $\{Y_{\ell,k} \;:\; k = 1,\ldots,2\ell{+}1,\ \ell = 0,1,\ldots,t\}$ be a set of (real) spherical harmonics orthonormal with respect to the L_2 inner product,

$$(f,g)_{L_2} = \int_{\mathbb{S}^2} f(\mathbf{x})g(\mathbf{x})d\omega(\mathbf{x}),$$

where $Y_{\ell,k}$ is a spherical harmonic of degree ℓ [20]. It is well known that the addition theorem for spherical harmonics on $\mathbb{S}^2$ gives

$$\sum_{k=1}^{2\ell+1} Y_{\ell,k}(\mathbf{x})Y_{\ell,k}(\mathbf{y}) = \frac{2\ell+1}{4\pi} P_\ell\left(\mathbf{x}\cdot\mathbf{y}\right) \quad \text{for all } \mathbf{x},\mathbf{y} \in \mathbb{S}^2, \tag{2.1}$$

where $\mathbf{x}\cdot\mathbf{y}$ is the inner product in $\mathbb{R}^3$ and $P_\ell : [-1,1] \to \mathbb{R}$ is the Legendre polynomial of degree ℓ normalized so that $P_\ell\left(1\right) = 1$.

For $t \geq 1$ and $N \geq (t+1)^2$, let $\mathbf{Y}_t^0 \in \mathbb{R}^{((t+1)^2-1)\times N}$ be the $((t+1)^2-1)\times N$ matrix defined by

$$\mathbf{Y}_t^0(\mathcal{X}_N) := [Y_{\ell,k}(\mathbf{x}_j)], \qquad k = 1,\ldots,2\ell+1, \quad \ell = 1,\ldots,t, \qquad j = 1,\ldots,N, \tag{2.2}$$

and let $\mathbf{Y}_t(\mathcal{X}_N)$ be a matrix with an added leading row consisting of the degree 0 spherical harmonic, that is,

$$\mathbf{Y}_t(\mathcal{X}_N) := \begin{bmatrix} \frac{1}{\sqrt{4\pi}}\mathbf{e}^T \\ \\ \mathbf{Y}_t^0(\mathcal{X}_N) \end{bmatrix} \in \mathbb{R}^{(t+1)^2\times N}, \tag{2.3}$$

where $\mathbf{e} = [1,\ldots,1]^T \in \mathbb{R}^N$.

It is well known (see, for example, [4, 9]) that there are many equivalent conditions for a set $\mathcal{X}_N \subset \mathbb{S}^2$ to be a spherical t-design. Among these equivalent statements, one that plays an important role in the subsequent discussion is the following proposition.

PROPOSITION 2.1 (see [29]). *A finite set $\mathcal{X}_N = \{\mathbf{x}_1, \ldots, \mathbf{x}_N\} \subset \mathbb{S}^2$ is a spherical t-design if and only if*

$$\sum_{j=1}^{N} Y_{\ell,k}(\mathbf{x}_j) = 0, \qquad k = 1, \ldots, 2\ell+1, \quad \ell = 1, \ldots, t. \tag{2.4}$$

Using (2.2), the condition (2.4) can be written in matrix-vector form as

$$\mathbf{r}_t(\mathcal{X}_N) := \mathbf{Y}_t^0(\mathcal{X}_N)\mathbf{e} = \mathbf{0}, \tag{2.5}$$

where $\mathbf{r}_t(\mathcal{X}_N) \in \mathbb{R}^{(t+1)^2-1}$.

Next we define the nonnegative quantity

$$\begin{aligned} A_{N,t}(\mathcal{X}_N) :&= \frac{4\pi}{N^2}\mathbf{r}_t(\mathcal{X}_N)^T\mathbf{r}_t(\mathcal{X}_N) \\ &= \frac{4\pi}{N^2}\mathbf{e}^T\mathbf{Y}_t^0(\mathcal{X}_N)^T\mathbf{Y}_t^0(\mathcal{X}_N)\mathbf{e} \\ &= \frac{4\pi}{N^2}\sum_{j=1}^{N}\sum_{i=1}^{N}\sum_{\ell=1}^{t}\frac{2\ell+1}{4\pi}P_\ell(\mathbf{x}_j\cdot\mathbf{x}_i). \end{aligned}$$

It is easy to see that, as pointed out in [29], $\mathcal{X}_N$ is a spherical t-design if and only if $A_{N,t}(\mathcal{X}_N) = 0$. The computational difficulty is in knowing when using computer arithmetic whether or not a small number truly corresponds to zero. Therefore, following [29], we also consider conditions expressed in terms of stationary point sets of $A_{N,t}(\mathcal{X}_N)$.

DEFINITION 2.2. *A point $\mathbf{x} \in \mathbb{S}^2$ is a stationary point of $f \in C^1(\mathbb{S}^2)$ if $(\nabla^* f)(\mathbf{x}) = 0$, where ∇^* is the surface gradient* [12] *of f. Similarly $\mathcal{X}_N = \{\mathbf{x}_1, \ldots, \mathbf{x}_N\} \subset \mathbb{S}^2$ is a stationary point set of $A_{N,t}$ if*

$$\left(\nabla^*_{\mathbf{x}_i} A_{N,t}\right)(\mathcal{X}_N) = 0, \qquad i = 1, \ldots, N.$$

Sloan and Womersley [29] used a condition based on the mesh norm to help determine if a stationary point set of $A_{N,t}(\mathcal{X}_N)$ is a spherical t-design. The mesh norm is expressed in terms of the geodesic distance between two points $\mathbf{x}$ and $\mathbf{y}$ on the unit sphere $\mathbb{S}^2$, defined by $\operatorname{dist}(\mathbf{x},\mathbf{y}) := \cos^{-1}(\mathbf{x}\cdot\mathbf{y}) \in [0,\pi]$.

DEFINITION 2.3. *The mesh norm $h_{\mathcal{X}_N}$ of a point set $\mathcal{X}_N \subset \mathbb{S}^2$ is*

$$h_{\mathcal{X}_N} := \max_{\mathbf{y}\in\mathbb{S}^2}\min_{\mathbf{x}_i\in\mathcal{X}_N} \operatorname{dist}(\mathbf{y},\mathbf{x}_\mathrm{i}). \tag{2.6}$$

PROPOSITION 2.4 (see [29]). *If $\mathcal{X}_N \subset \mathbb{S}^2$ is a stationary point of $A_{N,t}(\mathcal{X}_N)$ for which the mesh norm satisfies*

$$h_{\mathcal{X}_N} < \frac{1}{t+1}, \tag{2.7}$$

then $\mathcal{X}_N$ is a spherical t-design.

Since many optimization methods are efficient for finding a stationary point but not a global optimal solution, Proposition 2.4 provides a good way to use existing optimization software to find spherical t-designs. However, the mesh norm condition (2.7) is very strong. The mesh norm is the covering radius, that is, the smallest radius for N identical spherical caps centered at the points $\mathbf{x}_i$ so that the caps cover the sphere. Thus the whole area of all the caps must be at least that of the sphere, giving

$$N2\pi(1-\cos h_{\mathcal{X}_N}) = N4\pi\sin^2\frac{h_{\mathcal{X}_N}}{2} \geq 4\pi.$$

From the inequality $\sin x \leq x$, for $x \geq 0$, we have the lower bound $h_{\mathcal{X}_N} \geq 2N^{-\frac{1}{2}}$ on the mesh norm. Thus the condition (2.7) in Proposition 2.4 implies that $N > 4(t+1)^2$, an inequality that is far from sharp. This means that Proposition 2.4 requires more than $4(t+1)^2$ points to ensure that $\mathcal{X}_N$ is a spherical t-design.

Chen and Womersley [7] reformulated the problem of finding a spherical t-design with $N=(t+1)^2$ points as a system of underdetermined nonlinear equations. The nonlinear function $\mathbf{C}_t : (\mathbb{S}^2)^N \to \mathbb{R}^{N-1}$ is defined by

$$\mathbf{C}_t(\mathcal{X}_N) := \mathbf{E}\mathbf{G}_t(\mathcal{X}_N)\mathbf{e}, \tag{2.8}$$

where

$$\mathbf{E} := [\mathbf{1}, -\mathbf{I}_{N-1}] \in \mathbb{R}^{(N-1)\times N}, \tag{2.9a}$$

$$\mathbf{G}_t\left(\mathcal{X}_N\right) := \mathbf{Y}_t\left(\mathcal{X}_N\right)^T \mathbf{Y}_t\left(\mathcal{X}_N\right), \tag{2.9b}$$

$$\text{and } \mathbf{1} := [1,\ldots,1]^T \in \mathbb{R}^{N-1}. \tag{2.9c}$$

PROPOSITION 2.5 (see [7]). *Let $N=(t+1)^2$. Suppose the Gram matrix $\mathbf{G}_t(\mathcal{X}_N)$ is nonsingular. Then $\mathcal{X}_N$ is a spherical t-design if and only if $\mathbf{C}_t\left(\mathcal{X}_N\right) = \mathbf{0}$.*

We shall later prove a generalization of Proposition 2.5 for $N \geq (t+1)^2$; see Theorem 3.10. It is easily seen that the condition $\mathbf{C}_t\left(\mathcal{X}_N\right) = \mathbf{0}$ in Proposition 2.5 is equivalent to the statement that the row sums of $\mathbf{G}_t(\mathcal{X}_N)$ are all equal.

