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Numerical Verification Methods for Spherical *t*-Designs

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The construction of spherical t-designs with $(t+1)^2$ points on the unit sphere S^2 in $\mathbb{R}^3$ can be reformulated as an underdetermined system of nonlinear equations. This system is highly nonlinear and involves the evaluation of a degree t polynomial in $(t+1)^4$ arguments. This paper reviews numerical verification methods using the Brouwer fixed point theorem and Krawczyk interval operator for solutions of the underdetermined system of nonlinear equations. Moreover, numerical verification methods for proving that a solution of the system is a spherical t-design are discussed.

Key words: verification, spherical designs, system of nonlinear equations

1. Introduction

We denote the unit sphere by

$$S^2 = \{y \in R^3 \colon \|y\|_2 = 1\}.$$

Let $\mathbb{P}_t \equiv \mathbb{P}_t(S^2)$ be the linear space of restrictions of polynomials of degree $\leq t$ in 3 variables to the sphere S^2. *A spherical t-design,* introduced in [6], is a set of N points $\{y_1, y_2, \ldots, y_N\} \subset S^2$ such that

$$\int_{S^2} p(y)\, dy = \frac{4\pi}{N} \sum_{l=1}^{N} p(y_l)$$

for every polynomial $p \in \mathbb{P}_t$. For $t \geq 1$, the existence of a spherical t-design was proved in [20]. However, finding a concrete spherical t-design for any given t is very challenging. Numerical methods for finding spherical t-designs attract considerable attention. The main interest is in the number of points required to form a spherical t-design, efficient numerical algorithms for finding approximate spherical t-designs, and numerical methods for verifying spherical t-designs.

The 7-design with 24 points was first found by McLaren in 1963 [15]. Hardin and Sloane [9] suggested a sequence of putative spherical t-design with $\frac{1}{2}t^2 + o(t^2)$ points by using interval methods and the fact that a set of N points $\{y_1, y_2, \ldots, y_N\}$

forms a spherical t-design if and only if the polynomial identities

$$\frac{1}{N}\sum_{i=1}^{N}(y_i^{\mathrm{T}}y)^{2s} = \left(\prod_{j=0}^{s-1}\frac{2j+1}{2j+3}\right)(y^{\mathrm{T}}y)^{s}$$

and

$$\frac{1}{N}\sum_{i=1}^{N}(y_i^{\mathrm{T}}y)^{2\bar{s}+1} = 0$$

hold, where s and $\bar{s}$ are defined by $\{2s, 2\bar{s}+1\} = \{t-1, t\}$. Maier [14] studied an approach for the numerical calculation of spherical designs using methods of multiobjective optimization. Sloan and Womersley [22] established a new variational characterization of spherical designs and showed that a set of N points $\{y_1, y_2, \ldots, y_N\} \subset S^2$ is a spherical design if and only if a certain non-negative quantity takes the minimum value 0. The best known construction for spherical t-design on S^2 is given by Korevaar and Meyers [12] who obtained spherical t-design with $O(t^3)$ points. Recently, Chen and Womersley [3] reformulated the construction of spherical t-design with $(t+1)^2$ points as an underdetermined system of nonlinear equations with $2(t+1)^2-3$ variables and $(t+1)^2-1$ equations. Moreover, they proposed a numerical verification method for enclosure of solutions of the system. Note that the dimension of the space $\mathbb{P}_t$ is $(t+1)^2$. The lower bound on the smallest number of points required to form a spherical t-design is

$$N_t^* \geq \frac{(t+1)(t+3)}{4} \quad \text{if } t \text{ is odd,}$$

$$N_t^* \geq \frac{(t+2)^2}{4} \quad \text{if } t \text{ is even.}$$

See [6]. A spherical t-design whose number achieves the lower bounds is called a tight spherical t-design. However for all $t \geq 2$, it is known that tight spherical t-designs do not exist. The spherical t-design given by the reformulation of the underdetermined system of nonlinear equations in [3] has the same order $O(t^2)$ as the lower bounds N_t^*. However, the system is highly nonlinear which involves a degree t polynomial at $N^2 = (t+1)^4$ arguments. Verifying the existence of solution of the system for large t requires high performance computing. Lang, Beelitz, Frommer and Willems [13] developed an efficient algorithm to verify the existence solution of the underdetermined system of nonlinear equations. They were able to obtain verified solution of the system up to $t = 80$. If the Gram matrix at the $(t+1)^2$ points corresponding to the solution of the system is nonsingular, then the set of the $(t+1)^2$ points is a spherical t-design. In Section 2, we illustrate the construction of spherical t-designs by using the underdetermined system of nonlinear equations. In Section 3, we review verification methods for the underdetermined system of nonlinear equations, and discuss how to verify the nonsingularity of the Gram matrix at a solution of the system. Finally, we give some remarks on numerical verification for spherical t-designs.

