Interdisciplinary Information Sciences Vol. 24, No. 2 (2018) 181–184

ISSN 1340-9050 print/1347-6157 online
DOI 10.4036/iis.2018.S.02

SHORT COMMUNICATION

On Explicit Construction of Simplex t-designs

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A finite subset X of the n-dimensional simplex is called a simplex t-design if the integral of any polynomial of degree at most t over the simplex is equal to the average value of the polynomial over the set X. Although these designs on a simplex are tightly connected to several other topics in mathematics, such as spherical designs, an explicit construction of such designs is not well-studied. In this paper, we will explicitly construct such designs using a union of sets consisting of elements whose coordinates are a cyclic permutation of a particular point. By choosing such a set, the conditions of a set to be a simplex t-design can be reduced to a system of t equations. Solving these system of equations, we managed to explicitly construct simplex 2-designs on a simplex of an arbitrary dimension.

KEYWORDS: simplex, cubature formula, spherical design, averaging sets, explicit construction

1. Introduction

In 1955, Claringbold [4] coined the term simplex design in his study of joint action by means of an appropriate experimental design. This term is used for any N experimental points on the simplex. A related study on polynomials on simplex is also studied in [8]. Inspired by these results, we define simplex design in a more formal term. For a positive integer n, we define the simplex in $\mathbb{R}^n$ as follows:

$$\Delta^{n-1} = \left\{ (x_1, \ldots, x_n) \in \mathbb{R}^n \mid \sum_{i=1}^{n} x_i = 1 \text{ and } x_i \geq 0 \text{ for all } i \right\}.$$

A *simplex t-design* on Δ^{n-1} is defined as a finite set of points $X \subseteq \Delta^{n-1}$ for which

$$\frac{1}{\sigma(\Delta^{n-1})} \int_{\Delta^n} f(x) \mathrm{d}\sigma(x) = \frac{1}{|X|} \sum_{x \in X} f(x) \tag{1.1}$$

holds for all polynomials $f(x) = f(x_1, x_2, \ldots, x_n)$ of degree at most t, where σ denotes the surface measure on Δ^{n-1}. This definition can also be seen as a cubature rule of degree t on the n-dimensional simplex as thoroughly studied in [7]. Designs on a simplex are also tightly connected to several other topics in mathematics, such as spherical designs and isometric embeddings of the classical finite dimensional Banach spaces [5, 6].

Our interest in this topic originated from the fact that such a simplex t-design is closely related to the construction of spherical t-designs [1]. An explicit construction of such designs will result in an explicit construction of spherical designs with varied strength and dimensions. The most straightforward way of constructing a simplex t-design is to solve the moment equations that match the integral and the cubature sum for all polynomials up to degree t. The difficulty, however, lies in that the number of equations increase exponentially as t increase. To prevent this, we will restrict the set of points such that the number of equations to be solved is equal to the strength of the design. These equations then can be solved, even mostly only by numerical means and for cubature rules of moderate degrees in lower dimensions (see, for example, [10] for one of the latest effort in this direction). In the later section, we will also provide some explicit solutions for small t and n.

The organization of this paper is as follows. The next section is preliminary, where we sum up the background on cubature rules, mainly using a generalization of the beta function. Our main result and its accompanying lemma are given in Section 3. The explicit result then is given in in Section 4.

2. Preliminaries

Our construction of simplex designs is tightly related to some manipulation of the gamma and beta functions. In this

Received July 17, 2018; Accepted July 23, 2018; J-STAGE Advance published August 25, 2018
2010 Mathematics Subject Classification: Primary 05B30, Secondary 65D32
As International Research Fellow of the Japan Society for the Promotion of Science, this work is supported by Open Partnership Joint Research Project "Extremal graph theory, algebraic graph theory and mathematical approach to network science" (2017–2018).
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section, we will provide some basic facts about those two functions and some related identities.

