Chapter 11
Uniform Design on Manifold

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Abstract Uniform design aims to scatter points as evenly as possible on certain domain. Although in real applications, the experimental domain is often quite arbitrary, the discrepancies frequently used to measure the uniformity of experimental designs are often defined on the unit cube. In this paper, we will introduce a unified framework to measure the uniformity of an experimental design on manifold. We will give some examples to illustrate the construction of uniform designs on some specific manifolds and provide a stochastic algorithm to construct uniform designs on the unit semi-spherical surface and on the unit spherical surface. Numerical results show that the algorithm performs well.

11.1 Background

Uniform design has been applied to various fields since it was proposed in Fang [4], Wang and Fang [22]. As its name implies, the basic idea of a uniform design is to seek design points scattered uniformly on certain domain. So in general, the combinatorial structure of a uniform design (or a low-discrepancy design) is quite arbitrary, which is different from that of an orthogonal array. To evaluate uniformity of a design, one must need a criterion, named discrepancy in uniform design theory. In fact, the concept of discrepancy came from number theory (quasi-Monte Carlo) method. As indicated in Fang and Wang [7], Fang et al. [6], many discrepancies including star discrepancy, L_p-discrepancy, and modified discrepancies proposed in Hickernell [10, 11] have their clear geometrical meanings. Uniform designs based on various discrepancies have been investigated extensively in existing literatures. Many properties and construction methods related to uniform design can be found in Fang et al. [5, 6]. To make it easier, most discrepancies are defined on the unit cube $C^s = [0, 1)^s$, but in some real problems, the experimental domain may be quite complicated. For example, Chuang and Hung [1] proposed the centered composite

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discrepancy for a general domain, and Lin et al. [14] used it to construct uniform designs on the flexible region

$$R_m = \{(x_1, \ldots, x_s) \in [-1, 1]^s \big| |x_1|^m + |x_2|^m + \cdots + |x_s|^m \leq 1\},$$

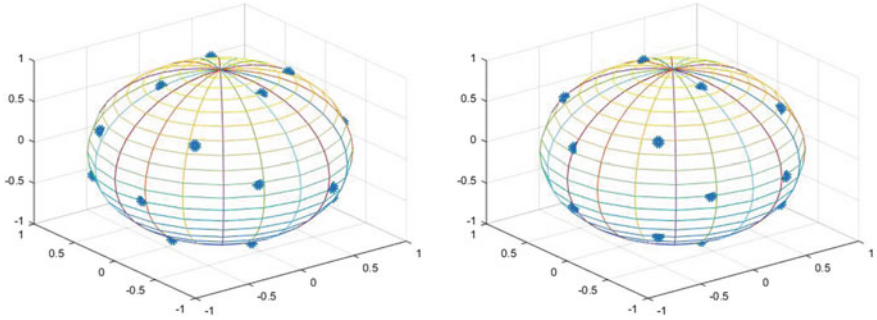
which was considered in Draper and Guttman [2]. The centered composite discrepancy can be regarded as a generalization of the centered L_2-discrepancy. Although it has no close form for an arbitrary domain, it can still be numerically calculated using efficient algorithms, just showed in Lin et al. [14]. Liu and Liu [15] considered uniform designs for mixture experiments with complex constraints, which could also be regarded as uniform designs on irregular domain. However, in some scenarios, the experimental domain will be even special. For example, in aerospace and military fields, people often want to scatter points on certain manifolds [3, 9]. To solve such problems, we need to further generalize the definition of discrepancy. Fang and Wang [7] suggests using inverse transformation to construct uniform design for some symmetrical domain including the unit spherical surface. For simplicity, throughout the paper, we only consider the three-dimensional case. Denote the unit spherical surface

$$\mathscr{U}^3 = \{(z_1, z_2, z_3) : z_1^2 + z_2^2 + z_3^2 = 1\}.$$

Let $\mathscr{P} = \{x^{(k)} = (x_{k1}, x_{k2}), k = 1, \ldots, n\}$ be a set of n points uniformly distributed on $\mathscr{C}^2 = [0, 1)^2$. Consider a transformation from $\mathscr{C}^2$ to $\mathscr{U}^3$ defined as

$$\begin{cases} z_{k1} = 1 - 2x_{k1}, \\ z_{k2} = 2\sqrt{x_{k1}(1 - x_{k1})}\cos(2\pi x_{k2}), \\ z_{k3} = 2\sqrt{x_{k1}(1 - x_{k1})}\sin(2\pi x_{k2}), \end{cases}$$

