Spherical designs with close to the minimal number of points

Robert S. Womersley

School of Mathematics and Statistics, University of New South Wales, Sydney, NSW, 2052, Australia

Abstract

In this paper we consider a general class of potentials for characterizing spherical $L$-designs on $S^d$. These are used to calculate spherical $L$-designs on $S^2$ for all degrees $L = 1, \ldots, 140$ and symmetric spherical $L$-designs for degrees $L = 1, 3, \ldots, 181$. Both sets of $L$-designs have $N = \frac{L^2}{2}(1 + o(1))$ points. The number of points $N$ is of the optimal order, but greater than the unachievable lower bound of $\frac{L^2}{4}(1 + o(1))$.

These new $L$-designs provide practical equal weight cubature rules for the two sphere with a high degree of polynomial exactness, and hence high accuracy for smooth integrands. The computed spherical designs also have good mesh norms, separation and (Coulomb) energy. A spherical $L$-design with these numbers of points also has its worst case cubature error in the Sobolev space $H^s$, $s > 1$, bounded by $cL^{-s}$ or $cN^{-s/2}$.

Key words: spherical design, symmetric spherical design, equal weight cubature, 2-sphere, mesh norm, covering radius, packing radius, worst case integration error, discrepancy

Email address: r.womersley@unsw.edu.au (Robert S. Womersley).

1 The support of the Australian Research Council and the programming assistance of Dave Dowsett are gratefully acknowledged. Many fruitful discussion with Ian Sloan are also acknowledged.

2 This work was completed while visiting the Department of Applied Mathematics, The Hong Kong Polytechnic University.

Preprint submitted to Elsevier 29 October 2009
1 Introduction

A spherical $L$-design on the unit sphere $S^d \subset \mathbb{R}^{d+1}$ is a finite set $X_N := \{x_1, \ldots, x_N\} \subset S^d$ with the property

$$\frac{1}{N} \sum_{j=1}^{N} p(x_j) = \frac{1}{\omega_d} \int_{S^d} p(x) d\omega(x) \quad \forall p \in \mathbb{P}_L, \quad (1.1)$$

where $d\omega(x)$ denotes surface measure on $S^d$, $\omega_d = \omega(S^d)$ is the surface measure of the whole unit sphere $S^d$, and $\mathbb{P}_L = \mathbb{P}_{L,d}$ is the set of spherical polynomials on $S^d$ of degree $\leq L$; that is, $\mathbb{P}_L$ is the restriction to $S^d$ of the set of polynomials in $\mathbb{R}^{d+1}$ of total degree $\leq L$. A spherical design is thus an $N$-point equal weight cubature rule with degree of precision $L$.

Collected works of Sobolev [12]

A symmetric (or antipodal) set of points has an even number of points $N$ and

$$x \in X_N \iff -x \in X_N. \quad (1.2)$$

Symmetric point sets have the advantage of integrating all odd functions, and in particular all odd polynomials, exactly.

The concept of a spherical design was introduced by Delsarte, Goethals and Seidel [11] in 1977. They established the following lower bound on $N$:

$$N \geq \begin{cases} 2 \binom{d+s}{s} & \text{if } L = 2s + 1, \\ \binom{d+s}{s} + \binom{d+s-1}{s-1} & \text{if } L = 2s. \end{cases} \quad (1.3)$$

By now many particular spherical designs are known for smaller values of $L$; See the survey of Bannai and Bannai [3], Hardin and Sloane [17] and Sloane’s web pages [16].

The question of the existence of spherical designs for all values of $d$ and $L$ was settled in the affirmative by Seymour and Zaslavsky [23] in 1984, but the non-constructive proof in that paper gives no information about the number of points $N$ needed to construct a spherical $L$-design. Bajnok [2] and Korevaar and Meyers [19] give tensor product constructions of a spherical $L$ design for $S^2$ with $N = O(L^3)$ points, based on equal weight quadrature for the interval $[-1, 1]$ using $L^2$ points. The extra power of $L$ comes from the fact that equal
weight quadrature rules for $[-1, 1]$ with degree of precision $L$ require $O(L^2)$ points [14].

A set of points which achieves the bounds (1.3) is known as a tight spherical $L$-design. Bannai and Damerell [4,5] show that tight spherical designs do not exist except for some special cases. In particular they do not exist in $\mathbb{S}^2$ except for for $L = 1, 2, 3, 5$. An example of a tight spherical 2-design is formed by the vertices of the regular tetrahedron.

A major gap in our knowledge is that it is not known whether, for fixed $d \geq 2$ and $L \to \infty$, spherical $L$-designs exist with $N$ of order $(L + 1)^d$, which is the order of the lower bound (1.3). For the case $d = 2$ there are numerical proofs based on interval techniques [8,7] that spherical designs exist with $N = (L + 1)^2$ points and $0 \leq L \leq 100$. Hardin and Sloane [17] propose a set of $L$-designs with $N = \frac{L^2}{2}(1 + o(1))$ points with icosahedral symmetry, but only give examples for $N$ up to 240. This paper gives computed spherical $L$-designs without any particular symmetry or with the reflection symmetry (1.2, and with $N = \frac{L^2}{2}(1 + o(1))$ points.