2. Reformulation

In this section we illustrate how to reformulate the construction of spherical t-designs as an underdetermined system of nonlinear equations.

Let $L_l\colon [-1,1] \to R$ be the usual Legendre polynomial [1]. The Rodrigues reprensetation yields

$$L_l(z) = \frac{1}{2^l} \sum_{k=0}^{[l/2]} \frac{(-1)^k (2l-2k)!}{k!\,(l-k)!\,(l-2k)!} z^{l-2k}, \tag{2.1}$$

where $[l/2]$ is the floor function. We define

$$J_t(z) = \frac{1}{4\pi} \sum_{l=0}^{t} (2l+1) L_l(z), \quad z \in [-1,1].$$

For a set of points $Y = \{y_1, \ldots, y_{d_t}\} \subset S^2$, we have

$$y_i^{\mathrm{T}} y_j \in [-1,1], \quad i,j = 1, \ldots, d_t.$$

The polynomials

$$g_i(y) = J_t(y_i^{\mathrm{T}} y), \quad i = 1, \ldots, d_t,\ y \in S^2$$

belong to $\mathbb{P}_t$. Since $\dim(\mathbb{P}_t) = (t+1)^2$, in order to make $\{g_1, \ldots, g_{d_t}\}$ a basis for $\mathbb{P}_t$, the number of points in Y should be

$$d_t = (t+1)^2.$$

Moreover, if the $d_t \times d_t$ Gram matrix G with elements

$$G_{ij}(Y) = g_i(y_j)$$

is nonsingular, then $\{g_1, \ldots, g_{d_t}\}$ is a basis for $\mathbb{P}_t$.

For a given arbitrary function $f \in C(S^2)$, we define the unique polynomial interpolant Λf for the set Y by

$$(\Lambda f)(y) = \sum_{i=1}^{d_t} v_i g_i(y).$$

Here the vector of weights $v = (v_1, \ldots, v_{d_t})$ is the solution of the following linear system of equations

$$G(Y)v = b, \tag{2.2}$$

where $b_i = f(y_i)$, $i = 1, \ldots, d_t$. By the nonsingularity, the zero polynomial is the only member of $\mathbb{P}_t$ that vanishes at each point $y_1, \ldots, y_{d_t}$. Hence, the set of points $Y = \{y_1, \ldots, y_{d_t}\} \subset S^2$ is a fundamental system.[1]

[1] A set of points $Y = \{y_1, \ldots, y_{d_t}\} \subset S^2$ is called a fundamental system if the zero polynomial is the only member of $\mathbb{P}_t$ that vanishes at each point $y_1, \ldots, y_{d_t}$.

If w is the solution of (2.2) with $b = e = (1, \dots, 1)^{\mathrm{T}}$, then the cubature rule

$$Q_{d_t}(f) = \sum_{i=1}^{d_t} w_i f(y_i)$$

for numerical integral

$$\int_{S^2} f(y)\, dy$$

is exact for all polynomials f of degree $\leq t$. This can be shown as follows. For any $p \in \mathbb{P}_t$, there are scalars α_i, $i = 1, \dots, d_t$ such that

$$p(y) = \sum_{i=1}^{d_t} \alpha_i g_i(y).$$

Using the following property of the basis $\{g_1, \dots, g_{d_t}\}$ [18]

$$\int_{S^2} g_i(y)\, dy = 1, \quad i = 1, \dots, d_t,$$

we obtain

$$\begin{aligned}
\int_{S^2} p(y)\, dy &= \sum_{i=1}^{d_t} \alpha_i \\
&= \sum_{i=1}^{d_t} \alpha_i \sum_{j=1}^{d_t} G_{ij}(Y) w_j \\
&= \sum_{j=1}^{d_t} w_j \sum_{i=1}^{d_t} G_{ij}(Y) \alpha_i \\
&= \sum_{j=1}^{d_t} w_j \sum_{i=1}^{d_t} g_i(y_j) \alpha_i \\
&= \sum_{j=1}^{d_t} w_j p(y_j).
\end{aligned}$$

