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Article

A REFINEMENT OF THE CONJECTURE ON THE PSEUDO COMPONENT TRANSFORMATION ON THE LATTICE POINTS IN THE SIMPLEX

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Abstract: We consider mixture experiments in which the proportions of the components must be non-negative and their sum must equal one. Thus, the experimental region for a mixture of components is a simplex. Li and Zhang (2017) made the conjecture that the pseudo component transformation of the lattice points in the simplex has a special property. In this paper, we show that this conjecture is not true in general. Furthermore, we refine this conjecture and prove the refined conjecture.

Keywords: Mixture experiments; Lattice points; Pseudo component transformation

1. Introduction

Mixture experiments are performed in many areas of product development and improvement (see, for example, [2,7]). In a mixture experiment, two or more ingredients (or components) are mixed or blended together in varying proportions to form an end product. In this experiment, the response is a function of the proportions of the components, i.e., the response depends only on the proportion of the components in the mixture and not on the total amount of the mixture. These proportions must be non-negative and their sum must equal one. The experimental region of a mixture experiment can usually be expressed as

$$\mathcal{X} = \left\{ (x_1, \ldots, x_q) : \sum_{i=1}^{q} x_i = 1, x_i \geq 0, i = 1, \ldots, q, C\text{'s} \right\},$$

where there are q components involved in the experiment, x_i represents the proportion of the ith component in the total amount of the mixture, $i = 1, \ldots, q$, and C's are some other constraints for $x_1, \ldots, x_q$ (see Liu and Liu [6]). Note that the conditions $\sum_{i=1}^{q} x_i = 1$ and $x_i \geq 0$, $i = 1, \ldots, q$ are the necessary conditions for a mixture experiment, but the conditions C's are not necessary and can have any form according to the practical situation.

We will focus on the case when the mixture components are subject to the only constraint that they must sum to one. In this case, i.e., if $\mathcal{X}$ is without constraints C's, we will represent $\mathcal{X}$ as S^{q-1}, which is called a $(q-1)$-dimensional simplex. The design of mixture experiments has been investigated by many authors. For the construction of mixture designs on S^{q-1}, Scheffé [8] introduced the so-called simplex lattice design, which gives a uniformly spaced distribution of points (called $\{q, m\}$ lattice points) over the simplex. Let $\mathcal{L}\{q, m\}$ be the $\{q, m\}$ simplex lattice, which consists of $\{q, m\}$ lattice points in S^{q-1}. Based on the method of Scheffé type design, Li and Zhang [5] extended

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it and defined a kind of design, named pseudo component transformation design. For $\lambda \geq 0$ and $\mathbf{x}_0 = (\frac{1}{q}, \ldots, \frac{1}{q}) \in S^{q-1}$, let $\mathcal{Z}(\mathcal{L}\{q,m\}, \mathbf{x}_0, \lambda)$ be a pseudo component transformation of $\mathcal{L}\{q,m\}$. Li and Zhang [5] made the conjecture about $MD(\mathcal{L}\{q,m\})$ and $MD(\mathcal{Z}(\mathcal{L}\{q,m\}, \mathbf{x}_0, \lambda))$, where MD denotes the maximum (squared) distance. The formal definitions of $\mathcal{L}\{q,m\}$, $\mathcal{Z}(\mathcal{L}\{q,m\}, \mathbf{x}_0, \lambda)$, $MD(\mathcal{L}\{q,m\})$ and $MD(\mathcal{Z}(\mathcal{L}\{q,m\}, \mathbf{x}_0, \lambda))$ will be given in Section 2.