This paper exploits various variational characterizations of spherical designs from the following class: A set $X_N = \{x_1, \ldots, x_N\}$ is a spherical $L$-design if and only if the quantity

$$A_{L,N,\psi}(X_N) := \frac{1}{N^2} \sum_{i=1}^{N} \sum_{j=1}^{N} \psi_L(x_i \cdot x_j)$$

(1.4)

takes the minimum possible value, namely 0. Here

$$\psi_L(z) := \sum_{\ell=1}^{L} a_{L,\ell} P_{d+1}^{\ell}(z) \quad z \in [-1, 1]$$

(1.5)

where the coefficients satisfy

$$a_{L,\ell} > 0, \quad \ell = 1, \ldots, L,$$

(1.6)

but are otherwise unrestricted. Here $P_{d+1}^{\ell}(z)$ is the Legendre polynomial in $\mathbb{R}^{d+1}$ normalized to $P_{d+1}^{\ell}(1) = 1$. They key here is the strict positivity for $\ell = 1, \ldots, L$ of the coefficients in the Legendre expansion of $\psi_L$. Note that the constant term $\ell = 0$ is not included, so

$$\int_{-1}^{1} \psi_L(z)dz = 0.$$
Indeed, as $P_{\ell+1}^{d+1}(z) = 1$, the term that must be subtracted from a polynomial $p$ of degree $L$ is just

$$a_0 = \frac{1}{2} \int_{-1}^{1} p(z) dz.$$ 

It will be useful to express quantities in terms of the (real) spherical harmonics $\{Y_{\ell,k} : k = 1, \ldots, M(d, \ell), \ \ell = 0, 1, \ldots\}$, where

$$M(d, \ell) = \frac{(2\ell + d - 1)(\ell + d - 2)!}{(d - 1)!\ell!}, \ \ell \geq 0. \quad (1.7)$$

The spherical harmonics provide an orthonormal basis for $\mathbb{P}_L$, where orthonormality is with respect to the $L_2$ inner product

$$(u, v) := \int_{S^d} u(x)v(x)d\omega(x).$$

Note that the normalisation is such that $Y_{0,1} = 1/\sqrt{\omega_d}$. Thus $Y_{\ell,k}$ is a spherical harmonic of degree $\ell$,

$$\mathbb{P}_L = \text{span}\{Y_{\ell,k} : k = 1, \ldots, M(d, \ell), \ \ell = 0, \ldots, L\},$$

and

$$\dim \mathbb{P}_{L,d} = \sum_{\ell=0}^{L} M(d, \ell) = M(d + 1, L) \sim (L + 1)^d.$$

Here $a_L \sim b_L$ means that positive constants $c_1, c_2$ exist, independently of $L$ (but possibly depending on $d$), such that $c_1a_L \leq b_L \leq c_2a_L$. It is also well known that the spherical harmonics satisfy the addition theorem

$$\sum_{k=1}^{M(d,\ell)} Y_{\ell,k}(x)Y_{\ell,k}(y) = \frac{M(d, \ell)}{\omega_d} P_{\ell+1}^{d+1}(x \cdot y), \quad x, y \in S^d,$$

where $x \cdot y$ is the inner product in $\mathbb{R}^{d+1}$. Thus for $x, y \in S^d$

$$\psi_L(x \cdot y) = \sum_{\ell=1}^{L} a_{L,\ell} P_{\ell+1}^{d+1}(x \cdot y) = \sum_{\ell=1}^{L} \frac{\omega_d}{M(d, \ell)} \sum_{k=1}^{M(d,\ell)} Y_{\ell,k}(x)Y_{\ell,k}(y). \quad (1.8)$$

For the class of potentials defined by (1.4), (1.5), (1.6), we first show that

$$0 \leq A_{L,N,\psi}(X_N) \leq \psi(1) = \sum_{\ell=1}^{L} a_{L,\ell},$$

4
and that $X_N$ is a spherical $L$-design if and only if $A_{L,N,\psi}(X_N) = 0$. This relatively elementary result, which is based on the fact that $A_{L,N,\psi}(X_N)$ is a positive weighted sum of the squares of the Weyl sums

$$r_{\ell,k}(x_N) := \sum_{j=1}^{N} Y_{\ell,K}(x_j), \quad k = 1, \ldots, M(d, \ell), \quad \ell = 1, \ldots, L. \quad (1.9)$$

A point set is a spherical $L$-design if and only if $r_{\ell,k}(X_N) = 0$ for $\ell = 1, \ldots, L$, $k = 1, \ldots, M(d, \ell)$. Major issues are knowing that solutions always exist for a sequence of point sets as $L \to \infty$ and knowing when a local minimizer with $A_{L,N,\psi}(X_N) > 0$ is a global minimizer, so spherical $L$-designs with $N$ points do not exist. This is made more difficult as optimization problems on the sphere typically have many local minima.