The condition in Proposition 2.5 that $\mathbf{G}_t(\mathcal{X}_N)$ is nonsingular is essential, as shown by Example 2 of [6]. In that example, $t=1$, and $\mathcal{X}_4$ consists of the following four points:

$$\mathbf{x}_1 = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}, \quad \mathbf{x}_2 = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}, \quad \mathbf{x}_3 = \frac{1}{2}\begin{bmatrix} 1 \\ -\sqrt{2} \\ 1 \end{bmatrix}, \quad \mathbf{x}_4 = \frac{1}{2}\begin{bmatrix} 1 \\ \sqrt{2} \\ 1 \end{bmatrix}.$$

The Gram matrix $\mathbf{G}_1$ for these points is

$$\mathbf{G}_1(\mathcal{X}_4) = \frac{1}{4\pi}\begin{bmatrix} 4 & 1 & 2.5 & 2.5 \\ 1 & 4 & 2.5 & 2.5 \\ 2.5 & 2.5 & 4 & 1 \\ 2.5 & 2.5 & 1 & 4 \end{bmatrix}$$

which is singular. Since the row sums are each equal to $2.5/\pi$, we have $\mathbf{C}_1(\mathcal{X}_4) = \mathbf{0}$, yet $\mathcal{X}_4$ is not a spherical 1-design since it fails to give the correct integral 0 for the polynomial $p \in \mathbb{P}_1$ defined by $p(\mathbf{x}) = x$, where $\mathbf{x} \in [x,y,z]^T \in \mathbb{S}^2$, as

$$\frac{4\pi}{4}\sum_{j=1}^{4} p(\mathbf{x}_j) = \pi\left(0+1+\frac{1}{2}+\frac{1}{2}\right) \neq 0 = \int_{\mathbb{S}^2} p(\mathbf{x})d\omega(\mathbf{x}).$$

Based on Proposition 2.5 and interval arithmetic, Chen, Frommer, and Lang [6] proved the existence of spherical t-designs with $N=(t+1)^2$ points for t up to 100.

3. Fundamental systems and spherical *t*-designs. The concept of a fundamental system plays a key role in this paper.

DEFINITION 3.1. *The set $\mathcal{X}_N = \{\mathbf{x}_1, \ldots, \mathbf{x}_N\} \subset \mathbb{S}^2$ is a fundamental system for $\mathbb{P}_t$ if the zero polynomial is the only element of $\mathbb{P}_t$ that vanishes at each point in $\mathcal{X}_N$, that is, if*

$$p \in \mathbb{P}_t, \qquad p(\mathbf{x}_i) = 0, \qquad i = 1, \ldots, N \tag{3.1}$$

implies $p(\mathbf{x}) = 0$ *for all* $\mathbf{x} \in \mathbb{S}^2$.

The simplest situation is when $N = (t+1)^2$, in which case $\mathcal{X}_N$ is a fundamental system for $\mathbb{P}_t$ if and only if $\mathbf{Y}_t(\mathcal{X}_N)$ is nonsingular or equivalently if and only if $\mathbf{G}_t(\mathcal{X}_N) = \mathbf{Y}_t(\mathcal{X}_N)^T\mathbf{Y}_t(\mathcal{X}_N)$ is nonsingular. The definition can also be applied when $N > (t+1)^2$, in which case the next lemma states that Definition 3.1 is equivalent to the condition that $\mathbf{Y}_t(\mathcal{X}_N) \in \mathbb{R}^{(t+1)^2\times N}$ has full row rank. Note that a fundamental system $\mathcal{X}_N$ for $\mathbb{P}_t$ must have $N \geq (t+1)^2$.

LEMMA 3.2. *A set $\mathcal{X}_N \subset \mathbb{S}^2$ is a fundamental system for $\mathbb{P}_t$ if and only if $\mathbf{Y}_t(\mathcal{X}_N)$ is of full row rank $(t+1)^2$.*

Proof. First, suppose that, for some $\mathcal{X}_N = \{\mathbf{x}_1, \ldots, \mathbf{x}_N\} \subset \mathbb{S}^2$, we have row $\operatorname{rank}(\mathbf{Y}_t(\mathcal{X}_N)) < (t+1)^2$. Then the rows of $\mathbf{Y}_t(\mathcal{X}_N)$ are linearly dependent, so there exist $\lambda_{\ell,k} \in \mathbb{R}$ not all zero such that

$$\sum_{\ell=0}^{t}\sum_{k=1}^{2\ell+1} \lambda_{\ell,k} Y_{\ell,k}(\mathbf{x}_j) = 0, \qquad j = 1, \ldots, N. \tag{3.2}$$

Define $p_t \in \mathbb{P}_t$ by

$$p_t(\mathbf{x}) = \sum_{\ell=0}^{t}\sum_{k=1}^{2\ell+1} \lambda_{\ell,k} Y_{\ell,k}(\mathbf{x}) \qquad \text{for all } \mathbf{x} \in \mathbb{S}^2. \tag{3.3}$$

Then p_t is a nonzero polynomial satisfying (3.1), and thus $\mathcal{X}_N$ is not a fundamental system.

On the other hand, suppose there exists $p_t \in \mathbb{P}_t$, $p_t \not\equiv 0$, such that (3.1) holds. Then, as $Y_{\ell,k},\ k = 1, \ldots, 2\ell+1,\ \ell = 0, \ldots, t$, form a basis for $\mathbb{P}_t$, there exist scalars $\lambda_{\ell,k}$ such that (3.3) holds. Then (3.1) gives

$$\sum_{\ell=0}^{t}\sum_{k=1}^{2\ell+1} \lambda_{\ell,k} Y_{\ell,k}(\mathbf{x}_i) = p_t(\mathbf{x}_i) = 0, \qquad i = 1, \ldots, N. \tag{3.4}$$

Thus the rows of $\mathbf{Y}_t(\mathcal{X}_N)$ are linearly dependent, and hence row $\operatorname{rank}(\mathbf{Y}_t(\mathcal{X}_N)) < (t+1)^2$. ▯

Later, for $N \geq (t+1)^2$, we will use both of the matrices

$$\mathbf{H}_t(\mathcal{X}_N) := \mathbf{Y}_t(\mathcal{X}_N)\mathbf{Y}_t(\mathcal{X}_N)^T \in \mathbb{R}^{(t+1)^2\times(t+1)^2}, \tag{3.5a}$$

$$\mathbf{G}_t(\mathcal{X}_N) := \mathbf{Y}_t(\mathcal{X}_N)^T\mathbf{Y}_t(\mathcal{X}_N) \in \mathbb{R}^{N\times N}. \tag{3.5b}$$

The following result is an immediate consequence of Lemma 3.2.

COROLLARY 3.3. *A set $\mathcal{X}_N \subset \mathbb{S}^2$ is a fundamental system for $\mathbb{P}_t$ if and only if $\mathbf{H}_t(\mathcal{X}_N)$ is nonsingular.*

A system of $N = (t+1)^2$ points can be fundamental but of very poor quality in other respects. This is even more true when $N \geq (t+1)^2$ since, once a system of points is fundamental, the addition of further points at arbitrary locations cannot change the fundamental nature of the system. Some fundamental systems of good quality are the extremal fundamental systems of $N = (t+1)^2$ points of Sloan and Womersley [28], which maximize the determinant of $\mathbf{G}_t(\mathcal{X}_N)$. As pointed out in [28], extremal systems are good for polynomial interpolation and have good geometrical properties.

Chen and Womersley [7] and then Chen, Frommer, and Lang [6] verified that a spherical t-design exists in a neighborhood of an extremal system. This leads to the idea of *extremal spherical t-designs*, which first appeared in [7] for the special case $N = (t+1)^2$. We here extend the definition to $N \geq (t+1)^2$.

DEFINITION 3.4. *A set $\mathcal{X}_N = \{\mathbf{x}_1, \dots, \mathbf{x}_N\} \subset \mathbb{S}^2$ of $N \geq (t+1)^2$ points is an extremal spherical t-design if the determinant of the matrix $\mathbf{H}_t(\mathcal{X}_N) := \mathbf{Y}_t(\mathcal{X}_N)\mathbf{Y}_t(\mathcal{X}_N)^T \in \mathbb{R}^{(t+1)^2 \times (t+1)^2}$ is maximal subject to the constraint that $\mathcal{X}_N$ is a spherical t-design.*

Definition 3.4 is a generalization of the concept of an extremal spherical t-design, defined originally in [7] only for $N = (t+1)^2$ since, in that special case, the fact that the matrix is square allows us to write

$$\det(\mathbf{H}_t(\mathcal{X}_N)) = \det(\mathbf{Y}_t(\mathcal{X}_N)\mathbf{Y}_t(\mathcal{X}_N)^T) = \det(\mathbf{Y}_t(\mathcal{X}_N))^2 \tag{3.6a}$$

$$= \det(\mathbf{Y}_t(\mathcal{X}_N)^T\mathbf{Y}_t(\mathcal{X}_N)) = \det(\mathbf{G}_t(\mathcal{X}_N)). \tag{3.6b}$$

Note that, for $N > (t+1)^2$, maximizing $\det(\mathbf{G}_t(\mathcal{X}_N)) = \det(\mathbf{Y}_t(\mathcal{X}_N)^T\mathbf{Y}_t(\mathcal{X}_N))$ would make no sense as $\mathbf{G}_t(\mathcal{X}_N)$ always has $N - (t+1)^2$ zero eigenvalues.

For $N \geq (t+1)^2$, the squares of the singular values $\sigma_i(\mathbf{Y}_t(\mathcal{X}_N))$ of $\mathbf{Y}_t(\mathcal{X}_N)$ have a fixed sum since

$$\sum_{i=1}^{(t+1)^2} \sigma_i^2(\mathbf{Y}_t(\mathcal{X}_N)) = \operatorname{trace}(\mathbf{Y}_t(\mathcal{X}_N)\mathbf{Y}_t(\mathcal{X}_N)^T) \tag{3.7a}$$

$$= \sum_{\ell=0}^{t}\sum_{k=1}^{2\ell+1}\sum_{j=1}^{N} Y_{\ell,k}^2(\mathbf{x}_j) \tag{3.7b}$$

$$= \frac{N(t+1)^2}{4\pi}, \tag{3.7c}$$

where the last step uses the addition theorem and $P_\ell(1) = 1$. From (3.7c) and the inequality of the arithmetic and geometric means, we have

$$\det(\mathbf{H}_t(\mathcal{X}_N)) = \det(\mathbf{Y}_t(\mathcal{X}_N)\mathbf{Y}_t(\mathcal{X}_N)^T) = \prod_{i=1}^{(t+1)^2} \sigma_i^2(\mathbf{Y}_t(\mathcal{X}_N)) \leq \left(\frac{(t+1)^2}{4\pi}\right)^N. \tag{3.8}$$

The constrained maximization of the product of the singular values when the sum of the singular values is fixed has the effect of producing well conditioned matrices $\mathbf{H}_t(\mathcal{X}_N)$ [8].