The maximum distance is one of the criteria proposed for measuring the uniformity of designs in experimental regions. In general, it is difficult to calculate the maximum distance in most practical problems. In this paper, we calculate $MD(\mathcal{L}\{q,m\})$ and $MD(\mathcal{Z}(\mathcal{L}\{q,m\}, \mathbf{x}_0, \lambda))$. By using the formulas for $MD(\mathcal{L}\{q,m\})$ and $MD(\mathcal{Z}(\mathcal{L}\{q,m\}, \mathbf{x}_0, \lambda))$, we prove that the conjecture of Li and Zhang [5] is not true in general. Furthermore, we refine this conjecture and prove the refined conjecture.

The simplex lattice designs have natural symmetric properties and are the most natural designs for mixture experiments. This paper investigates the uniformity of the design in experimental regions in relation to the pseudo component transformation of the simplex lattice design. The symmetric properties inherent in the simplex lattice designs and the pseudo component transformations of the designs are used in the proof of our results.

The paper is organized as follows. In Section 2, we describe the conjecture of Li and Zhang [5] in detail. In Sections 3 and 4, we derive the formulas for $MD(\mathcal{L}\{q,m\})$ and $MD(\mathcal{Z}(\mathcal{L}\{q,m\}, \mathbf{x}_0, \lambda))$, respectively. By using these formulas, we refine the conjecture of Li and Zhang [5] in Section 5. Conclusions are given in Section 6.

2. Conjecture on the pseudo component transformation

Recall that the $(q-1)$-dimensional simplex, S^{q-1}, is given by

$$S^{q-1} = \Big\{\mathbf{x} = (x_1, \ldots, x_q) \in \mathbb{R}^q : \sum_{i=1}^{q} x_i = 1, x_i \geq 0, i = 1, \ldots, q\Big\}.$$

As mentioned in the Introduction, Scheffé [8] introduced the simplex lattice design (for applications and extensions see Gorman and Hinman [4]). The $\{q,m\}$ simplex lattice, denoted by $\mathcal{L}\{q,m\}$, is defined by

$$\mathcal{L}\{q,m\} = \Big\{\mathbf{x} \in \mathbb{R}^q : \mathbf{x} = (\frac{k_1}{m}, \ldots, \frac{k_q}{m}), \sum_{i=1}^{q} k_i = m, k_i \in \mathbb{Z}_+, i = 1, \ldots, q\Big\}.$$

The number of points in $\mathcal{L}\{q,m\}$ is $\binom{m+q-1}{m}$. Some $\{q,m\}$ simplex lattices for $q = 3$ and 4 are depicted in Scheffé [8] and Cornell [2].

Let $A \subset S^{q-1}$ and $\lambda \in [0, \infty)$ be the transform parameter. For a given reference point $\mathbf{x}_0 = (x_{01}, \ldots, x_{0q}) \in S^{q-1}$, a pseudo component transformation of the experimental region A is defined by

$$\mathcal{Z}(A, \mathbf{x}_0, \lambda) = \frac{\lambda}{\lambda+1}A + \frac{1}{\lambda+1}\mathbf{x}_0 = \Big\{\frac{\lambda}{\lambda+1}\mathbf{x} + \frac{1}{\lambda+1}\mathbf{x}_0 : \mathbf{x} \in A\Big\},$$

refer to Li and Zhang [5]. Many criteria have been proposed for measuring the uniformity of designs in experimental regions; for example, the mean squared error proposed by Fang and Wang [3], root mean squared distance, maximum distance, and average distance discrepancies proposed by Borkowski and Piepel [1]. We will focus on the maximum distance, which is defined below. Suppose $\mathcal{P} = \{\mathbf{y}_1, \ldots, \mathbf{y}_n\}$ denotes a design composed of n points in the simplex S^{q-1}, where $\mathbf{y}_i = (y_{i1}, \ldots, y_{iq})$, $1 \leq i \leq n$. The distance between a point $\mathbf{x} = (x_1, \ldots, x_q) \in S^{q-1}$ and the design $\mathcal{P}$ is defined as

$$d(\mathbf{x}, \mathcal{P}) = \min_{1 \leq i \leq n} d(\mathbf{x}, \mathbf{y}_i),$$