In particular, the cubature rule is exact for the constant polynomial $1 \in \mathbb{P}_t$. Thus

$$\int_{S^2} dy = |S^2| = 4\pi = \sum_{i=1}^{d_t} w_i.$$

Hence the average weight is

$$w_{\mathrm{avg}} = \frac{4\pi}{d_t}.$$

A spherical t-design is a set of points $Y^* = \{y_1^*, y_2^*, \ldots, y_{d_t}^*\}$ such that

$$\int_{S^2} p(y)\, dy = \sum_{i=1}^{d_t} w_i^* p(y_i)$$

for every polynomial $p \in \mathbb{P}_t$ with equal weights

$$w_i^* = \frac{4\pi}{d_t}, \quad i = 1, \ldots, d_t, \tag{2.3}$$

where w^* is the solution of

$$G(Y^*)w = e. \tag{2.4}$$

Hence, a spherical t-design can be found by solving the system of nonlinear equations on S^2

$$G(Y)e = \frac{d_t}{4\pi} e, \quad \text{for } Y \subset S^2. \tag{2.5}$$

Now we reformulate this problem as an underdetermined system of nonlinear equations without constraints. As the matrix G is rotationally invariant with respect to the angles, we set $\phi_1 = 0$, $\theta_1 = 0$ and $\phi_2 = 0$, that is, the first point y_1 is conveniently fixed at the north pole and the second point y_2 on the prime meridian. Hence a spherical parametrization $\theta_j \in [0, \pi]$ and $\phi_j \in [0, 2\pi)$ of the points y_j, $j = 1, 2, \ldots, d_t$ has $2d_t - 3$ variables.

Let

$$n = 2d_t - 3, \quad m = d_t - 1,$$

and let

$$\begin{aligned} x_{i-1} &= \theta_i, & i &= 2, 3, \ldots, d_t, \\ x_{d_t+i-3} &= \phi_i, & i &= 3, 4, \ldots, d_t. \end{aligned}$$

Then the relation between the set of points $\{y_1, \ldots, y_{d_t}\}$ and the vector of variables $x \in R^n$ is uniquely defined as

$$y_1 = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}, \quad y_2 = \begin{bmatrix} \sin x_1 \\ 0 \\ \cos x_1 \end{bmatrix}, \quad y_i = \begin{bmatrix} \sin\theta_i \cos\phi_i \\ \sin\theta_i \sin\phi_i \\ \cos\theta_i \end{bmatrix} = \begin{bmatrix} \sin x_{i-1} \cos x_{d_t+i-3} \\ \sin x_{i-1} \sin x_{d_t+i-3} \\ \cos x_{i-1} \end{bmatrix}.$$

The simple bounds on θ_i and ϕ_i can be ignored as the periodicity of the sin and cos functions. Hence the matrix $G(Y)$ can be regarded as a function of x whose elements are defined by

$$G_{ij}(Y) = G_{ij}(x) = J_t(y_i^{\mathrm{T}} y_j).$$

Let E be the following $m \times d_t$ matrix

$$E = \begin{pmatrix} 1 & -1 & 0 & \cdots & 0 \\ 1 & 0 & -1 & \ddots & \vdots \\ \vdots & \vdots & \ddots & \ddots & 0 \\ 1 & 0 & \cdots & 0 & -1 \end{pmatrix}.$$

We define a function $c\colon R^n \to R^m$ and consider the following underdetermined system of nonlinear equations

$$c(x) := EG(x)e = 0. \tag{2.6}$$

In [3], Chen and Womersley gave the following theorem, which states the relation between a spherical t-design and a solution of the underdetermined system of nonlinear equations (2.6).

THEOREM 2.1. *Suppose that $G(x^*)$ is nonsingular. Then x^* corresponds to a spherical t-design with $(t+1)^2$ points if and only if $c(x^*) = 0$.*

3. Numerical verification of spherical t-designs

In this section, we review numerical verification methods for the underdetermined system of nonlinear equations (2.6) and discuss how to verify the nonsingularity of $G(x)$ at a solution of (2.6).

For a given $x \in R^n$, let $\mathcal{B} = \{k_1, k_2, \dots, k_m\}$ be an index set such that the submatrix $c'_{\mathcal{B}}(x)$ whose entries lie in the columns of $c'(x) \in R^{m\times n}$ indexed by $\mathcal{B}$ is nonsingular. Let $x_{\mathcal{B}}$ be the subvector of x whose entries of x are indexed by $\mathcal{B}$. Let $\mathcal{N} = \{1, 2, \dots, n\} \setminus \mathcal{B}$.