where $k = 1, 2, \ldots, n$. Although it can be proved that the resultant point set $\{z^{(k)} = (z_{k1}, \ldots, z_{ks}), k = 1, \ldots, n\}$ is uniformly scattered on the unit spherical surface $\mathscr{U}^s$, the actual result of the inverse transformation method does not seem effective, especially when the number of points is small. As Fang and Wang [7] pointed out, the indirect method using inverse transformation may not measure the uniformity of designs accurately. Figure 11.1 will illustrate it. The left part (a) in Fig. 11.1 indicates 20 points on the unit spherical surface obtained using the inverse transformation, while the right part (b) shows the 20 vertices of a regular dodecahedron, whose circumscribed sphere is the unit spherical surface. Intuitively, the latter seems more uniform compared with the former. It is well-known that there are only five different types of regular polyhedrons. Thus when the number of points is other than four, six, eight, twelve and twenty, we need consider other construction methods. Moreover, we will also show that even when a regular polyhedron exists, it will not always be the best one given some specific criterion. The paper is organized as follows. We will first define a general discrepancy based on geodesic distance for uniform design on manifold in Sect. 11.2. In Sects. 11.3 and 11.4, we consider uniform designs on the unit semi-spherical surface and the unit spherical surface,



(a). Transferred from $\mathscr{C}^2$ (b). Regular dodecahedron

Fig. 11.1 Two methods to construct uniform designs on $\mathscr{U}^3$

respectively. We also propose an algorithm to construct uniform designs for these two cases. Numerical examples will show that the algorithm is quite effective. Finally, we will give some conclusion and discussion in the last section.

11.2 General Discrepancy on Manifold

The concept of discrepancy arises in the Quasi-Monte Carlo method, which is used to solve multivariate integration problem. In many cases, we want to obtain the integration of certain function $f(x)$ over a specific domain $\mathscr{D}$. However, since the function $f(x)$ may be much complicated and we cannot get the exact value of the integration

$$I(f) \equiv \int_{\mathscr{D}} f(x)\, dx,$$

we will sometimes use the approximation to evaluate $I(f)$. A simple and easy way of doing so is to choose a set of n-point, P, which is uniformly scattered on the domain $\mathscr{D}$, and calculate all the values of $f(x)$ on these points, sum up them all and divide by n, i.e.,

$$Q(f; P) \equiv \frac{1}{n} \sum_{z \in P} f(z).$$

The approximation part $Q(f; P)$ is often called quadrature rule. Obviously, different set of points P may result in different quadrature rule. So we need to define a criterion to evaluate the uniformity of the point set P. As discussed in the previous section, some modified L_2-discrepancies, including the centered L_2-discrepancy and the wrap-around L_2-discrepancy, are often used in practice. However, most of them are defined on the unit cube and cannot be directly used when the experimental domain is a manifold. In Li [13], the author proposed the λ-discrepancy for uniform

design on a general domain. In this paper, we will generalize the λ-discrepancy, in order to let it be suitable for uniform design on manifold.

Definition 11.1 Let $\mathscr{D}$ be a domain and $\partial\mathscr{D}$ be its boundary. For any point $z \in \mathscr{D}$, define

$$\mathscr{B}_z = \bigvee_{x \in \partial\mathscr{D}} \boldsymbol{d}_B(z, x), \tag{11.1}$$

where $\boldsymbol{d}_B(\cdot,\cdot)$ is a well-defined distance function and the notation "$\bigvee$" represents an overall function (such as summation, integral, maximum or minimum), then $\mathscr{B}_z$ is called the **boundary deviation of** z.

Definition 11.2 Let $\mathscr{D}$ be a domain, and $\mathscr{Z} = \{z^{(1)}, z^{(2)}, \ldots, z^{(n)}\}$ be an n-point set, where each $z^{(i)} \in \mathscr{D}$. For any point $z \in \mathscr{D}$, define

$$\mathscr{P}_z = \bigvee_{z^{(i)} \in \mathscr{Z}} \boldsymbol{d}_P(z, z^{(i)}), \tag{11.2}$$

where $\boldsymbol{d}_P(\cdot,\cdot)$ also represents a well-defined distance function and "$\bigvee$" represents an overall function (such as summation, integral, maximum or minimum), then $\mathscr{P}_z$ is called the **point deviation of** z.