The computational construction of extremal spherical t-designs is discussed in section 4. There we maximize instead of $\det(\mathbf{H}_t(\mathcal{X}_N))$ its logarithm,

$$\log\det(\mathbf{H}_t(\mathcal{X}_N)) = 2\sum_{i=1}^{(t+1)^2} \log\sigma_i(\mathbf{Y}_t(\mathcal{X}_N)). \tag{3.9}$$

It needs to be emphasized that we can never know if a computed set of points is a global rather than a local maximizer. Thus, in practice, we prefer to say that the computed sets are *well conditioned spherical designs* rather than to claim that they are truly extremal spherical designs. Section 4 discusses the use of interval methods to prove there exists a true well conditioned spherical design close to the computed spherical design and to provide rigorous bounds on $\log\det(\mathbf{H}_t(\mathcal{X}_N))$.

3.1. Mesh norm and fundamental system. Theorem 3.5 below shows that $h_{\mathcal{X}_N} < 1/t$ implies $\mathcal{X}_N$ is a fundamental system for $\mathbb{P}_t$; thus the mesh norm condition in Proposition 2.4 (which is that $h_{\mathcal{X}_N} < 1/(t+1)$) is much stronger than the condition that $\mathcal{X}_N$ is a fundamental system for $\mathbb{P}_t$. Theorem 3.6 shows that, for $N \geq (t+2)^2$, if $\mathcal{X}_N$ is both a fundamental system for $\mathbb{P}_{t+1}$ and a stationary point of $A_{N,t}(\mathcal{X}_N)$, then $\mathcal{X}_N$ is a spherical t-design.

THEOREM 3.5. *For t a positive integer, if the mesh norm of the point set $\mathcal{X}_N \subset \mathbb{S}^2$ satisfies $h_{\mathcal{X}_N} < \frac{1}{t}$, then $\mathcal{X}_N$ is a fundamental system for $\mathbb{P}_t$.*

The idea of the proof is adapted from the proof of Theorem 5 in [29].

Proof. Suppose, on the contrary, that row rank$(\mathbf{Y}_t(\mathcal{X}_N)) < (t+1)^2$. Then from Lemma 3.2 there is a nonzero polynomial $p_t \in \mathbb{P}_t$ defined by (3.3) which vanishes at all points in $\mathcal{X}_N$. Now we show that such a p_t cannot exist. Assume p_t takes its maximum absolute value at $\mathbf{x}_0 \in \mathbb{S}^2$. By definition of the mesh norm $h_{\mathcal{X}_N}$ of $\mathcal{X}_N = \{\mathbf{x}_1, \ldots, \mathbf{x}_N\}$, there exists $\mathbf{x}_{i^*}$, $i^* \in \{1, \ldots, N\}$, such that

$$\operatorname{dist}(\mathbf{x}_{i^*}, \mathbf{x}_0) \leq h_{\mathcal{X}_N} < \frac{1}{t}.$$

Now let q be the restriction of p_t to the great circle through $\mathbf{x}_0$ and $\mathbf{x}_{i^*}$. Then q is a trigonometric polynomial of degree $\leq t$, which satisfies both

$$q(\mathbf{x}_0) = p_t(\mathbf{x}_0) = \pm \|p_t\|_\infty \quad \text{and} \quad q(\mathbf{x}_{i^*}) = 0.$$

The Bernstein inequality

$$\sup |q'| \leq t \|q\|_\infty$$

implies

$$|q(\mathbf{x}_0) - q(\mathbf{x}_{i^*})| \leq \sup |q'| \operatorname{dist}(\mathbf{x}_{i^*}, \mathbf{x}_0) \leq t||q||_\infty \operatorname{dist}(\mathbf{x}_{i^*}, \mathbf{x}_0),$$

and hence

$$\|p_t\|_\infty = |q(\mathbf{x}_0)| = |q(\mathbf{x}_0) - q(\mathbf{x}_{i^*})| \leq t||q||_\infty \operatorname{dist}(\mathbf{x}_{i^*}, \mathbf{x}_0) < t\|q\|_\infty \frac{1}{t} = \|p_t\|_\infty,$$

which is a contradiction. ∎

The following example shows that the conditions $h_{\mathcal{X}_N} < 1/(t+1)$ in Proposition 2.4 and $h_{\mathcal{X}_N} < 1/t$ in Theorem 3.5, although sufficient, are not necessary.

Example 3.1 (regular tetrahedron). We consider the regular tetrahedron vertices $\mathcal{X}_4^* = \{\mathbf{x}_1^*, \mathbf{x}_2^*, \mathbf{x}_3^*, \mathbf{x}_4^*\} \subset \mathbb{S}^2$, where

$$\mathbf{x}_1^* = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}, \ \mathbf{x}_2^* = \begin{bmatrix} \sqrt{8}/3 \\ 0 \\ -1/3 \end{bmatrix}, \ \mathbf{x}_3^* = \begin{bmatrix} -\sqrt{2}/3 \\ \sqrt{2/3} \\ -1/3 \end{bmatrix}, \ \mathbf{x}_4^* = \begin{bmatrix} -\sqrt{2}/3 \\ -\sqrt{2/3} \\ -1/3 \end{bmatrix};$$

see Figure 3.1. It is well known that $\mathcal{X}_4^*$ is a spherical 2-design and a fundamental system for $\mathbb{P}_1$, that $\mathbf{G}_1(\mathcal{X}_4^*) = \frac{1}{\pi}\mathbf{I}_4$, and hence $\det(\mathbf{G}_1(\mathcal{X}_4^*)) = (1/\pi)^4$. The set $\mathcal{X}_4^*$ is also an extremal spherical 1-design. Yet $h_{\mathcal{X}_N} < 1/t$ fails for every positive integer t as the mesh norm is $h_{\mathcal{X}_4^*} = \cos^{-1}(1/3) \approx 1.2310 > 1$.

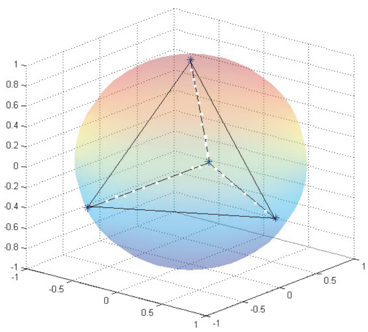

FIG. 3.1. *Regular tetrahedron on* $\mathbb{S}^2$.

3.2. Stationary points and spherical designs. This subsection gives sufficient conditions for a stationary point set of $A_{N,t}$ to be a spherical t-design. (See section 2 for definitions.)

THEOREM 3.6. *Let* $t \geq 1$ *and* $N \geq (t+2)^2$, *and suppose* $\mathcal{X}_N = \{\mathbf{x}_1, \ldots, \mathbf{x}_N\} \subset \mathbb{S}^2$ *is a stationary point set of* $A_{N,t}$. *Then either* $\mathcal{X}_N$ *is a spherical* t*-design or there exists a nonzero polynomial* $p \in \mathbb{P}_{t+1}$ *such that* $p(\mathbf{x}_j) = 0$ *for* $j = 1, \ldots, N$.

This theorem rests on the following lemma taken from [29].

LEMMA 3.7 (see [29]). *Let* $t \geq 1$, *and suppose* $\mathcal{X}_N = \{\mathbf{x}_1, \ldots, \mathbf{x}_N\}$ *is a stationary point set of* $A_{N,t}$. *Then either* $\mathcal{X}_N$ *is a spherical* t*-design or there exists a nonconstant polynomial* $p \in \mathbb{P}_t$ *with a stationary point at each point* $\mathbf{x}_i \in \mathcal{X}_N, i = 1, \ldots, N$.

The proof of Theorem 3.6 follows the lines of Theorem 5 in [29].

Proof of Theorem 3.6. Suppose $\mathcal{X}_N$ is a stationary point set of $A_{N,t}(\mathcal{X}_N)$ but is not a spherical t-design. Then, by Lemma 3.7, there exists a nonconstant polynomial $q \in \mathbb{P}_t$ with a stationary point at each $\mathbf{x}_i \in \mathcal{X}_N, i = 1, \ldots, N$, i.e.,

$$\nabla^* q(\mathbf{x}_j) = 0, \qquad j = 1, \ldots, N. \tag{3.10}$$

Now define

$$p_i = \mathbf{e}_i \cdot \nabla^* q, \qquad i = 1, 2, 3,$$

where $\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3$ are the unit vectors in the direction of the (fixed) coordinate axes for $\mathbb{R}^3$ and the dot indicates the inner product in $\mathbb{R}^3$. By the stationary property of q, each p_i for $i = 1, 2, 3$ satisfies

$$p_i(\mathbf{x}_j) = 0, \qquad j = 1, \ldots, N.$$

Since q is not a constant polynomial, at least one component of $\nabla^* q$ does not vanish identically, and hence at least one of p_1, p_2, p_3 is not identically zero. Assume

$$p := p_{i_0} \tag{3.11}$$

is not identically zero. Because q is a linear combination of spherical harmonics $Y_{\ell,k}$ with $\ell = 1, \ldots, t$ of degree ℓ, then (see [12], Chapter 12) $p = p_{i_0} = \mathbf{e}_{i_0} \cdot \nabla^* q$ is a linear combination of spherical harmonics of degrees $\ell - 1$ and $\ell + 1$. Since $q \in \mathbb{P}_t$, it follows that $p \in \mathbb{P}_{t+1}$. Finally (3.10) gives

$$p(\mathbf{x}_j) = 0\ , \qquad j = 1, \ldots, N, \tag{3.12}$$

completing the proof. $\square$

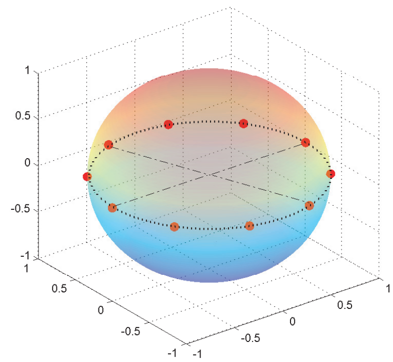

FIG. 3.2. *Ten points distributed equally on the equator.*

Remark 1. The statement that there exists a nonzero polynomial $p \in \mathbb{P}_{t+1}$ such that $p(\mathbf{x}_j) = 0$ for $j = 1, \ldots, N$ is equivalent to the condition that $\mathcal{X}_N$ is not a fundamental system for $\mathbb{P}_{t+1}$ or that $\mathbf{Y}_{t+1}(\mathcal{X}_N)$ is not of full row rank.