If $A_{L,N,\psi}(X_N) > 0$ it may be useful to think of $A_{L,N,\psi}(X_N)$ as a measure of the extent to which $X_N$ differs from a spherical $L$-design. Theorem 2.3, which gives an explicit expression for the mean of $A_{L,N}$ over all choices of $x_1, \ldots, x_N$, helps to set a scale by which the departure of $X_N$ from a spherical $L$-design may be measured. The mean $\bar{A}_{L,N}$ is defined by

$$\bar{A}_{L,N,\psi} := \frac{1}{\omega_d^N} \int_{S^d} \cdots \int_{S^d} A_{L,N,\psi}(x_1, \ldots, x_N) d\omega(x_1) \cdots d\omega(x_N). \quad (1.10)$$

Theorem 2.3 states that

$$\bar{A}_{L,N} \quad \frac{1}{N} \sum_{\ell=1}^{L} a_{L,\ell} = \frac{\psi(1)}{N} = A_{L,N}^{\text{max}}.$$ 

In particular, if for fixed $d$ we choose $N$ to be of exactly the order of $M(d + 1, L) \sim (L + 1)^d$, then $\bar{A}_{L,N,\psi}$ is bounded by a constant.

For the particular case of $S^2$ a number of different potentials are discussed. Any of these can be minimized to try to calculate a spherical $L$-design.

A number of properties of the spherical designs are discussed. Let

$$\text{dist}(x, y) = \cos^{-1}(x \cdot y)$$

denote the geodesic distance between $x$ and $y \in S^d$. A spherical cap with centre $z$ and radius $\gamma$ is

$$C(z, \gamma) = \left\{ x \in S^d : \text{dist}(z, x) \leq \gamma \right\}.$$

These properties include
• mesh norm \( ( \text{the covering radius for spherical cap with centres } x_j ) \)
  \[
h_{X_N} := \max_{x \in \mathbb{S}^d} \min_{j=1, \ldots, N} \text{dist} (x, x_j).
\]

• separation \( ( \text{twice the packing radius for spherical cap with centres } x_j ) \)
  \[
  \delta_{X_N} = \min_{i \neq j} \text{dist} (x_i, x_j).
\]

• mesh ratio
  \[
  \rho_{X_N} = \frac{2h_{X_N}}{\delta_{X_N}} \geq 1.
\]

• Riesz \( s \)-energy
  \[
  E_{X_N}^s = \sum_{1 \leq i < j} \frac{1}{|x_i - x_j|^s}.
\]

• spherical cap discrepancy
  \[
  \delta_{X_N} = \sup_{C(z, \gamma)} \left| \frac{|X_N \cap C(z, \gamma)|}{N} - \frac{|C(z, \gamma)|}{\omega_d} \right|.
\]

• worst case error for integrating functions from a space \( H \)
  \[
  \sup_{\|f\|_{H} \leq 1} \left| \frac{\omega_d}{N} \sum_{j=1}^{N} f(x_j) - \int_{\mathbb{S}^d} f(x) \, d\omega(x) \right|
  \]

Section 2 states and proves the characterizations of spherical \( L \)-designs using \( A_{L,N,\psi}(X_N) \). Section 3 specializes to \( d = 2 \), and considers several potentials that have been used. Sections 4 presents the calculated \( L \)-designs and considers the evidence that they are indeed \( L \)-designs, as well as other properties. \( A_{L,N,\psi}(X_N) \) achieves the global lower bound of 0 if and only if the point set is a spherical \( L \)-design. However if for particular values of \( N \) and \( L \) it is very difficult to identify cases where the global minimum of \( A_{L,N,\psi}(X_N) \) is positive, so not spherical \( L \)-designs exist for that number of points. The calculated \( L \)-designs for \( L = 1, \ldots, 131 \) and symmetric \( L \)-designs for \( L = 1, 3, \ldots, 181 \) still provide practical equal weight cubature rules for \( \mathbb{S}^2 \). Section 5 considers various properties of the calculated spherical designs, included their mesh norm, separation and cubature error.