Definition 11.3 Let $\mathscr{D}$ be a domain, and $\mathscr{Z} = \{z^{(1)}, z^{(2)}, \ldots, z^{(n)}\}$ be an n-point set, where each $z^{(i)} \in \mathscr{D}$. Define

$$\mathscr{M}_\lambda(\mathscr{Z}) = C + \bigvee_{z^{(i)} \in \mathscr{Z}} \mathscr{B}_{z^{(i)}} + \lambda \bigvee_{z^{(i)} \in \mathscr{Z}} \mathscr{P}_{z^{(i)}}, \tag{11.3}$$

where C is a constant, λ is a positive parameter and "$\bigvee$" represents an overall function (such as summation, integral, maximum or minimum), then $\mathscr{M}_\lambda(\mathscr{Z})$ is called the **λ*e*-discrepancy of set** $\mathscr{Z}$.

Definition 11.4 Let $\mathscr{D}$ be a domain, and $\mathscr{Z} = \{z^{(1)}, z^{(2)}, \ldots, z^{(n)}\}$ be an n-point set, where each $z^{(i)} \in \mathscr{D}$. If $\mathscr{M}_\lambda(\mathscr{Z})$ can achieve the best value (minimum or maximum with respect to the choices of the overall function "$\bigvee$") over $\mathscr{D}$, then $\mathscr{Z}$ will be called a unform design on $\mathscr{D}$ under the λ-discrepancy.

Remark 11.1 the two distance function $\boldsymbol{d}_B(\cdot,\cdot)$ and $\boldsymbol{d}_P(\cdot,\cdot)$ in the above definitions can be different. Obviously, uniform designs under the λ-discrepancy may vary from different choices of the two distance functions $\boldsymbol{d}_B(\cdot,\cdot)$ and $\boldsymbol{d}_P(\cdot,\cdot)$. However, for uniform design on manifold, the natural selection of $\boldsymbol{d}_B(\cdot,\cdot)$ and $\boldsymbol{d}_P(\cdot,\cdot)$ is the geodesic distance function. Throughout this paper, we will take both of these two functions as the same geodesic distance function defined on the unit spherical surface.

Remark 11.2 different overall function "$\bigvee$" can be chosen for different purpose. Hickernell [10, 11] defined many modified discrepancies, i.e, overall functions, based

on different types of kernels, i.e, distance functions, on the unit cube. However, these discrepancies may not be suitable for uniform designs on manifolds. Throughout this paper, we will follow the idea of Johnson et al. [12], and use the maximin criterion to define the overall function. That is to say, we will first define the overall boundary deviation as the minimum distance over the domain boundary, and define the overall point deviation as the minimum distance among all distinct (otherwise the overall point deviation shall always be zero) pairwise points in the point set $\mathscr{Z}$. Then we try to maximize these two overall functions.

The λ-discrepancy in Definition 11.2 tries to balance the both the boundary effect and the point effect simultaneously, and thus has clear geometrical meanings. For clarity, we will divide into two cases to investigate uniform designs on spherical surface and on semi-spherical surface, respectively.

11.3 Uniform Design on Semi-spherical Surface

In this section, we will use the λ-discrepancy defined in the previous section as the measure of uniformity to consider uniform designs on the unit semi-spherical surface. To make it clear, throughout this section, the unit semi-spherical surface considered will always be assumed to be the above one, i.e, the point set of the domain is

$$\mathscr{U}_+^3 = \{(z_1, z_2, z_3) : z_3 \geq 0 \text{ and } z_1^2 + z_2^2 + z_3^2 = 1\}.$$

So the boundary of the domain is a circle:

$$\partial\mathscr{U}_+^3 = \{(z_1, z_2, z_3) : z_3 = 0 \text{ and } z_1^2 + z_2^2 + z_3^2 = 1\}.$$

As stated in the previous section, here we use maximin criterion [12] to measure the uniformity of the design. That is to say, the λ-discrepancy in (11.3) becomes the following form:

$$\mathscr{M}_\lambda(\mathscr{Z}) = C + \min_{z^{(i)}\in\mathscr{Z}} \min_{z^{(j)}\in\partial\mathscr{U}_+^3} \boldsymbol{d}_B(z^{(i)}, z^{(j)}) + \lambda \min_{z^{(i)}\in\mathscr{Z}} \min_{z^{(j)}\neq z^{(i)}} \boldsymbol{d}_P(z^{(i)}, z^{(j)}). \quad (11.4)$$

Here the distance functions $\boldsymbol{d}_B(\cdot,\cdot)$ and $\boldsymbol{d}_P(\cdot,\cdot)$ in (11.4) are both chosen to be the geodesic distance on the unit spherical surface. It is well-known that the geodesics on spherical surface are great circles.