When the points of $\mathcal{X}_N$ coincide, $A_{N,t}(\mathcal{X}_N)$ achieves its maximum value $(t+1)^2-1$ (see [29, Theorem 3]), in which case $\mathcal{X}_N$ is a stationary point set of $A_{N,t}$ but is neither a spherical t-design nor a fundamental system for any $\mathbb{P}_t$, $t \geq 1$.

COROLLARY 3.8. *Let $t \geq 1$ and $N \geq (t+2)^2$. Assume $\mathcal{X}_N \subset \mathbb{S}^2$ is a stationary point set of $A_{N,t}$ and $\mathcal{X}_N$ is a fundamental system for $\mathbb{P}_{t+1}$. Then $\mathcal{X}_N$ is a spherical t-design.*

Since a fundamental system for $\mathbb{P}_{t+s}$ with $s \geq 1$ is a fundamental system for $\mathbb{P}_{t+1}$, we also have the following corollary.

COROLLARY 3.9. *Let $t \geq 1$, $s \geq 1$, and $N = (t+s+1)^2$. Assume $\mathcal{X}_N \subset \mathbb{S}^2$ is a stationary point set of $A_{N,t}$ and $\mathcal{X}_N$ is a fundamental system for $\mathbb{P}_{t+s}$. Then $\mathcal{X}_N$ is a spherical t-design.*

The following example shows that the fundamental system assumption in Corollary 3.8 is, although a sufficient condition, not necessary for the existence of spherical t-designs.

Example 3.2 (equator points). Let us choose 10 points on the equator distributed equally; see Figure 3.2. It is easy to see the point set $\mathcal{X}_{10}$ is a spherical 1-design and hence a stationary point set for $A_{10,1}$. Indeed, any pair of antipodal points is a spherical 1-design, and hence any union of antipodal pairs is also a spherical 1-design. However, $\mathcal{X}_{10}$ is not a fundamental system for $\mathbb{P}_1$ because the third component of $\mathbf{x} = [x, y, z]^T \in \mathbb{S}^2$ vanishes at every point on the equator.

3.3. Fundamental systems with at least $(t+1)^2$ points. From [7, 6], Proposition 2.5 can characterize spherical t-designs with $N = (t+1)^2$ points via $\mathbf{C}_t(\mathcal{X}_N) = \mathbf{0}$ under the assumption that $\mathbf{G}_t(\mathcal{X}_N)$ is nonsingular or equivalently that $\mathcal{X}_N$ is a fundamental system for $\mathbb{P}_t$. Now we generalize the characterization to $N \geq (t+1)^2$ and $\mathcal{X}_N$ a fundamental system for $\mathbb{P}_t$. The extra points give additional degrees of freedom which can be used to satisfy not only the spherical t-design constraints but also other desired criteria. The next theorem shows that when $\mathcal{X}_N$ is a fundamental system for $\mathbb{P}_t$, $\mathcal{X}_N$ is a spherical t-design if and only if $\mathbf{C}_t(\mathcal{X}_N) = \mathbf{0}$, generalizing Proposition 2.5. The definition of $\mathbf{C}_t(\mathcal{X}_N)$ through (2.8) and (2.9) remains unchanged for $N \geq (t+1)^2$.

THEOREM 3.10. *Let $N \geq (t+1)^2$, and suppose that $\mathcal{X}_N = \{\mathbf{x}_1, \ldots, \mathbf{x}_N\}$ is a fundamental system for $\mathbb{P}_t$. Then $\mathcal{X}_N$ is a spherical t-design if and only if $\mathbf{C}_t(\mathcal{X}_N) = \mathbf{0}$.*

Proof. From (2.9b), we have

$$\mathbf{G}_t(\mathcal{X}_N) = \left[\frac{1}{\sqrt{4\pi}}\mathbf{e} \quad \mathbf{Y}_t^0(\mathcal{X}_N)^T\right] \begin{bmatrix} \frac{1}{\sqrt{4\pi}}\mathbf{e}^T \\ \\ \mathbf{Y}_t^0(\mathcal{X}_N) \end{bmatrix} = \frac{1}{4\pi}\mathbf{e}\mathbf{e}^T + \mathbf{Y}_t^0(\mathcal{X}_N)^T \mathbf{Y}_t^0(\mathcal{X}_N).$$

Hence, from (2.8) and $\mathbf{r}_t(\mathcal{X}_N) := \mathbf{Y}_t^0(\mathcal{X}_N)\mathbf{e}$, we obtain, using $\mathbf{E}\mathbf{e} = \mathbf{0}$,

$$\mathbf{C}_t(\mathcal{X}_N) = \mathbf{E}\mathbf{Y}_t^0(\mathcal{X}_N)^T\mathbf{Y}_t^0(\mathcal{X}_N)\mathbf{e} = \mathbf{E}\mathbf{Y}_t^0(\mathcal{X}_N)^T\mathbf{r}_t(\mathcal{X}_N). \tag{3.13}$$

We are given that $\mathcal{X}_N = \{\mathbf{x}_1, \ldots, \mathbf{x}_N\}$ is a fundamental system for $\mathbb{P}_t$. Assume first that $\mathbf{C}_t(\mathcal{X}_N) = \mathbf{0}$, so we have from (3.13)

$$\mathbf{E}\mathbf{Y}_t^0(\mathcal{X}_N)^T\mathbf{r}_t(\mathcal{X}_N) = \mathbf{0}.$$

Then all elements of $\mathbf{Y}_t^0(\mathcal{X}_N)^T\mathbf{r}_t(\mathcal{X}_N)$ are equal, i.e., there is a scalar ν such that

$$\mathbf{Y}_t^0(\mathcal{X}_N)^T\mathbf{r}_t(\mathcal{X}_N) = \nu\mathbf{e}.$$

This implies

$$\mathbf{Y}_t(\mathcal{X}_N)^T \begin{bmatrix} -\sqrt{4\pi}\nu \\ \\ \mathbf{r}_t(\mathcal{X}_N) \end{bmatrix} = \left[\frac{1}{\sqrt{4\pi}}\mathbf{e} \quad \mathbf{Y}_t^0(\mathcal{X}_N)^T\right] \begin{bmatrix} -\sqrt{4\pi}\nu \\ \\ \mathbf{r}_t(\mathcal{X}_N) \end{bmatrix} = \mathbf{0}.$$

Since $\mathbf{Y}_t(\mathcal{X}_N)^T$ is of full (column) rank $(t+1)^2$, the only solution is the zero vector, implying

$$\nu = 0, \qquad \mathbf{r}_t(\mathcal{X}_N) = \mathbf{0}.$$

Hence $\mathcal{X}_N$ is a spherical t-design by Proposition 2.1. Conversely, suppose $\mathcal{X}_N$ is a spherical t-design. By Proposition 2.1 we have $\mathbf{r}_t(\mathcal{X}_N) = \mathbf{0}$. From (3.13) it follows that

$$\mathbf{C}_t(\mathcal{X}_N) = \mathbf{0},$$

completing the proof. ∎

4. Computational construction of well conditioned spherical *t*-designs. In this section we discuss the computational construction of well conditioned spherical t-designs for $N \geq (t+1)^2$. Interval methods [1, 6, 25] are then used to prove the existence of a well conditioned true spherical t-design in a narrow interval and to place relatively close upper and lower bounds on the determinant of the matrix $\mathbf{H}_t(\mathcal{X}_N)$ over the interval.

We seek to maximize the $\log\det(\mathbf{H}_t(\mathcal{X}_N))$ subject to the constraint $\mathbf{C}_t(\mathcal{X}_N) = \mathbf{0}$. We know already from inequality (3.8) that, even without the constraint, the log of the determinant is bounded above by

$$\log\det(\mathbf{H}_t(\mathcal{X}_N)) \leq N\log\left(\frac{(t+1)^2}{4\pi}\right). \tag{4.1}$$

We do not know the maximum of $\log\det(\mathbf{H}_t(\mathcal{X}_N))$ for the constrained maximization problem considered here, and in any case it almost certainly has many local maxima. Thus, in reality, the best we can hope for is to find a good local maximum of the constrained problem. More precisely, we want to find an interval for the point set $\mathcal{X}_N$ that contains a solution of $\mathbf{C}_t(\mathcal{X}_N) = \mathbf{0}$ and is such that there exist a lower bound $\underline{b}$ and an upper bound $\overline{b}$ on $\log\det(\mathbf{H}_t(\mathcal{X}_N))$ for $\mathcal{X}_N$ in this interval with $\overline{b} - \underline{b}$ very small and $\underline{b}$ as large as possible. By Theorem 3.10, as long as $\underline{b} > -\infty$, a solution of

$\mathbf{C}_t(\mathcal{X}_N) = \mathbf{0}$ is a true spherical t-design. Thus, if $\underline{b}$ is large, there is guaranteed to be a well conditioned spherical t-design in the interval.