2 Characterizing spherical \( L \)-designs

It is well known (see for example [3]) that there are many equivalent conditions for a set \( X = X_N \subset \mathbb{S}^d \) to be a spherical \( L \)-design. Among these equivalent
Proposition 1 The set $X_N = \{x_1, \ldots, x_N\} \subset S^d$ is a spherical $L$-design if and only if

$$
\sum_{j=1}^{N} Y_{\ell,k}(x_j) = 0 \quad \text{for } k = 1, \ldots, M(d, \ell), \ \ell = 1, \ldots, L. \quad (2.1)
$$

The necessity of the condition follows from the fact that if $X_N$ is a spherical $L$-design then we have, for $1 \leq \ell \leq L$,

$$
\sum_{j=1}^{N} Y_{\ell,k}(x_j) = \frac{N}{\omega_d} \int_{S^d} Y_{\ell,k}(x) \omega(x) = \frac{N}{\omega_d^{1/2}} \int_{S^d} Y_{\ell,k}(x) Y_{0,1}(x) \omega(x) = 0.
$$

Sufficiency follows from the fact that an arbitrary $p \in \mathbb{P}_L$ can be represented (uniquely) as

$$
p = \sum_{\ell=0}^{L} \sum_{k=1}^{M(d, \ell)} \alpha_{\ell,k} Y_{\ell,k} = \alpha_{0,1} Y_{0,1} + \sum_{\ell=1}^{L} \sum_{k=1}^{M(d, \ell)} \alpha_{\ell,k} Y_{\ell,k}.
$$

If (2.1) holds we therefore have

$$
\frac{1}{N} \sum_{j=1}^{N} p(x_j) = \alpha_{0,1} Y_{0,1} + 0 = \frac{1}{\omega_d} \int_{S^d} p(x) \omega(x) \quad \forall p \in \mathbb{P}_L,
$$

which is the condition for $X_N$ to be a spherical $L$-design.

2.1 The variational quantity $A_{L,N,\psi}(X_N)$

For each $L \geq 1$, we are given a polynomial $\psi_L \in \mathbb{P}_L[-1,1]$ with positive Legendre coefficients, so

$$
\psi_L(z) := \sum_{\ell=1}^{L} a_{L,\ell} P_{\ell}(z), \quad (2.2)
$$

with

$$
a_{L,\ell} > 0 \quad \text{for } \ell = 1, \ldots, L. \quad (2.3)
$$
Then we define
\[ A_{L,N,\psi}(x) := \frac{1}{N^2} \sum_{i=1}^{N} \sum_{j=1}^{N} \psi_L(x_i \cdot x_j). \]

The quantity \( A_{L,N,\psi}(X_N) \) is a generalization of the variational quantity \( A_{L,N} \) used in [25] which corresponds to
\[ a_{L,\ell} = M(d, \ell), \quad \ell = 1, \ldots, L, \]
so for \( d = 2 \), \( a_{L,\ell} = 2\ell + 1 \).

Using the addition theorem for spherical harmonics, we can write \( A_{L,N,\psi}(X_N) \) in the obviously non-negative form
\[ A_{L,N,\psi}(X_N) = \frac{\omega_d}{N^2} \sum_{\ell=1}^{L} \frac{a_{L,\ell}}{M(d, \ell)} \sum_{k=1}^{M(d, \ell)} (r_{\ell,k}(X_N))^2, \quad (2.4) \]
where \( r_{\ell,k} \) is defined by (1.9).

A strictly positive sum of squares is always non-negative and moreover it is equal to zero if and only if each term \( \alpha_{\ell,k} \) is zero. Thus the following theorems may be proved in exactly the same way as the corresponding theorems in [25]. We omit the proofs.

**Theorem 2.1** Let \( L \geq 1 \) and \( X_N = \{x_1, \ldots, x_N\} \subset S^2 \), and let \( \psi_L \) be as in (2.2), (2.3). Then
\[ 0 \leq A_{L,N,\psi}(X_N) \leq L \sum_{\ell=1}^{L} a_{L,\ell} = \psi_L(1). \]

Moreover, \( X_N \) is a spherical design if and only if \( A_{L,N,\psi}(X_N) = 0 \).

Note that the maximum is attained for \( N \) points which all coincide.

**Theorem 2.2** Let \( L \geq 1 \), and let \( \psi_L \) be as in (2.2), (2.3). Assume \( X_N := \{x_1, \cdots, x_N\} \subset S^2 \) is a stationary point set for \( A_{L,N,\psi} \) for which the mesh norm satisfies \( h_{X_N} < 1/(L + 1) \). Then \( X_N \) is a spherical \( L \)-design.

The next theorem gives the average value of \( A_{L,N,\psi}(X_N) \).
\[ \overline{A}_{L,N,\psi} := \frac{1}{(\omega_d)^N} \int_{S^d} \cdots \int_{S^d} A_{L,N,\psi}(x_1, \cdots, x_N) d\omega(x_1) \cdots d\omega(x_N). \]
Theorem 2.3 Let $L \geq 1$, and let $\psi_L$ be as in (2.2), (2.3). Then

$$A_{L,N,\psi} = \frac{1}{N} \sum_{\ell=1}^{L} a_{L,\ell} = \frac{\psi_L(1)}{N}.$$ 