Let Γ be the gamma function. It is well-known that $\Gamma(\frac{1}{2}) = \sqrt{\pi}$ and for $x > 1$, $\Gamma(x) = (x-1)\Gamma(x-1)$. For $\alpha_i > 1$, $1 \le i \le n$, we define the multivariate beta function as follows:

$$\mathrm{B}((\alpha_i)_{i=1}^n) := \frac{\prod_{i=1}^n \Gamma(\alpha_i)}{\Gamma\left(\sum_{i=1}^n \alpha_i\right)}.$$

We can also check that

$$\mathrm{B}((\alpha_l)_{l=1}^n) = \sum_{l=1}^n \mathrm{B}(\alpha_1 + \delta_{l1}, \alpha_2 + \delta_{l2}, \ldots, \alpha_n + \delta_{ln}) \tag{2.1}$$

where δ_{li} is the Kronecker delta. An integral representation of this beta function can be given as follows.

$$\mathrm{B}((\alpha_i)_{i=1}^n) = \frac{1}{(n-1)!\sigma(\Delta^{n-1})} \int_{\Delta^{n-1}} \left(\prod_{i=1}^n x_i^{\alpha_i - 1}\right) \mathrm{d}\sigma(x). \tag{2.2}$$

The detail of this representation can be found in [9, p. 222]. One can notice that the right-hand side of this equation is in the form of an integral over a simplex and we will use this to simplify our requirements for a set to be a simplex design.

We note that due to the linearity of the summation and integral in (1.1), to show that a set $X \subseteq \Delta^{n-1}$ is a simplex t-design, it is enough to verify (1.1) for all monomials of degree at most t. Now by (2.2), this is equivalent to

$$\frac{1}{|X|} \sum_{x \in X} x_1^{k_1} x_2^{k_2} \cdots x_n^{k_n} = (n-1)!\mathrm{B}((k_i + 1)_{i=1}^n) \qquad \left(0 \le \sum_{i=1}^n k_i \le t\right). \tag{2.3}$$

3. Method of Construction

In this section, we manipulate both sides of (1.1) using some properties of the beta function, then the number of required equations is reduced to t. Throghout this section, let C_n denote a cyclic group of order n.

Lemma 3.1. *Let $n, k \in \mathbb{Z}_{>0}$, $r_1, r_2 \in \mathbb{R}$. Define*

$$V := \mathbb{R}[x_1, x_2, \ldots, x_n] \Big/ \left(\sum_{i=1}^n x_i - 1\right),$$

$$F(k_1, k_2, \ldots, k_n) := r_1 \sum_{\pi \in C_n} x_{\pi(1)}^{k_1} x_{\pi(2)}^{k_2} \cdots x_{\pi(n)}^{k_n} - r_2 \mathrm{B}((k_i + 1)_{i=1}^n) \in V.$$

Let V_k be a subspace of V spanned by $F(j, 0, \ldots, 0)$, $0 \le j \le k$. Then, for non-negative integers $k_1, \ldots, k_n$ such that $\sum_{i=1}^n k_i = k$, one has $F(k_1, \ldots, k_n) \in V_k$.

Proof. As an element in V,

$$\begin{aligned}\sum_{\pi \in C_n} x_{\pi(1)}^{k_1} x_{\pi(2)}^{k_2} \cdots x_{\pi(n)}^{k_n} &= \left(\sum_{\pi \in C_n} x_{\pi(1)}^{k_1} x_{\pi(2)}^{k_2} \cdots x_{\pi(n)}^{k_n}\right)\left(\sum_{j=1}^n x_j\right) \\ &= \sum_{l=1}^n \sum_{\pi \in C_n} x_{\pi(1)}^{k_1 + \delta_{l1}} x_{\pi(2)}^{k_2 + \delta_{l2}} \cdots x_{\pi(n)}^{k_n + \delta_{ln}}.\end{aligned}$$

Then, by (2.1),

$$F(k_1, k_2, \ldots, k_n) = \sum_{l=1}^n F(k_1 + \delta_{l1}, k_2 + \delta_{l2}, \ldots, k_n + \delta_{ln}). \tag{3.1}$$

Let $>_l$ be the lexicographical ordering on $\mathbb{Z}_{\ge 0}^n$. We will prove $F(k_1, \ldots, k_n) \in V_k$ by double induction on k and the reverse lexicographical ordering of $(k_1, \ldots, k_n)$ whose sum is k.