In [6, 7] it was verified that, for $t \le 100$, a spherical t-design with $N = (t+1)^2$ exists in a neighborhood of an extremal system. Theorem 3.10 shows, for $N \ge (t+1)^2$, that if $\mathcal{X}_N$ is a fundamental system for $\mathbb{P}_t$, then the system of nonlinear constraints $\mathbf{C}_t(\mathcal{X}_N) = \mathbf{0}$ characterizes a spherical t-design. Maximizing the (log of) the determinant of $\mathbf{H}_t(\mathcal{X}_N)$ subject to these constraints ensures that we get a provably fundamental system of points and hence a spherical t-design. Thus we consider the following optimization problem:

$$\begin{array}{ll} \max & \log\det(\mathbf{H}_t(\mathcal{X}_N)) \\ \mathcal{X}_N \subset \mathbb{S}^2 & \\ \text{subject to} & \mathbf{C}_t(\mathcal{X}_N) = \mathbf{0}. \end{array} \tag{4.2}$$

Problem (4.2) is a nonlinear programming problem with both a nonlinear objective and nonlinear constraints. An additional difficulty is that the objective and the constraints $\mathbf{C}_t(\mathcal{X}_N) = \mathbf{0}$ are well defined only for $\mathcal{X}_N \subset \mathbb{S}^2$, yet many nonlinear programming algorithms allow intermediate iterates to be infeasible in order to make greater improvements in the objective function.

We represent the points $\mathbf{x}_i$ on the sphere by spherical coordinates with θ_i (the angle $\mathbf{x}_i$ makes with the positive z-axis, $0 \le \theta_i \le \pi$) and φ_i (the angle $\mathbf{x}_i$ makes with the plane $y = 0$, $0 \le \varphi_i < 2\pi$). We use normalized point sets $\mathcal{X}_N$ in which the first point is fixed at the north pole ($\theta_1 = 0$, φ_1 not defined) and the second point is fixed on the prime meridian ($\varphi_2 = 0$). Fixing the first point of $\mathcal{X}_N$ at the north pole avoids any difficulties there, but care must be taken with a point at the south pole.

The following strategy is adopted. Choose a nonnegative integer t, $N \ge (t+1)^2$, and a fundamental system $\mathcal{X}_N^0$ as a starting point set.

1. Use the Gauss–Newton method (see [21], page 256) to find an approximate solution $\tilde{\mathcal{X}}_N$ of $\mathbf{C}_t(\mathcal{X}_N) = \mathbf{0}$ starting from $\mathcal{X}_N^0$.
2. Use a nonlinear programming method to find
$$\hat{\mathcal{X}}_N \approx \arg\max\{\log\det(\mathbf{H}_t(\mathcal{X}_N)) \mid \mathbf{C}_t(\mathcal{X}_N) = \mathbf{0}\}$$
starting from $\tilde{\mathcal{X}}_N$.

Repeat as desired. The choice of a good starting point set is critical. For the $N = (t+1)^2$ case, a suitable starting point set $\mathcal{X}_N^0$ is an extremal system [28].

Finally we use the verification method discussed in the next subsection to find a narrow interval that contains both the computed spherical design and a true spherical t-design.

4.1. Numerical verification. Generalizing the computational existence proofs for spherical t-designs with $N = (t+1)^2$ in [6], we show how to construct a narrow interval that contains a well conditioned true spherical t-design $\mathcal{X}_N$ with $N \ge (t+1)^2$. Moreover, using a preconditioned interval method, we give close upper and lower bounds for $\det(\mathbf{H}_t(\mathcal{X}_N))$.

By $\mathbb{IR}^n$, we denote the space of all compact real interval vectors $[a] = [\underline{a}, \overline{a}]$, $\underline{a}, \overline{a} \in \mathbb{R}^n$, $\underline{a} \le \overline{a}$ componentwise. The arithmetic operations $+, -, *, /$ can be extended from $\mathbb{R}^n$ to $\mathbb{IR}^n$ and from $\mathbb{R}^{n\times n}$ to $\mathbb{IR}^{n\times n}$. The bounds of the resulting intervals can be computed from the bounds of the operands. Let $\mathtt{mid}[a] = (\underline{a} + \overline{a})/2$ componentwise.

Let $\mathbf{F} : D \subseteq \mathbb{R}^n \to \mathbb{R}^n$ be a continuously differentiable function. Let $[d\mathbf{F}] \in \mathbb{IR}^{n\times n}$ be an interval matrix containing $\mathbf{F}'(\xi)$ for all $\xi \in [\mathbf{z}] \subseteq D$, i.e.,

$$\{\mathbf{F}'(\mathbf{z}) : \mathbf{z} \in [\mathbf{z}]\} \subseteq [d\mathbf{F}]([\mathbf{z}]). \tag{4.3}$$

Such a $[d\mathbf{F}]$ can be obtained by an interval arithmetic evaluation of (expressions for) the Jacobian $\mathbf{F}'$ at the interval vector $[\mathbf{z}]$.

Now let $\mathbf{z}, \mathbf{y} \in [\mathbf{z}]$. Then, by the mean value theorem, there is $\alpha_i \in [0,1]$ such that

$$F_i(\mathbf{y}) = F_i(\mathbf{z}) + \mathbf{F}'_i(\xi_i)^T(\mathbf{y} - \mathbf{z}), \qquad \xi_i = \alpha_i \mathbf{z} + (1-\alpha_i)\mathbf{y}, \qquad i = 1, \dots, n$$

for each component F_i of $\mathbf{F}$, $i = 1, \dots, n$. By (4.3), we obtain

$$\{\mathbf{F}(\mathbf{y}) : \mathbf{y} \in [\mathbf{z}]\} \subseteq \mathbf{F}(\mathbf{z}) + [d\mathbf{F}]\,([\mathbf{z}] - \mathbf{z}).$$

Given a nonsingular matrix $\mathbf{B} \in \mathbb{R}^{n\times n}$, $\check{\mathbf{z}} \in [\mathbf{z}] \subseteq D$, and $[d\mathbf{F}] \in \mathbb{IR}^{n\times n}$, the *Krawczyk operator* [18] is defined by

$$k_{\mathbf{F}}(\check{\mathbf{z}}, [\mathbf{z}], \mathbf{B}, [d\mathbf{F}]) := \check{\mathbf{z}} - \mathbf{B}\mathbf{F}(\check{\mathbf{z}}) + (\mathbf{I}_n - \mathbf{B}\cdot[d\mathbf{F}])([\mathbf{z}] - \check{\mathbf{z}}). \tag{4.4}$$

It is known that $k_{\mathbf{F}}(\check{\mathbf{z}}, [\mathbf{z}], \mathbf{B}, [d\mathbf{F}])$ is an interval extension of the function $\psi(\mathbf{z}) := \mathbf{z} - \mathbf{B}\mathbf{F}(\mathbf{z})$ over $[\mathbf{z}]$, that is, $\mathbf{z} - \mathbf{B}\mathbf{F}(\mathbf{z}) \in k_{\mathbf{F}}(\check{\mathbf{z}}, [\mathbf{z}], \mathbf{B}, [\mathbf{F}])$ for all $\mathbf{z} \in [\mathbf{z}]$.

LEMMA 4.1 (see [18, 19]). *Let $\mathbf{F} : D \subset \mathbb{R}^n \to \mathbb{R}^n$ be a continuously differentiable function. Choose $[\mathbf{z}] \in \mathbb{IR}^n$, $\check{\mathbf{z}} \in [\mathbf{z}] \subseteq D$, an invertible matrix $\mathbf{B} \in \mathbb{R}^{n\times n}$, and $[d\mathbf{F}] \in \mathbb{IR}^{n\times n}$ such that $\mathbf{F}'(\xi) \in [d\mathbf{F}]$ for all $\xi \in [\mathbf{z}]$. Assume that*

$$k_{\mathbf{F}}(\check{\mathbf{z}}, [\mathbf{z}], \mathbf{B}, [d\mathbf{F}]) \subseteq [\mathbf{z}].$$

Then $\mathbf{F}$ has a zero $\mathbf{z}^*$ in $k_{\mathbf{F}}(\check{\mathbf{z}}, [\mathbf{z}], \mathbf{B}, [d\mathbf{F}])$.

In computation, we represent the points $\mathbf{x}_i$ on the sphere by spherical coordinates with θ_i and φ_i as stated before. We seek intervals $[\theta_i]$, $[\varphi_i]$ such that there is a solution of $\mathbf{C}_t(\mathcal{X}_N) = \mathbf{0}$ in the interval point set $[\mathcal{X}_N]$, in which the interval for each point is defined by

$$[\mathbf{z}_i] = [\sin([\theta_i])\cos([\varphi_i]),\ \sin([\theta_i])\sin([\varphi_i]),\ \cos([\theta_i])]^T, \quad i = 1, \dots, N.$$

We fix the first point at the north pole ($\theta_1 = 0, \varphi_1 = 0$) and the second point on the prime meridian ($\varphi_2 = 0$). Hence $\mathbf{C}_t(\mathcal{X}_N)$ is redefined as a system of nonlinear equation

$$\tilde{\mathbf{F}}(\mathbf{y}) = \mathbf{0}.$$

The components of $\mathbf{y}$ are $y_{i-1} = \theta_i,\ i = 2, \dots, N,\ y_{N+i-3} = \varphi_i,\ i = 3, \dots, N$. As in [6], we use a QR-factorization method at each step to determine the $N-2$ least important components of $\mathbf{y}$, which we label collectively by $\mathbf{y}_N$, then write $\mathbf{y} := (\mathbf{z}, \mathbf{y}_N)$, and define a new function $\mathbf{F}(\mathbf{z}) = \tilde{\mathbf{F}}(\mathbf{z}, \mathbf{y}_N)$, where $\mathbf{F} : \mathbb{R}^{N-1} \to \mathbb{R}^{N-1}$. Using the Krawczyk operator with $\mathbf{B} = (\mathtt{mid}[d\mathbf{F}])^{-1}$, we can verify the existence of a fixed point of $\mathbf{z} - \mathbf{B}\mathbf{F}(\mathbf{z})$, which is a solution of $\mathbf{F}(\mathbf{z}) = \mathbf{0}$. For more details, see [6].

To prove the existence of well conditioned spherical t-designs in $[\mathcal{X}_N]$, we have to show that all matrices $\mathbf{H}_t(\mathcal{X}_N)$ are well conditioned for $\mathcal{X}_N \in [\mathcal{X}_N]$. To show it, we compute interval enclosures of $\mathbf{H}_t$ such that

$$\{\mathbf{H}_t(\mathcal{X}_N), \quad \mathcal{X}_N \in [\mathcal{X}_N]\} \subseteq [\mathbf{H}_t(\mathcal{X}_N)],$$

where $[\mathbf{H}_t(\mathcal{X}_N)]$ denotes an interval of symmetric matrices. To verify that all matrices in $[\mathbf{H}_t(\mathcal{X}_N)]$ are nonsingular, the following lemma was used in [6].