Suppose that $\hat{x}$ is an approximate solution of (2.6) close to a vector $\bar{x}$ corresponding to an extremal fundamental system $\bar{Y}$.[2]

We consider two verification methods for solution of the underdetermined system of nonlinear equations (2.6) on the set

$$X = \{x \mid \|x_{\mathcal{B}} - \hat{x}_{\mathcal{B}}\| \le r,\ x_{\mathcal{N}} = \hat{x}_{\mathcal{N}}\}.$$

Kantorovich-type method

1. Calculate $c'_{\mathcal{B}}(\hat{x})$ and K such that

$$\|c'_{\mathcal{B}}(x) - c'_{\mathcal{B}}(\hat{x})\| \le K\|x - \hat{x}\|, \quad x \in X.$$

[2] A set of points $\bar{Y} = \{\bar{y}_1, \dots, \bar{y}_{d_t}\}$ defined by

$$\log\det G(\bar{Y}) = \max_{Y\subset S^2} \log\det(G(Y))$$

is called an extremal fundamental system.

2. Check the following inequality

$$\rho := K\|c'_{\mathcal{B}}(\hat{x})^{-1}c(\hat{x})\| \, \|c'_{\mathcal{B}}(\hat{x})^{-1}\| \le \frac{1}{2}. \tag{3.1}$$

If it is TRUE and

$$r_1 := \frac{1-\sqrt{1-2\rho}}{K\|c'_{\mathcal{B}}(\hat{x})^{-1}\|} \le r,$$

then there is a solution of (2.6) in the set

$$X = \{x \mid \|x_{\mathcal{B}} - \hat{x}_{\mathcal{B}}\| \le r_1, \ x_{\mathcal{N}} = \hat{x}_{\mathcal{N}}\}.$$

If (3.1) fails and

$$r_2 := \frac{\sqrt{1+2\rho}-1}{K\|c'_{\mathcal{B}}(\hat{x})^{-1}\|} \le r,$$

then (2.6) has no solution in

$$X = \{x \mid \|x_{\mathcal{B}} - \hat{x}_{\mathcal{B}}\| \le r_2, \ x_{\mathcal{N}} = \hat{x}_{\mathcal{N}}\}.$$

Now we consider the Krawczyk interval operator defined in the interval

$$X = \{x \mid \|x_{\mathcal{B}} - \hat{x}_{\mathcal{B}}\|_\infty \le r, \ x_{\mathcal{N}} = \hat{x}_{\mathcal{N}}\}.$$

Krawczyk-type method

1. Compute an interval matrix $[C_{\mathcal{B}}]$ which contains $\{c'_{\mathcal{B}}(x) \mid x \in X\}$.
2. Compute an approximation R of $(\mathrm{mid}([C_{\mathcal{B}}]))^{-1}$.
3. Check the following enclosure

$$K(\hat{x}_{\mathcal{B}}, X_{\mathcal{B}}) := \hat{x}_{\mathcal{B}} - Rc(\hat{x}) + (I_{\mathcal{B}} - R[C_{\mathcal{B}}])(X_{\mathcal{B}} - \hat{x}_{\mathcal{B}}) \subseteq X_{\mathcal{B}}. \tag{3.2}$$

If it is TRUE, then there is a solution of (2.6) in the set X. If $K(\hat{x}_{\mathcal{B}}, X_{\mathcal{B}}) \cap X_{\mathcal{B}} = \emptyset$, then there is no solution in X.

Suppose that the exstence of solution of (2.6) in X has been verified. To ensure the solution of (2.6) in X corresponds to a spherical t-design, we have to verify the nonsingularity of the Gram matrix G at the solution. We suggest a verification process as follows.

Compute an interval $[G]$ which contains $\{G(x) \mid x \in X\}$. For any $G \in [G]$, we have

$$\|G - \mathrm{mid}([G])\| \le \|\mathrm{radius}([G])\|.$$

By Theorem 2.3.4 in [8], if $\mathrm{mid}([G])$ is nonsingular and

$$\|(\mathrm{mid}([G]))^{-1}\| \, \|\mathrm{radius}([G])\| < 1,$$

then all matrices in $[G]$ is nonsingular. In this case, we can claim that the solution of the underdetermined system of nonlinear equations (2.6) in X is a spherical t-design. Using this process with the truncated multi-point Horner scheme proposed in [7], we were able to prove the existence of $(t+1)^2$ point spherical designs for t values up to $t = 80$ [2].

4. Final remarks

Interpolation on the sphere and numerical integration on the sphere have many applications in engineering and science, for examples, global climate models for the earth, modeling viruses, computer graphics, computational geometry, etc. The interpolatory cubature rule associated with a spherical t-design provides high-order numerical integration on the sphere. The construction of spherical t-designs is interesting in mathematical theory and real practice. Moreover, finding spherical t-designs can be used as a test problem for algorithms for global minimization problems and nonlinear equations, as the function c is highly nonlinear, the natural residual $\|c(x)\|_2$ has many local minimizers, and selection of an appropriate nonsingular submatrix $c_{\mathcal{B}}(x)$ effects the efficiency of the algorithms.

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