The latter result follows immediately from (2.4) and

$$\frac{1}{\omega_d} \int_{S^d} \cdots \int_{S^d} r_{\ell,k}(X_N)^2 d\omega(x_1) \cdots d\omega(x_N)$$

$$= \frac{1}{\omega_d} \int_{S^d} \cdots \int_{S^d} \sum_{i=1}^{N} Y_{\ell,k}(x_i) \sum_{j=1}^{N} Y_{\ell,k}(x_j) d\omega(x_1) \cdots d\omega(x_N)$$

$$= \frac{1}{(\omega_d)^2} \sum_{i=1}^{N} \sum_{j=1}^{N} \int_{S^d} \int_{S^d} Y_{\ell,k}(x_i) Y_{\ell,k}(x_j) d\omega(x_i) d\omega(x_j)$$

$$= \frac{\omega_d}{(\omega_d)^2} \sum_{i=1}^{N} \int_{S^d} Y_{\ell,k}(x_i)^2 d\omega(x_i)$$

$$= \frac{N}{\omega_d},$$

where we used

$$\int_{S^d} Y_{\ell,k}(x) d\omega(x) = 0 \quad \text{for} \quad \ell \geq 1, \quad \int_{S^d} Y_{\ell,k}(x)^2 d\omega(x) = 1.$$

3 Practical spherical designs for $d = 2$

For $d = 2$, the dimension of the space of spherical polynomials with exact degree $\ell$ is $M(2, \ell) = 2\ell + 1$, the dimension of $P_L = M(d + 1, L) = (L + 1)^2$, and $P_\ell$ is the usual Legendre polynomial.

3.1 Specific potentials

We need a polynomial of degree $L$ with all the Legendre coefficients $a_{L,\ell} > 0$ for $\ell = 1, \ldots, L$. Note that $z^L$ has the Legendre expansion [1]

$$z^L = \sum_{\ell=L,L-2,\ldots} a_{L,\ell} P_\ell(z), \quad a_{L,\ell} = \frac{(2\ell + 1)!!}{2^{(L-\ell)/2} ((L+1)!!)^2} > 0. \quad (3.1)$$

with positive coefficients, but only odd or even degrees.
Example 3.1

\[ \psi_L(z) = z^L + z^{L-1} - a_{L,0} \]  
(3.2)

where

\[ a_{L,0} = \begin{cases} 
\frac{1}{L} & \text{if } L \text{ odd}, \\
\frac{1}{L+1} & \text{if } L \text{ even.}
\end{cases} \]

From the expansion (3.1) the Legendre expansion of \( z^L + z^{L-1} \) has strictly positive coefficients for \( \ell = 1, \ldots, L \). For symmetric set of points, which integrate all odd degree polynomials exactly, only the even term \( z^L \) or \( z^{L+1} \) needs to be included. This form was used by Grabner and Tichy [15]. Brauchart [6] also used this potential.

Example 3.2

\[ \psi_L(z) = (1 + z)^L - \frac{2^L}{L+1}. \]  
(3.3)

As a binomial expansion of \( (1 + z)^L \) includes all powers of \( z^\ell \) for \( \ell = 1, \ldots, L \) with positive coefficients, the Legendre expansion (3.1) shows that all the coefficients \( a_{L,\ell}, \ell = 1, \ldots, L \) are strictly positive. This is a scaled version of

\[ f(r) = (4 - r)^L, \quad r = |x - y|^2 = 2(1 - x \cdot y) \]

used by Cohn and Kumar [9].

Example 3.3

\[ \psi_L(z) = \frac{1}{\omega_d} J_L^{(1,0)}(z) - 1 = \sum_{\ell=1}^{L} (2\ell + 1)P_\ell(z) \]  
(3.4)

and \( J_L^{(1,0)} \) is the Jacobi polynomial \( J_L^{(\alpha,\beta)} \) with parameters \( \alpha = 1, \beta = 0 \). This function arises naturally from the summation formula and was used in Sloan and Womersley [25].

Example 3.4

\[ \psi_L(z) = z + z^2 + \cdots + z^L - a_0 = \begin{cases} 
z\frac{(1-z^L)}{1-z} - a_0 & \text{if } -1 \leq z < 1, \\
L - a_0 & \text{if } z = 1.
\end{cases} \]

where

\[ a_0 = \begin{cases} 
0 & \text{if } L = 1; \\
\frac{1}{3} + \frac{1}{5} + \cdots + \frac{1}{L+1} & \text{if } L \text{ is even}; \\
\frac{1}{3} + \frac{1}{5} + \cdots + \frac{1}{L} & \text{if } L > 1 \text{ is odd.}
\end{cases} \]
Example 3.5  Cui and Freeden [10] use

\[
\sum_{\ell=1}^{\infty} \frac{1}{\ell(\ell+1)} P_\ell(z) = 1 - 2 \log \left( 1 + \sqrt{\frac{1-z}{2}} \right)
\]

to define a discrepancy. This suggests using

\[
\psi_L(z) = \sum_{\ell=1}^{L} \frac{1}{\ell(\ell+1)} P_\ell(z).
\]