LEMMA 4.2 (see [6]). *Let $[\mathbf{A}] \in \mathbb{IR}^{n\times n}$ be an interval matrix, and let $\mathbf{M} \in \mathbb{R}^{n\times n}$. Then if*

$$\|\mathbf{I}_n - \mathbf{M}\,[\mathbf{A}]\,\|_\infty < 1, \tag{4.5}$$

then $\mathbf{M}$ as well as all matrices $\mathbf{A} \in [\mathbf{A}]$ are nonsingular.

Noting that $\mathbf{H}_t(\mathcal{X}_N)$ is symmetric, we need to consider only all symmetric matrices in the interval. This allows us to use a preconditioning technique to provide a sharp error bound for the determinant of all symmetric matrices in the interval.

PROPOSITION 4.3. *Let* $\mathbf{U}$ *be a nonsingular upper triangular matrix. Assume that*

$$\|\mathbf{I}_n - \mathbf{U}^T[\mathbf{A}]\mathbf{U}\|_\infty \le r < 1. \tag{4.6}$$

Let $\beta = (\Pi_{j=1}^N \mathbf{U}_{jj})^{-2}$. *Then*

$$0 < \beta(1-r)^N \le \det(\mathbf{A}) \le \beta(1+r)^N \quad \textit{for} \quad \mathbf{A} \in [\mathbf{A}] \ \textit{and} \ \mathbf{A}^T = \mathbf{A}. \tag{4.7}$$

Proof. We consider a symmetric matrix $\mathbf{A} \in [\mathbf{A}]$. Noting that $\mathbf{U}^T\mathbf{A}\mathbf{U}$ preserves the symmetric structure, we denote its (real) eigenvalues by $\lambda_i(\mathbf{U}^T\mathbf{A}\mathbf{U})$. Since

$$\max_{1\le i\le N} |\, 1 - \lambda_i(\mathbf{U}^T\mathbf{A}\mathbf{U}) \,| = \rho\left(\mathbf{I}_n - \mathbf{U}^T\mathbf{A}\mathbf{U}\right) \le \|\mathbf{I}_n - \mathbf{U}^T\mathbf{A}\mathbf{U}\|_\infty \le r,$$

where ρ is the spectral radius, we have

$$0 < 1 - r \le \lambda_i(\mathbf{U}^T\mathbf{A}\mathbf{U}) \le 1 + r, \qquad i = 1, \ldots, N.$$

Hence,

$$(1-r)^N \le \det\left(\mathbf{U}^T\mathbf{A}\mathbf{U}\right) \le (1+r)^N.$$

Noting that $\det(\mathbf{U})\det(\mathbf{U}^T) = (\Pi_{j=1}^N \mathbf{U}_{jj})^2 = \beta^{-1}$, from

$$0 < (1-r)^N \le \beta^{-1}\det(\mathbf{A}) \le (1+r)^N,$$

we obtain (4.7). □

To overcome the problem of overflow, in the computation we consider $\log\det(\mathbf{A})$ instead of $\det(\mathbf{A})$. Letting

$$\underline{b} = \log\beta + N\log(1-r) \quad \text{and} \quad \overline{b} = \log\beta + N\log(1+r),$$

we obtain from Proposition 4.3

$$\log\det(\mathbf{A}) \in \left[\underline{b},\ \overline{b}\right], \quad \mathbf{A} \in [\mathbf{A}], \text{ and } \mathbf{A}^T = \mathbf{A}. \tag{4.8}$$

Applying Proposition 4.3 and the above results to $\mathbf{A} = \mathbf{H}_t(\mathcal{X}_N)$, we obtain the interval for $\log\det(\mathbf{H}_t(\mathcal{X}_N))$ with a preconditioning matrix $\mathbf{U}$

$$[\log\det(\mathbf{H}_t(\mathcal{X}_N))] \subseteq \left[\underline{b},\ \overline{b}\right] \tag{4.9}$$

for all $\mathcal{X}_N \in [\mathcal{X}_N]$.

In an actual computation, we choose $\mathbf{U}$ such that $(\mathbf{U}^{-1})^T\mathbf{U}^{-1} \approx \mathtt{mid}[\mathbf{H}_t]$. We conduct all operations in machine interval arithmetic and get an interval containing $\|\mathbf{I}_n - \mathbf{U}^T[\mathbf{H}_t]\mathbf{U}\|_\infty$ with $(\mathbf{U}^{-1})^T\mathbf{U}^{-1}$ the Cholesky factorization of $\mathtt{mid}[\mathbf{H}_t]$; see [10]. If the upper bound r of the interval satisfies $r < 1$, then we have computationally proved that (4.9) holds.

4.2. Numerical results. Based on the code in [6] and INTLAB [25], we have used the numerical verification technique to prove the existence of a spherical t-design close to the computed point set for $N = (t+1)^2$ points for t up to 60. As in [6], we choose to work with $\mathbf{G}_t(\mathcal{X}_N)$ rather than $\mathbf{H}_t(\mathcal{X}_N)$, noting that $\det(\mathbf{H}_t(\mathcal{X}_N)) = \det(\mathbf{G}_t(\mathcal{X}_N))$. As a starting point set $\hat{\mathcal{X}}_N$ to solve problem (4.2), we use the extremal systems from [28] without any additional constraints. In Figure 4.1 we report, for

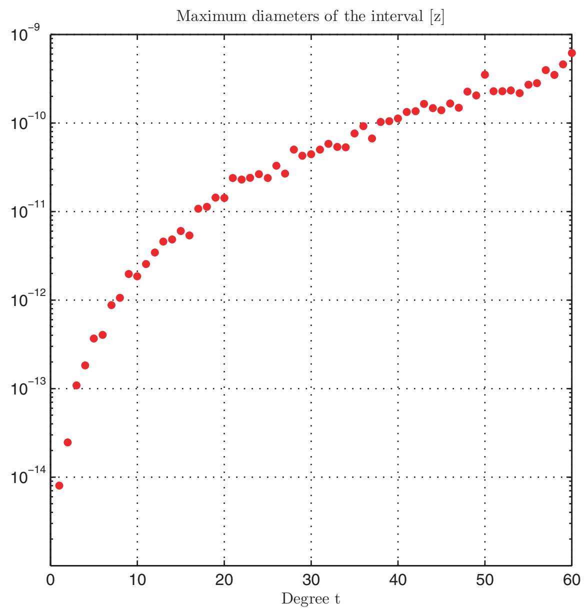

FIG. 4.1. *The maximum diameters of the interval* $[\mathbf{z}]$ *containing spherical coordinates corresponding to a true spherical* t*-design.*

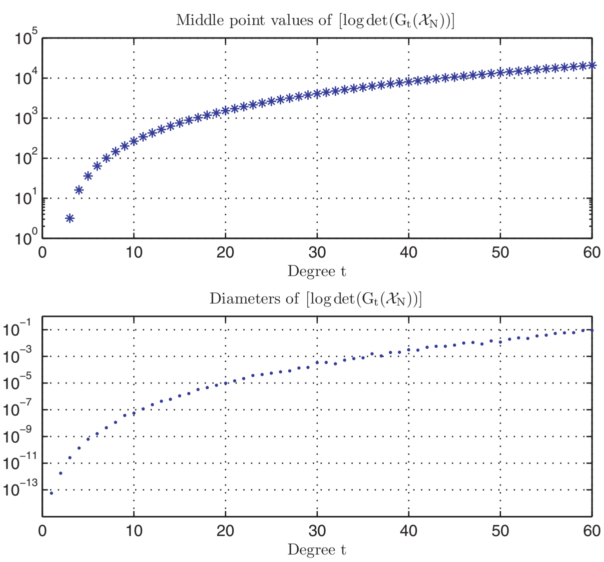

FIG. 4.2. *Middle point values of* $[\log\det(\mathbf{G}_t(\mathcal{X}_N))]$ *and diameters of* $[\log\det(\mathbf{G}_t(\mathcal{X}_N))]$.

each t, the maximum diameter of various interval quantities computed with the numerical verification algorithm. Here `max diam([z])` represents the diameter of the interval contains a true spherical design. We see that the diameter of the interval increases as t increases, but it is still less than 10^{-9} radians for the largest values of t. Furthermore, in Figure 4.2, the diameters $\texttt{diam}([\log\det(\mathbf{G}_t(\mathcal{X}_N))])$ are less than 10^{-1} for the largest t, yet the middle point value of $[\log\det(\mathbf{G}_t(\mathcal{X}_N))]$ is over 10^4

for the largest t. This implies that the estimate (4.9) is relatively tight given the large size of $\log\det(\mathbf{G}_t(\mathcal{X}_N))$. Note that Figure 4.2 does not show the middle values $\mathtt{mid}[\log\det(\mathbf{G}_1)] = -4.5789$ and $\mathtt{mid}[\log\det(\mathbf{G}_2)] = -3.2150$ as the values are in this case negative.

5. Well conditioned spherical *t*-designs and their geometry. In this section we concentrate on the geometrical properties of extremal spherical t-designs. Some properties are known theoretically, while other properties suggested by the known properties of the extremal fundamental systems [15, 16, 22] have not been proved.