Let $z^{(1)} = (x_1, x_2, x_3)$ and $z^{(2)} = (y_1, y_2, y_3)$ be two points on the unit spherical surface. Denote $\boldsymbol{d}_e(z^{(1)}, z^{(2)}) = \sqrt{((x_1 - y_1)^2 + (x_2 - y_2)^2 + (x_3 - y_3)^2)}$ as the Euclidean distance between $z^{(1)}$ and $z^{(2)}$. Then the geodesic distance between $z^{(1)}$ and $z^{(2)}$ is actually the length of arc $\overset{\frown}{z^{(1)}z^{(2)}}$ on the unit spherical surface, i.e,

$$\boldsymbol{d}_P(z^{(1)}, z^{(2)}) = \arccos\left[1 - 0.5\,\boldsymbol{d}_e^2(z^{(1)}, z^{(2)})\right].$$

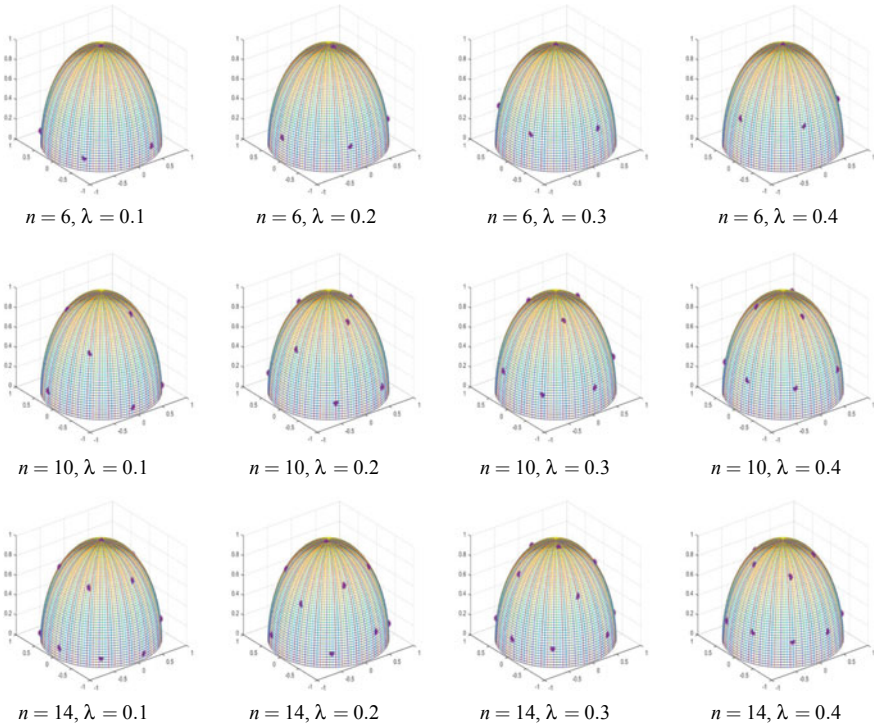


Fig. 11.2 Searching results for different number of points and λ's

Moreover, for any fixed point $\boldsymbol{z}^{(i)} = (x_1, x_2, x_3)$, its nearest point within the boundary $\partial\mathscr{U}_+^3$ will be $\boldsymbol{z}_0^{(i)} = (x_1', x_2', 0)$, where $x_1' = \frac{x_1}{\sqrt{x_1^2+x_2^2}}$ and $x_2' = \frac{x_2}{\sqrt{x_1^2+x_2^2}}$, thus

$$\min_{\boldsymbol{z}^{(j)} \in \partial\mathscr{U}_+^3} \boldsymbol{d}_B(\boldsymbol{z}^{(i)}, \boldsymbol{z}^{(j)}) = \boldsymbol{d}_P(\boldsymbol{z}^{(i)}, \boldsymbol{z}_0^{(i)}).$$

Now the objective function, i.e, the λ-discrepancy $\mathscr{M}_\lambda(\mathscr{Z})$ in (11.4), can be fully determined if an n-point set is given. So we can use a standard optimization algorithm to search for a design with less λ-discrepancy. The basic framework of the pseudo code is presented in Algorithm 5.