3.2 Spherical parametrization

For the two sphere we use the spherical parametrization \(\theta \in [0, \pi]\) and \(\phi \in [0, 2\pi]\), so

\[
\mathbf{x} = \begin{bmatrix}
\sin(\theta) \cos(\phi) \\
\sin(\theta) \sin(\phi) \\
\cos(\theta)
\end{bmatrix}.
\]

As a rotation of the whole point set \(X_N\) does not affect whether it is a spherical design as all the quantities can be expressed just in terms of the inner products \(\mathbf{x}_i \cdot \mathbf{x}_j\), equivalently the angles between the points. Thus following [13,27] the point set is normalized so that the first point is at the north pole \((\theta = 0, \phi \text{ not defined})\) and the second point on the prime meridian \((\phi = 0)\). Thus the point set \(X_N\) is parametrized by

\[
\theta_j, j = 1, \ldots, N, \quad \phi_j, j = 3, \ldots, N
\]

with \(\theta_1 = 0(\phi_1 = 0)\) and \(\phi_2 = 0\) fixed. Thus for \(N\) points there are \(n = 2N - 3\) parameters describing the point set.

Fixing a point at the north pole avoids the lack of differentiability with respect to \(\theta\) there. However there are still possible difficulties at the south pole \((\theta = \pi)\).

We will also want to work with symmetric point sets, in which case \(N\) is even and \(\mathbf{x} \in X_N \iff -\mathbf{x} \in X_N\). We then only work with a parametrization of half the points. Again a rotation can be used to normalize these \(N/2\) points so the first is at the north pole and the second on the prime meridian. The full
point set is recovered by symmetry, so it has (fixed) points at both the north and south poles. This avoids any issues with lack of differentiability there. In the symmetric case there are \( n = 2(N/2) - 3 = N - 3 \) parameters and \( N \) must be even.

### 3.3 Number of equations

The various potentials are all weighted sums of squares of the Weyl sums (1.9). A point set is a spherical \( L \)-design if and only if it satisfies the

\[
    r_{\ell,k}(X_N) := \sum_{j=1}^{N} Y_{\ell,k}(x_j) = 0 \quad k = 1, \ldots, 2\ell + 1, \quad \ell = 1, \ldots, L. \tag{3.5}
\]

Thus we have \( m = (L + 1)^2 - 1 \) equations to be satisfied. The simple condition \( n \geq m \) that there be at least as many variables as equations gives \( 2N - 3 \geq (L + 1)^2 - 1 \), or

\[
    N \geq N_1 := \begin{cases} \frac{(L+1)^2}{2} + 1 & \text{if } L \text{ is odd,} \\ \frac{(L+1)^2+1}{2} + 1 & \text{if } L \text{ is even.} \end{cases} \tag{3.6}
\]

This is roughly twice the Delsarte, Goethals and Seidel lower bound (1.3), which for \( d = 2 \) is

\[
    N \geq \begin{cases} \frac{(L+1)(L+3)}{4} & \text{if } L \text{ is odd,} \\ \frac{(L+2)^2}{4} & \text{if } L \text{ is even.} \end{cases} \tag{3.7}
\]

It is of the same order \( \frac{L^2}{2}(1 + o(1)) \) as suggested by Hardin and Sloane [17].

For \( \ell \) odd, \( Y_{\ell,k} \) is odd for \( k = 1, \ldots, 2\ell + 1 \). Thus for symmetric point sets the Weyl sums (3.5) for odd degrees \( \ell \) are automatically zero. Then number of equations, corresponding to the even degrees, is

\[
    m = \sum_{i=1}^{[L/2]} 2(2i + 1) = 2[L/2] (2 \lfloor L/2 \rfloor + 3).
\]

Again the simple requirement that there be at least as many variables as equations gives, for \( L \) odd so \( [L/2] = (L - 1)/2 \),

\[
    N \geq N_1^* := \begin{cases} \frac{(L-1)(L+2)}{2} + 3 & \text{if } L + 1 \text{ is divisible by 4,} \\ \frac{(L-1)(L+2)}{2} + 4 & \text{if } L + 1 \text{ is divisible by 2, but not 4.} \end{cases} \tag{3.8}
\]
Certainly there exist spherical $L$-designs with fewer points in certain special cases, see [17,16]. Our experiments have found spherical $L$-designs with $N_1(L)$ points for $L$ up to 138, except for $L = 3, 5, 7, 9, 11$. In these cases spherical $L$-designs with $N_1(L) - 1$ and $N_1(L) + 1$ points are known. Taking $N$ (slightly) larger made it much easier to find a spherical $L$ design.

Symmetric spherical $L$ designs with $N_s^1(L)$ points where found for $L = 1, 3, \ldots, 181$, except for $L = 7, 11, 15$ when $N_s^2 + 2$ points were required. These are available from the web page web.math.unsw.edu.au/~rsw/Sphere/Designs. The next subsections discuss the calculation of these, evidence that they are indeed spherical $L$ designs and their properties.