The points of an extremal fundamental system of $N = (t+1)^2$ are known theoretically (see Reimer [22, Theorem 6.13]) to be *well separated* with the *separation distance* $\delta_{\mathcal{X}_N}$ satisfying

$$\delta_{\mathcal{X}_N} := \min_{\mathbf{x}_i,\mathbf{x}_j\in\mathcal{X}_N, i\neq j} \operatorname{dist}(\mathbf{x}_i,\mathbf{x}_j) \geq \frac{\pi}{2t} \geq \frac{\pi}{2\sqrt{N}}. \tag{5.1}$$

The argument uses the Lagrange polynomials ℓ_j, which are the polynomials of degree t such that $\ell_j(\mathbf{x}_j) = 1$ and $\ell_j(\mathbf{x}_i) = 0$ for $i \neq j$. For extremal fundamental systems it is known that $|\ell_j(\mathbf{x})| \leq 1$ (see (6.1) below) so that $|\ell_j|$ attains its maximum value of 1 at $\mathbf{x}_j$. Noting that ℓ_j, when restricted to the great circle through $\mathbf{x}_i$ and $\mathbf{x}_j$, is a trigonometric polynomial of degree at most t, the bound (5.1) follows as a consequence of a result of Riesz; see, for example, Reimer [22, Lemma 6.12].

For extremal spherical t-designs, which must satisfy the additional nonlinear system of constraints, the argument fails since the maximum of $|\ell_j|$ no longer occurs at $\mathbf{x}_j$ but nearby, with a value (slightly) larger than one. Nevertheless, for the calculated extremal spherical t-designs, Figure 5.1 shows that the points are well separated. Figure 5.1 reports the separation distance for our well conditioned spherical t-designs as a function of t. The separation distance is close to $2\pi/(2t+1)$.

Spherical t-designs considered as quadrature rules have equal quadrature weights $w_j = 4\pi/N$, $j = 1,\ldots,N$. Consequently, we can adopt the results of Reimer and Yudin; see [22, Theorem 6.21], which state that if a positive weight cubature formula

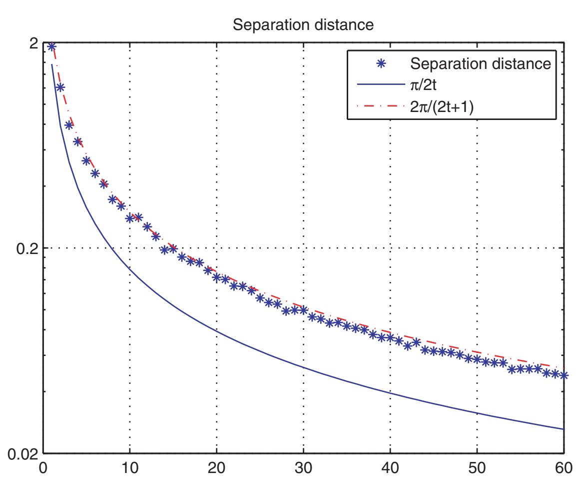

FIG. 5.1. *The separation distance for well conditioned spherical t-designs with $N = (t+1)^2$.*

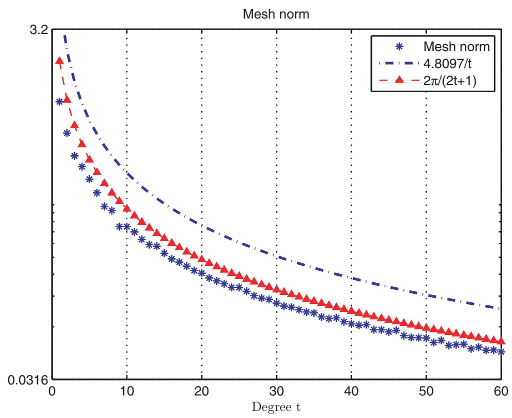

FIG. 5.2. *The mesh norm of well conditioned spherical t-designs with $N = (t+1)^2$.*

defined by a point set $\mathcal{X}_N$ is exact for all $p \in \mathbb{P}_t$, then the mesh norm $h_{\mathcal{X}_N}$ satisfies

$$h_{\mathcal{X}_N} \leq \cos^{-1}(z_t),$$

where z_t is the largest zero of the Legendre polynomial $P_{\lceil t/2 \rceil}$. From [15, 22] we know that

$$\frac{\pi}{2\lceil t/2 \rceil + 1} \leq \cos^{-1}(z_t) \leq \frac{2\pi}{2\lceil t/2 \rceil + 1}. \tag{5.2}$$

A better upper bound on the mesh norm for positive weight cubature rules with degree of precision t is [28]

$$h_{\mathcal{X}_N} \leq \frac{2j_0}{t} \simeq \frac{4.8097}{t},$$

where j_0 is the smallest zero of the Bessel function J_0. Figure 5.2 gives the mesh norms for the calculated extremal spherical t-designs. The computed mesh norms are smaller than the latter bound and smaller than $2\pi/(2t+1)$.

The mesh norm is the covering radius for covering the sphere with identical spherical caps of the smallest possible radius centered at the points in $\mathcal{X}_N$, while the separation distance $\delta_{\mathcal{X}_N}$ is twice the packing radius, so $h_{\mathcal{X}_N} \geq \delta_{\mathcal{X}_N}/2$. The *mesh ratio* $\rho_{\mathcal{X}_N}$ defined by

$$\rho_{\mathcal{X}_N} := \frac{2h_{\mathcal{X}_N}}{\delta_{\mathcal{X}_N}} \geq 1$$

is a good measure of the quality of the geometric distribution of $\mathcal{X}_N$: the smaller $\rho_{\mathcal{X}_N}$ is, the more uniformly are the points distributed on $\mathbb{S}^2$ [16]. Figure 5.3 shows that the mesh ratio satisfies $\rho_{\mathcal{X}_N} < 2$ for all the well conditioned spherical t-designs with $N = (t+1)^2$ points and $t = 1, \dots, 60$.

A reasonable conjecture is that $\rho_{\mathcal{X}_N}$ is bounded above by a constant close to 2 since natural bounds on $\mathbb{S}^2$ for $\delta_{\mathcal{X}_N}$ and $h_{\mathcal{X}_N}$, supported by the computational experiments, take the form

$$\delta_{\mathcal{X}_N} \geq C_\delta N^{-\frac{1}{2}}$$

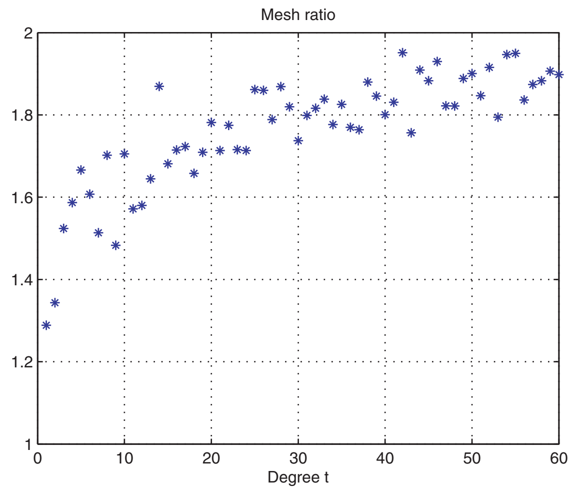

FIG. 5.3. *The mesh ratio of well conditioned spherical t-designs with $N = (t+1)^2$.*

and

$$h_{\mathcal{X}_N} \leq C_h N^{-\frac{1}{2}}$$

which together would give the uniform bound

$$\rho_{\mathcal{X}_N} \leq \frac{2C_h}{C_\delta} \quad \text{independent of} \quad N. \tag{5.3}$$

6. The Lebesgue constant for interpolation. In this section we consider polynomial interpolation with respect to the computed well conditioned spherical designs, and we discuss the *Lebesgue constants* for interpolation. The Lebesgue constant (defined in (6.3)) plays a similar role to the condition number of a matrix: errors in the data can be magnified in the interpolation process by at most a factor equal to the Lebesgue constant (see [23]). In this section we show that our well conditioned spherical designs lead to small Lebesgue constants.

Given a fundamental system $\mathcal{X}_N = \{\mathbf{x}_1, \ldots, \mathbf{x}_N\} \subset \mathbb{S}^2$ for $\mathbb{P}_t$ with $N = (t+1)^2$, we define the kernel polynomial [27]

$$g_i(\mathbf{x}) := \sum_{\ell=0}^{t} \frac{2\ell+1}{4\pi} P_\ell(\mathbf{x}\cdot\mathbf{x}_i) = \frac{t+1}{4\pi} P_t^{(1,0)}(\mathbf{x}\cdot\mathbf{x}_i) \in \mathbb{P}_t, \qquad i = 1, \ldots, N,$$

where $P_t^{(1,0)}(z),\ z \in [-1,\ 1]$ is the Jacobi polynomial (in the notation of Szegö [31]) corresponding to the weight function $(1-z)$. Furthermore, we define the vector valued function $\mathbf{g} :\ \mathbb{S}^2 \to \mathbb{R}^N$ by

$$\mathbf{g}(\mathbf{x}) = \begin{bmatrix} g_1(\mathbf{x}) \\ \vdots \\ g_N(\mathbf{x}) \end{bmatrix} = \frac{t+1}{4\pi} \begin{bmatrix} P_t^{(1,0)}(\mathbf{x}\cdot\mathbf{x}_1) \\ \vdots \\ P_t^{(1,0)}(\mathbf{x}\cdot\mathbf{x}_N) \end{bmatrix}.$$

Then the matrix $\mathbf{G}_t(\mathcal{X}_N)$ in (2.9b) can be written as [33]

$$\mathbf{G}_t(\mathcal{X}_N) = [\ \mathbf{g}(\mathbf{x}_1), \ldots, \mathbf{g}(\mathbf{x}_N)\ ].$$

The Lagrange polynomials $\{\ell_1, \ldots, \ell_N\}$ are defined, as usual, by

$$\ell_j \in \mathbb{P}_t, \qquad \ell_j(\mathbf{x}_i) = \delta_{ji}, \qquad i,\ j = 1, \ldots, N,$$

where δ_{ji} is the Kronecker delta. An explicit representation for ℓ_j is

$$\ell_j(\mathbf{x}) = \frac{\det\left(\mathbf{G}_t\left(\mathbf{x}_1, \ldots, \mathbf{x}_{j-1}, \mathbf{x}, \mathbf{x}_{j+1}, \ldots, \mathbf{x}_N\right)\right)}{\det\left(\mathbf{G}_t\left(\mathbf{x}_1, \ldots, \mathbf{x}_{j-1}, \mathbf{x}_j, \mathbf{x}_{j+1}, \ldots, \mathbf{x}_N\right)\right)}. \tag{6.1}$$

For given $f \in C\left(\mathbb{S}^2\right)$, the classical expression for the interpolant $\Lambda_t f$, defined by

$$\Lambda_t f \in \mathbb{P}_t, \qquad \Lambda_t f\left(\mathbf{x}_j\right) = f\left(\mathbf{x}_j\right), \qquad j = 1, \ldots, N,$$

is

$$\Lambda_t f = \sum_{j=1}^{N} f\left(\mathbf{x}_j\right) \ell_j. \tag{6.2}$$

From this it follows easily that

$$\|\Lambda_t\| := \sup_{f \in C(\mathbb{S}^2)} \frac{\|\ \Lambda_t f\ \|_\infty}{\|\ f\ \|_\infty} = \max_{\mathbf{x} \in \mathbb{S}^2} \sum_{j=1}^{N} \left|\ell_j(\mathbf{x})\right|, \tag{6.3}$$

the usual expression for the *Lebesgue constant* for interpolation.