Note that for any $(k_1, \ldots, k_n) \in \mathbb{Z}_{\ge 0}^n$, with $\sum_{i=1}^n k_i = k$,

$$(k, 0, \ldots, 0) >_l (k_1, \ldots, k_n)$$

unless $k_2 = k_3 = \cdots = k_n = 0$ and the statement is trivially true for $(k, 0, \ldots, 0)$. Now, assume that $F(k_1', \ldots, k_n') \in V_k$ for $(k_1', \ldots, k_n') \in \mathbb{Z}_{\ge 0}^n$ such that $\sum_{i=1}^n k_i' \le k - 1$ or $\sum_{i=1}^n k_i' = k$ and $(k_1', \ldots, k_n') >_l (k_1, \ldots, k_n)$. Pick $a \in \{2, \ldots, n\}$ so that $k_a \neq 0$. Choose $\pi \in C_n$ in such a way that $\pi(n) = a$. Then,

$$\begin{aligned} F(k_1,k_2,\dots,k_n) &= F(k_{\pi(1)},k_{\pi(2)},\dots,k_{\pi(n)}) \\ &= F(k_{\pi(1)},\dots,k_{\pi(n-1)},k_{\pi(n)}-1) - \sum_{i=1}^{n-1} F(k_{\pi(1)}+\delta_{i1},\dots,k_{\pi(n-1)}+\delta_{i,n-1},k_{\pi(n)}-1) \end{aligned}$$

by (3.1). Since $\sum_{i=1}^{n} k_{\pi(i)} - 1 = k-1$, we have $F(k_{\pi(1)},\dots,k_{\pi(n-1)},k_{\pi(n)}-1) \in V_{k-1}$. Also, for $i \in \{1,\dots,n-1\}$, we have

$$(k_{\pi(1)}+\delta_{i1},\dots,k_{\pi(n-1)}+\delta_{i,n-1},k_{\pi(n)}-1) >_l (k_{\pi(1)},\dots,k_{\pi(n-1)},k_{\pi(n)}).$$

Then, by induction hypotheses, $F(k_{\pi(1)}+\delta_{i1},\dots,k_{\pi(n-1)}+\delta_{i,n-1},k_{\pi(n)}-1) \in V_k$. Thus,

$$F(k_{\pi(1)},\dots,k_{\pi(n-1)},k_{\pi(n)}-1) - \sum_{i=1}^{n-1} F(k_{\pi(1)}+\delta_{i1},\dots,k_{\pi(n-1)}+\delta_{i,n-1},k_{\pi(n)}-1) \in V_k.$$

This completes the induction. □

Theorem 3.2. *Let $n,s,t \in \mathbb{Z}_{>0}$, $n \geq 2$, $(x_{i,j})_{1\leq i\leq s,1\leq j\leq n} \in (0,1)^{s\times n}$ where $\sum_{j=1}^{n} x_{i,j} = 1$ for all i. Also, let*

$$X = \{(x_{i,\pi(1)},x_{i,\pi(2)},\dots,x_{i,\pi(n)}) \in \mathbb{R}^n \mid 1 \leq i \leq s, \pi \in C_n\}.$$

Then, the multiset X is a simplex t-design if and only if

$$\frac{1}{sn}\sum_{i=1}^{s}\sum_{j=1}^{n} x_{i,j}^k = \frac{\Gamma(n)\Gamma(k+1)}{\Gamma(n+k)} \quad (2 \leq k \leq t). \tag{3.2}$$

Proof. Let $2 \leq k \leq t$ and $(k_1,\dots,k_n) \in \mathbb{Z}_{\geq 0}^n$ such that $\sum_{j=1}^{n} k_j = k$. Define

$$F_i(k_1,\dots,k_n) = \frac{1}{n}\sum_{\pi\in C_n} x_{i,\pi(1)}^{k_1}x_{i,\pi(2)}^{k_2}\cdots x_{i,\pi(n)}^{k_n} - (n-1)!\mathrm{B}((k_j+1)_{j=1}^n) \quad (1 \leq i \leq s).$$

We can rewrite (3.2) as

$$\sum_{i=1}^{s} F_i(k,0,\dots,0) = 0 \quad (1 \leq k \leq t). \tag{3.3}$$

Note that by Lemma 3.1, with $r_1 = \frac{1}{n}$, $r_2 = (n-1)!$, there exists $c_j \in \mathbb{R}$, $0 \leq j \leq t$, such that

$$F(k_1,\dots,k_n) = \sum_{j=0}^{k} c_j F(j,0,\dots,0).$$

Since $X \subset \Delta^{n-1}$, we may evaluate both sides at $(x_{i,1},\dots,x_{i,n})$ to obtain

$$F_i(k_1,\dots,k_n) = \sum_{j=0}^{k} c_j F_i(j,0,\dots,0) \quad (1 \leq i \leq s). \tag{3.4}$$