3.4 Real spherical harmonics and sums of squares

For the special case of $d = 2$, it is convenient to use the real spherical harmonic basis for $\mathbb{P}_L$. Using the spherical parametrization $\theta \in [0, \pi]$ and $\phi \in [0, 2\pi)$,

$$Y_{\ell,k} = \begin{cases} N_{\ell,k} P_{\ell}^{[k]}(\cos \theta) \cos(k\phi) & k = -\ell, \ldots, -1 \\ N_{\ell,0} P_{\ell}^{0}(\cos \theta) & k = 0 \\ N_{\ell,k} P_{\ell}^{k}(\cos \theta) \cos(k\phi) & k = 1, \ldots, \ell \end{cases}$$

where $N_{\ell,k}$ are the normalization coefficients

$$N_{\ell,k} = \sqrt{\frac{2\ell + 1 (\ell - k)!}{4\pi (\ell + k)!}}$$

and $P_{\ell}^{[k]}$ are the associated Legendre polynomials.

Add the $m$ by $n$ Jacobian matrix $J$ of $r : \mathbb{R}^n \rightarrow \mathbb{R}^m$.

$$\frac{\partial r_{\ell,k}(y)}{\partial y_j} =$$

The gradient and the Hessian of the sum of squares $f = r^T r$ can be written as

$$\nabla f = 2J^T r, \quad \nabla^2 f = 2J^T J + \sum_{i=1}^m r_i(y)\nabla^2 r_i(y) \quad (3.9)$$

Thus any method for nonlinear least squares can be used to minimize $r^T r$. 

13
An alternative is to use any unconstrained optimization method to minimize $A_{L,N,\psi}(X_N)$ as a function of a spherical parametrization of the variables. The closed form expressions for the potential $\psi_L(z)$ can be used to derive expressions for the gradient and possibly the Hessian of $A_{L,N,\psi}(X_N)$.

3.5 Evaluating $A_{L,N,\psi}(X_N)$

Consider the matrix $Y$ of size $M(d+1,L) - 1$ by $N$ defined by

$$Y = [Y_{\ell,k}(x_j)], \quad \ell = 1, \ldots, L, \quad k = 1, \ldots, M(d,\ell), \quad j = 1, \ldots, N, \quad (3.10)$$

where the rows are labeled by $\ell, k$ and the columns by $j$. Note that a row for the degree $\ell = 0$ is not included. Also let the $N$ by $N$ matrix $\Psi$ be defined by

$$\Psi_{ij} = \psi_L(x_i, x_j), \quad i, j = 1, \ldots, N. \quad (3.11)$$

Again note that the definition of $\psi_L$ in (2.2) does not include the $\ell = 0$ term. Then equation (1.8) gives

$$\Psi = \omega_d Y^T W Y,$$

where

$$W = \text{diag}(w_{\ell,k}, k = 1, \ldots, M(d,\ell), \ell = 1, \ldots, L), \quad w_{\ell,k} = \frac{a_{L,\ell}}{M(d,\ell)}.$$

By Proposition 1 a spherical design is characterized by the $M(d+1,L) - 1$ equations

$$r := Ye = 0, \quad (3.12)$$

where $e \in \mathbb{R}^N$ is the vector in which every entry is 1. Thus

$$A_{L,N,\psi}(X_N) = \frac{1}{N^2} e^T \Psi e = \frac{\omega_d}{N^2} e^T Y^T W Ye = \frac{\omega_d}{N^2} r^T W r. \quad (3.13)$$

The first and third expressions for $A_{L,N,\psi}(X_N)$ suggest two different ways of evaluating $A_{L,N,\psi}(X_N)$. In the first we may use the closed form expressions for $\psi_L(z)$. For Example 3.3 there is a stable three-term recurrence for the Jacobi polynomial. The second alternative is to use the real spherical harmonics and form the weighted sum of squares of the residual $r = Ye$. Using sum over all the $\psi_L(x_i \cdots x_j)$ was found to result in significant cancelation between the off-diagonal elements of $\Psi$, sometimes producing the embarrassment of negative values for $A_{L,N,\psi}(X_N)$. The weighted sum of squares of the residual avoids the
problem of negative values, and so is the preferred method for our calculations for modest $L$.

![Spherical L-design with N = (L+2)^2/2 + 1 points](image)

Figure 1. Spherical designs for degrees $L = 1, \ldots, 138$

Figure 2 gives the values of the potentials in Examples 3.2, 3.1 and 3.4. Note that for Example 3.2 the term $2^L/(L+1)$ that must be subtracted from $(1+z)^L$ grows so rapidly with $L$, that this introduces significant rounding error for large value of $L$. **** Remove Example 1 from plot ?? ****

In [8] the authors were able to use interval-based methods for proving the existence of a nearby exact spherical design. Those arguments depend critically on being able to choose a well conditioned sub-matrix of the Jacobian of the system of nonlinear equations $\mathbf{r} = \mathbf{0}$. For $d = 2$, if as in [8] we take $N = (L+1)^2$ then the extra degrees of freedom can be used to achieve this, for example by starting from the extremal fundamental systems of [24].