We note from (6.2) that if there are data errors so that $f(\mathbf{x}_j)$ is replaced by $f(\mathbf{x}_j) + \epsilon_j$, then $\Lambda_t f$ is replaced by

$$\Lambda_t f + \sum_{j=1}^{N} \epsilon_j \ell_j, \tag{6.4}$$

giving an additional pointwise error of $\sum_{j=1}^{N} \epsilon_j \ell_j(\mathbf{x})$, and hence using (6.3) a uniform bound of $\|\Lambda_t\|\,\|\epsilon\|_\infty$, where $\epsilon = [\epsilon_1, \ldots, \epsilon_N]^T$, for the additional approximation error arising from data errors. Thus the Lebesgue constant is also a stability constant.

Define the vector valued function $\mathbf{l} : \mathbb{S}^2 \to \mathbb{R}^N$ by

$$\mathbf{l}(\mathbf{x}) = \begin{bmatrix} \ell_1(\mathbf{x}) \\ \vdots \\ \ell_N(\mathbf{x}) \end{bmatrix}.$$

As pointed out by [33], a concrete representation for $\mathbf{l}(\mathbf{x})$ is $\mathbf{l} = \mathbf{G}_t^{-1}\mathbf{g}$. Thus (6.3) can be written as

$$\|\Lambda_t\| = \max_{\mathbf{x} \in \mathbb{S}^2} \|\mathbf{l}(\mathbf{x})\|_1 = \max_{\mathbf{x} \in \mathbb{S}^2} \left\|\mathbf{G}_t^{-1}\mathbf{g}(\mathbf{x})\right\|_1. \tag{6.5}$$

The last equality suggests that maximizing $\det(\mathbf{G}_t(\mathcal{X}_N))$ (or equivalently, minimizing $\det(\mathbf{G}_t^{-1}(\mathcal{X}_N))$ subject to the spherical t-design condition will lead to a relatively small value of the Lebesgue constant.

For an extremal fundamental system, the explicit representation (6.1) gives immediately

$$\|\ell_j\|_\infty = 1, \quad j = 1, \ldots, (t+1)^2,$$

and hence from (6.3),

$$\|\Lambda_t\| \leq (t+1)^2.$$

This argument breaks down for extremal spherical designs, but in any case, this upper bound, which in practice is very loose, still seems to hold.

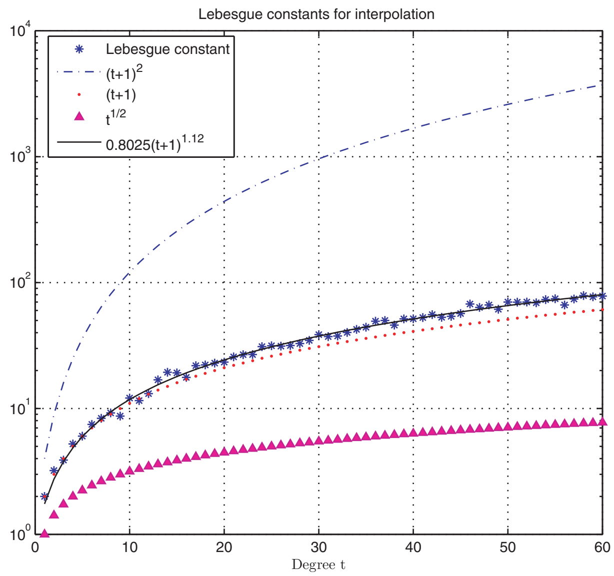

FIG. 6.1. *The Lebesgue constant of well conditioned spherical t-designs with $N = (t+1)^2$.*

Figure 6.1 reports the Lebesgue constant of the computed well conditioned spherical t-designs, showing it to lie between $(t+1)^2$ and $\sqrt{t}$ and lying rather close to $(t+1)$. Note that $\sqrt{t}$ is the growth rate of the Lebesgue constant for orthogonal projection [11], which is known to be a lower bound for the Lebesgue constant for interpolation [33]. Nonlinear data fitting estimates the growth of the Lebesgue constant in Figure 6.1 as $0.8025(t+1)^{1.12}$.

It is natural to compare the computed Lebesgue constants with those obtained in [28] for extremal systems; see http://web.maths.unsw.edu.au/∼rsw/Sphere. In practice they are almost indistinguishable, indicating that the added constraint of $\mathcal{X}_N$ being a spherical t-design has not had any detrimental effect on the Lebesgue constants. One can also compare the new results with the least possible Lebesgue constants for polynomial interpolation, computed in [33]. For all available values of t, the present Lebesgue constants are within a factor of 2 of the least possible Lebesgue constants.

7. Application to numerical integration and interpolation.

In this section we use the computed well conditioned spherical t-designs with $N = (t+1)^2$ points to evaluate integration and interpolation for a well known test function on $\mathbb{S}^2$.

We consider one of the Franke functions as adapted by Renka to the three-dimension case [24]:

$$\begin{aligned} f(x,y,z) = {} & 0.75\exp(-(9x-2)^2/4-(9y-2)^2/4-(9z-2)^2/4)\\ & + 0.75\exp(-(9x+1)/49-(9y+1)/10-(9z+1)/10)\\ & + 0.5\exp(-(9x-7)^2/4-(9y-3)^2/4-(9z-5)^2/4)\\ & - 0.2\exp(-(9x-4)^2-(9y-7)^2-(9z-5)^2), \quad (x,y,z)\in\mathbb{S}^2. \end{aligned}$$

The value of the integral on $\mathbb{S}^2$ computed by the mathematical software package Maple to 20 significant digits is

$$\int_{\mathbb{S}^2} f(\mathbf{x})d\omega(\mathbf{x}) = 6.6961822200736179523.$$

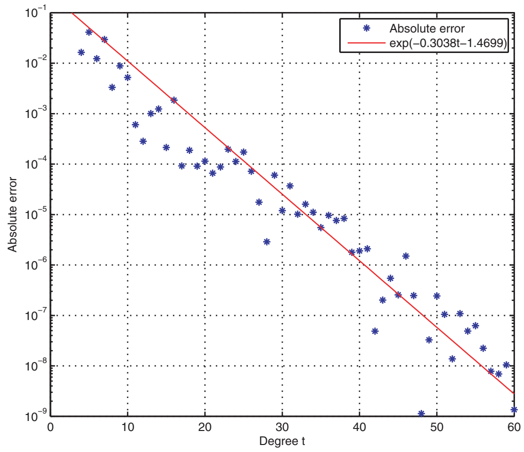

FIG. 7.1. *The absolute error.*

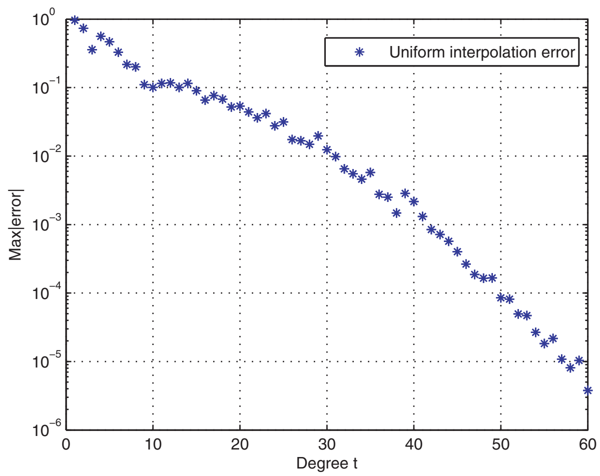

FIG. 7.2. *Uniform interpolation error for the Franke function.*

We show the absolute error of the equal weight quadrature rule applied to f in Figure 7.1 as a function of t. The absolute error decreases dramatically to around 10^{-9} at $t = 60$. And the nonlinear fitting curve is $\exp(-0.3038t - 1.4699)$, which is a rapidly decaying function. As expected, the high degree spherical t-designs deal successfully with a complicated function as long as it is smooth.

The uniform error of interpolation is estimated by

$$\|f(\mathbf{x}) - \Lambda_t f(\mathbf{x})\|_\infty \approx \max_{\mathbf{x}\in X} |f(\mathbf{x}) - \Lambda_t f(\mathbf{x})|, \tag{7.1}$$

where X is a large but finite set of well distributed points over the sphere, for instance, the Bauer points [5], with 10000 points. The uniform errors using the well conditioned spherical t-designs are shown in Figure 7.2.

8. Conclusion. This paper introduces the concept of extremal spherical t-designs for $N \geq (t+1)^2$. This is a new class of well conditioned spherical t-designs for which the determinant of a certain matrix is maximized. We provide a new sufficient condition for a stationary point of the variational characterization introduced by [29] to be a spherical t-design and extend the spherical design characterization of [6, 7] in terms of a nonlinear system to $N \geq (t+1)^2$. We show how, in practice, to compute an interval within which a well conditioned spherical design is guaranteed to lie and how to place close upper and lower bounds on the determinant. Numerical results show that the computed well conditioned spherical t-designs have good properties for integration and interpolation on the sphere. The computed well conditioned spherical t-designs may be found on the web site http://web.maths.unsw.edu.au/∼rsw/Sphere.

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