We assume (3.3) holds. By taking summation over i on both sides of (3.4), we have (2.3). Conversely, assume (2.3) holds. Then, (3.3) is just a special case $(k_1,\dots,k_n) = (k,0,\dots,0)$ of (2.3). □

In this theorem, if we set all x_is to be the same, except x_n, we have a system of t equations with t variables. We expect this system to have a solution, thus one can obtain a simplex t-design on Δ^n with $n(t-1)$ points.

4. Explicit Construction of Simplex t-design

Even though we managed to reduce the number of required equations for a set to be a simplex design, it is still difficult to solve moment equations that are nonlinear in the coordinate of points. Nevertheless, we will provide some explicit results for some small t.

With $t = 2$ and $s = 1$ in Theorem 3.2, we take all $x_i s$ to be the same, except x_n. We obtain the following corollary.

Corollary 4.1. *Let $n \in \mathbb{Z}_{>0}$, $n \geq 2$, and π be a cyclic permutation of order n. The set*

$$X = \{\pi^j(a,a,\dots,a,1-(n-1)a) \mid 0 \leq j \leq n-1\} \quad \text{with} \quad a \in \{\tfrac{1}{n} \pm \tfrac{1}{n\sqrt{n+1}}\}$$

is a simplex 2-design on Δ^{n-1}.

The following result can be obtained by taking $n = 3$ in Theorem 3.2:

Corollary 4.2. *Let $s,t \in \mathbb{Z}_{>0}$, $a_i,b_i \in (0,1]$ for $1 \leq i \leq s$. Also, let*

$$X = \bigcup_{i=1}^{s}\{(a_i,b_i,1-a_i-b_i),(1-a_i-b_i,a_i,b_i),(b_i,1-a_i-b_i,a_i)\}.$$

Then, the multiset X is a simplex t-design on Δ^2 *if and only if*

$$\frac{1}{3s}\sum_{i=1}^{s}(a_i^k + b_i^k + (1-a_i-b_i)^k) = \frac{2}{(k+2)(k+1)} \quad (2 \le k \le t). \tag{4.1}$$

Taking $s = 1$ and $t = 3$, the system of equations (4.1) can be reduced to the polynomial $60x^3 - 60x^2 + 15x - 1$ whose roots are $a_1, b_1, 1 - a_1 - b_1$. These roots all lie in interval $(0, 1]$, hence we obtain a simplex 3-design on Δ^2 with 3 points.

Further, if we take $a_i = b_i$ and $s = t - 1$ in Corollary 4.2, we will have a system of $t - 1$ equations with $t - 1$ variables. It turns out that these systems of equations do have a solution for small t. The following table shows the value of some t and its corresponding numerical solution a_is for a set X as in Corollary 4.2 to be a simplex t-design:

t	a_1	a_2	a_3	a_4	a_5
2	$\frac{1}{2}$ or $\frac{1}{6}$				
3	0.446334	0.126485			
4	0.476589	0.257088	0.094591		
4	0.456393	0.433938	0.092359		
5	0.489178	0.385410	0.184975	0.084132	
5	0.490566	0.270260	0.192580	0.083133	
6	0.499627	0.393244	0.211612	0.173352	0.074035

Although a better computational power is needed to find a_i for larger t, this experimental result shows that for small t, we only need $3(t-1)$ points to construct a simplex t-design on Δ^2. The fact that the number of points is linear in t allows us to construct a spherical t-design on S^5 of size $3(t+1)^3(t-1)$ (see [2]). If this is true for arbitrarily large t, it will give a better asymptotic bound than that of [3] which states that for each $N \ge ct^5$, there exists a spherical t-design in the sphere S^5 consisting of N points, where c is a constant.

Acknowledgments

The author would like to thank Prof. Akihiro Munemasa as the author's Ph.D advisor for giving continuous help and guidance throughout the research process. Also, as International Research Fellow of the Japan Society for the Promotion of Science, this work was supported by Open Partnership Joint Research Project "Extremal graph theory, algebraic graph theory and mathematical approach to network science" (2017–2018).

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