For the sake of simplicity, here we implement the algorithm on restricted lattice points. The candidates are equal distance grid points in the polar coordinate system. The searching results of Algorithm 5 are shown in Fig. 11.2. It can easily be seen that when the parameter λ becomes larger, the points tends to be scattered away from the boundary. This seems reasonable as we add more penalty to the boundary deviation when the points are near the boundary. Such a flexible solution can provide an alternative way to control the experimental points according to specific requirements in different real applications.

Algorithm 5 Pseudo code for prototype local search heuristic.

1: Initialize λ and τ (number of iterations)
2: Generate a starting design $\mathscr{Z}^c$ and let $\mathscr{Z}^{\max} := \mathscr{Z}^c$
3: **while** number of iterations $< \tau$ **do**
4: Generate $\mathscr{Z}^{\text{new}} \in \mathscr{N}(\mathscr{Z}^c)$ (neighbor to current solution)
5: Compute $\nabla = \mathscr{M}_\lambda(\mathscr{Z}^{\text{new}}) - \mathscr{M}_\lambda(\mathscr{Z}^c)$ and generate u (uniform random variable)
6: **if** $(\nabla > 0)$ or acceptance criterion(∇, u) met **then** $\mathscr{Z}^c = \mathscr{Z}^{\text{new}}$
7: **if** $\mathscr{Z}^c > \mathscr{Z}^{\max}$ **then** $\mathscr{Z}^{\max} := \mathscr{Z}^c$
8: **end while**

11.4 Uniform Design on Spherical Surface

Now we will consider uniform designs on the unit spherical surface. Similar with the case in the previous section, we also take the maximin criterion to define the λ-discrepancy. Since the unit spherical surface has no boundary, the λ-discrepancy of (11.3) will be equivalent with the following quantity:

$$\mathscr{M}_\lambda(\mathscr{Z}) = \min_{z^{(i)} \in \mathscr{Z}} \min_{z^{(j)} \neq z^{(i)}} \boldsymbol{d}_P(z^{(i)}, z^{(j)}), \tag{11.5}$$

where the distance function $\boldsymbol{d}_p(\cdot, \cdot)$ also represents the geodesic distance on the unit spherical surface.

Spherical trigonometry theory [21] tells us that there are many existing properties related to angles, sides and areas of spherical triangles and other configurations. These properties can not only help calculate the λ-discrepancies during our searching for uniform designs on the unit spherical surface numerically, but also provide upper bounds. In fact, Tammes [20] firstly considered the problem of arranging n points on a unit sphere which maximizes the minimum distance between any two distinct points. It is not an easy task to determine the best arrangement of the Tammes problem for some sporadic numbers of points, let alone to provide a systematical solution. For example, Musin and Tarasov [16, 17] provided final solutions to the Tammes problem when the numbers of points are thirteen and fourteen, respectively. The current paper does not study the Tammes problem theoretically and only aims to give an algorithmic solution to it. To evaluate our searching results, here we present some upper bounds of the λ-discrepancies.

Theorem 11.1 *Let $\mathscr{Z}$ be n points on the unit spherical surface $\mathscr{U}^3$, and $\mathscr{M}_\lambda(\mathscr{Z})$ be its λ-discrepancy as defined in (11.5). Then we have*

$$\mathscr{M}_\lambda(\mathscr{Z}) \leq 4 \arcsin(\sqrt{1/n}). \tag{11.6}$$

Proof Denote $r = \mathscr{M}_\lambda(\mathscr{Z})/2$. Since $0 \leq \mathscr{M}_\lambda(\mathscr{Z}) \leq 2\pi$, we have $0 \leq r \leq \pi$. For each point $z \in \mathscr{Z}$ on the unit spherical surface, define a set $\Omega_z = \{x \in \mathscr{U}^3 : \boldsymbol{d}_p(x, z) \leq r\}$. Easy to see, all points of Ω_z form a spherical crown. Thus the area of Ω_z is $A_z = 4\pi \sin^2(r/2)$. Sum up the area of all these spherical crowns, we