Add plot of condition number of basis matrix, and show bounds obtained from Chen and Womersley interval analysis.

For the spherical $L$-designs, Figure 3 gives the mesh norm, or covering radius
Fig. 2. Spherical design potentials $L = 1, \ldots, 138$

$h_{X_N}$, the minimum angle, or twice the packing radius, $d_{X_N}$ and the mesh ratio $\rho_{X_N} = 2h_{X_N}/d_{X_N} \geq 1$. A common assumption [20] is that the mesh ratio is bounded, which is the case for the degrees illustrated here. The mesh norm is bounded by the covering radius for the best covering, which empirically has $h_{X_N} = c_{c}/\sqrt{N}$ with $c \approx 2.3$. A simple argument based on the fact that the spherical caps of radius $h$ must cover the whole surface of the sphere gives the bound $h \geq 2/\sqrt{N}$. Yudin [28] showed that a spherical $L$-design has covering radius given by the largest zero $z_L = \cos(h)$ of the Jacobi polynomial $P^{(1,1)}$. Thus for spherical $L$-designs with $N \approx L^2/2$ points,

$$\frac{c_{c}}{\sqrt{N}} \leq h \leq \cos^{-1}(z_L) \sim \frac{2j_0}{L} \approx \frac{4.8}{\sqrt{N}},$$

where $j_0$ is the largest zero of the Bessel function $J_0$.

The minimum angle is bounded by the separation obtained for best packing
Fig. 3. Mesh norm, separation and mesh ratio for spherical $L$-designs, $L = 1, \ldots, 138$ (see [22] for example), so

$$d_{X_N} \leq d_N^* = \frac{c_p}{\sqrt{N}}, \quad c_p = \sqrt{\frac{8\pi}{\sqrt{3}}} \approx 3.8093$$

However, as two spherical $L$-designs is still a spherical $L$-design, the separation can be arbitrarily small (see [18]). However, from Figures 3, 4, the calculated spherical designs are well separated.

Figure 4 gives the corresponding data for the symmetric spherical $L$-designs.

Hesse and Leopardi [18] give an estimate for the Riesz energy of a spherical $L$-design that satisfies a separation condition of the form $d_{X_N} \geq c/\sqrt{N}$, which is true for the calculated spherical designs. Figure 5 show the Coulomb (Riesz $s = 1$) energy with the leading term removed, and compares it with the values for some low energy point chosen by minimizing the energy. (There is no guarantee these are global minimum energy points, as the problems have many local minima). The striking feature is how close to the conjectured asymptotic limit (see [22] for example) the energy of the spherical designs is to this limit.
Fig. 4. Mesh norm, separation and mesh ratio for symmetric spherical $L$-designs, $L = 1, 3, \ldots, 181$

Hesse and Sloan /citeHesS06 showed that cubature rules that satisfy a certain regularity property and are exact for all polynomials of degree $L$ have a worst case cubature error in the Sobolev space $H^s$ bounded by $c_s L^{-s}$. Reimer [21] showed the regularity property is automatically satisfied if the cubature rule has positive weights, so in particular it is satisfied by a spherical $L$-design. As our $L$-designs have $N = L^2/2 + O(L)$ points gives the bound on the worst case cubature error

$$\sup_{\|f\|_{H^s} \leq 1} \left| \omega_2 \sum_{j=1}^{N} f(x_j) - \int_{S^2} f(x) \, d\omega(x) \right| \leq c_s L^{-s} \approx c_s N^{-s/2}.$$ 

For the particular case of $s = 3/2$ the worst case error can be evaluated exactly using the Cui and Freeden [10] discrepancy. The results are given in Figure 6, suggesting $c_s \approx 0.26$.

Tensor product rules for cubature over $S^2$ are well known (see Stroud [26] for example). A Gauss-Legendre rule for $[-1,1]$ combined with an equally spaced points for the azimuthal angle $\phi$ gives a cubature rule with $N =$
Fig. 5. Coulomb (Riesz $s = 1$) energy and conjectured asymptotic limit $(L + 1) [ (L + 1)/2 ]$ points that is exact for polynomials of degree up to $L$ and has positive weights. This is also $\frac{L^2}{2} (1 + o(1))$ points as the calculated spherical designs, but the weights are not equal and the points are denser close to the poles (as with tensor product rule).

Finally to illustrate the performance of the calculated spherical designs they are used to approximate

$$\int_{S^2} \frac{1}{x^2 + y^2 + (z - 1/2)^2} d\omega(x) = \frac{5\pi \log(11)}{3}.$$ 

The results are illustrated in Figure 7 showing the exponential convergence expected for a smooth integrand.

References

Fig. 6. Worst case error for $H^{3/2}$


Fig. 7. Cubature error for \( f(x) = 1/(x^2 + y^2 + (z - 1.2)^2) \)