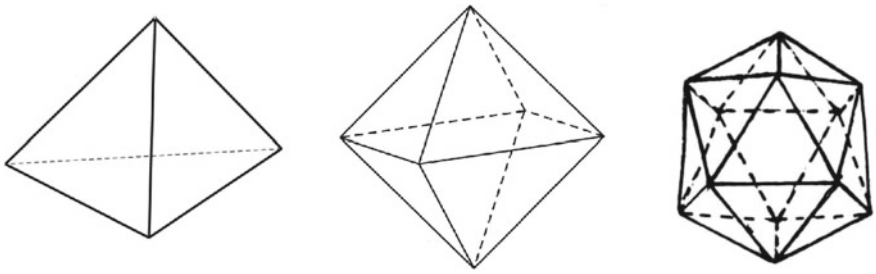


Fig. 11.3 Triangulations of regular polyhedrons with four, six and twelve points

have $nA_z \leq 4\pi$, where 4π represents the total area of the unit spherical surface. So $n \leq 1/\sin^2(r/2)$, i.e, $\mathscr{M}_\lambda(\mathscr{Z}) = 2r \leq 4\arcsin(\sqrt{1/n})$. □

The proof of Theorem 11.1 is quite intuitive, however, the bound of (11.6) can be further improved. As a matter of fact, many authors have provided upper bounds for the Tammes problem using graph theory, convex optimization and other techniques. Specifically, the following result was stated in Fejes-Tath [8].

Theorem 11.2 *Let $\mathscr{Z}$ be n points on the unit spherical surface, and $\mathscr{M}_\lambda(\mathscr{Z})$ be its λ-discrepancy as defined in (11.5). Then we have*

$$\mathscr{M}_\lambda(\mathscr{Z}) \leq \arccos[(cot^2\omega - 1)/2], \tag{11.7}$$

where $\omega = \frac{n}{n-2} \cdot \frac{\pi}{6}$.

The proof of Theorem 11.2 is not straightforward. Here we only give some explanation. The right hand side of (11.7) is the side length of an equilateral spherical triangle of area $\frac{4\pi}{(2n-4)}$, where 4π means the total area of the unit spherical surface and $2n-4$ represents the number of triangular faces induced by the n points. Theorem 11.2 says that when all the $2n-4$ triangular faces are equilateral spherical triangles with the same side length, the λ-discrepancy will achieve the upper bound (11.7). As it has been pointed out in many existing papers, when the number of points are four, six and twelve, the λ-discrepancies of the regular polyhedrons reach the upper bound (11.7). The triangulations of these regular polyhedrons are illustrated in Fig. 11.3, respectively.

Implement similar pseudo code as that of Algorithm 5, we can obtain a series of uniform designs on the unit spherical surface. Table 11.1 shows the numerical results for designs with different number of points. Notice that the values in the second and the third columns of Table 11.1 represent the λ-discrepancies of the resultant designs obtained by the inverse transformation from $\mathscr{C}^2$ and by implementing Algorithm 5, respectively. Easy to see, the algorithmic approach should be recommended. In fact, when the number of points are eight and twenty, the λ-discrepancies of the resultant

Table 11.1 Searching results of uniform designs on the unit spherical surface

#points	Transform	**Algorithm**	Bound (11.6)	Bound (11.7)	Polyhedron
4	1.633435	**1.908769**	2.094395	1.910633	1.910633
6	1.094689	**1.566865**	1.682137	1.570796	1.570796
8	0.822482	**1.299689**	1.445468	1.359080	1.230959
10	0.740723	**1.146458**	1.287002	1.214081	–
12	0.548902	**1.092115**	1.171371	1.107149	1.107149
14	0.525865	**0.950100**	1.082199	1.024176	–
16	0.461221	**0.888048**	1.010721	0.957398	–
18	0.358579	**0.834576**	0.951765	0.902163	–
20	0.434371	**0.795415**	0.902054	0.855491	0.7297277

designs are even better than those of polyhedrons. The fourth and the fifth columns of Table 11.1 list the upper bounds in (11.6) and (11.7), respectively. Compared with the former, the latter shall be much better.

11.5 Conclusion and Discussion

In this paper, we introduce a general definition of discrepancy based on geodesic distance to measure the uniformity of designs on manifold. We provide an algorithmic approach of a unified framework to search for low-discrepancy designs on the unit semi-spherical surface as well as on the unit spherical surface. Numerical results show the effectiveness of our proposed algorithm.

Some issues reported in this paper can be further investigated. For example, here we use the maximin criterion to define the overall function for the λ-discrepancy (11.3). However, using geodesic distance on specific manifold, criteria including minimax, mean squared-error [18] and entropy [19] can also be defined as the objective functions. Moreover, during the implementation of the algorithm, we restrict the candidates within equal distance grid points in the polar coordinate system. Such an approach may reduce the calculation burden, it can also bring negative effect on the λ-discrepancies of the designs.

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