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where $d(\mathbf{x}, \mathbf{y}_i) = \| \mathbf{x} - \mathbf{y}_i \| = \sqrt{\sum_{j=1}^{q} (x_j - y_{ij})^2}$. Then the maximum (squared) distance is defined as

$$MD(\mathcal{P}) = \sup_{\mathbf{x} \in S^{q-1}} d^2(\mathbf{x}, \mathcal{P}).$$

In general, for $B \subset S^{q-1}$, the maximum distance is defined as

$$MD(B) = \sup_{\mathbf{x} \in S^{q-1}} d^2(\mathbf{x}, B),$$

where $d^2(\mathbf{x}, B) = \inf_{\mathbf{y} \in B} d^2(\mathbf{x}, \mathbf{y})$ with $d^2(\mathbf{x}, \mathbf{y}) = \| \mathbf{x} - \mathbf{y} \|^2$. Specifically,

$$MD(\mathcal{L}\{q, m\}) = \sup_{\mathbf{x} \in S^{q-1}} d^2(\mathbf{x}, \mathcal{L}\{q, m\}),$$
$$MD(\mathcal{Z}(\mathcal{L}\{q, m\}, \mathbf{x}_0, \lambda)) = \sup_{\mathbf{x} \in S^{q-1}} d^2(\mathbf{x}, \mathcal{Z}(\mathcal{L}\{q, m\}, \mathbf{x}_0, \lambda)).$$

Li and Zhang [5] made the following conjecture on the pseudo component transformation of the lattice points in the simplex.

Conjecture 1. *Let* $\mathbf{x}_0 = (\frac{1}{q}, \ldots, \frac{1}{q})$ *be the reference point in the simplex* S^{q-1}*. Then,*

(i) $\arg\min_{\lambda \in [0,\infty)} MD(\mathcal{Z}(\mathcal{L}\{q, m\}, \mathbf{x}_0, \lambda)) = m$*;*
(ii) $MD(\mathcal{Z}(\mathcal{L}\{q, m\}, \mathbf{x}_0, m)) = MD(\mathcal{L}\{q, m+1\}) = \frac{q-1}{q(m+1)^2}$.

As mentioned before, it is difficult in general to calculate the maximum distance in most practical problems. In the following two sections, we derive the formulas for $MD(\mathcal{L}\{q, m\})$ and $MD(\mathcal{Z}(\mathcal{L}\{q, m\}, \mathbf{x}_0, \lambda))$, respectively. We prove that Conjecture 1 is true for some special cases. Furthermore, we refine this conjecture and prove the refined conjecture.

Remark 1. The original statement of the first part of Conjecture 1 in Li and Zhang [5] is

$$\arg\min_{\lambda \in [0,\infty)} MD(\mathcal{Z}(\mathcal{L}\{q, m+1\}, \mathbf{x}_0, \lambda)) = m. \quad (1)$$

However, this seems to be a printing error. The correct equation should be

$$\arg\min_{\lambda \in [0,\infty)} MD(\mathcal{Z}(\mathcal{L}\{q, m\}, \mathbf{x}_0, \lambda)) = m, \quad (2)$$

as described in Conjecture 1(i). We can see by using Euclidean geometry in the plane that (2) is true when $q \leq 3$. However, (1) is not true for any $q \leq 3$.

3. Derivation of the formula for $MD(\mathcal{L}\{q, m\})$

In this section, we derive the formula for $MD(\mathcal{L}\{q, m\})$, the maximum distance between any point $\mathbf{x}$ in S^{q-1} and the design point of $\mathcal{L}\{q, m\}$ nearest to $\mathbf{x}$, as shown below in Theorem 1. The proof is given at the end of this section.

Theorem 1. $MD(\mathcal{L}\{q, m\})$ *is given by*

$$MD(\mathcal{L}\{q, m\}) = \frac{p_{q,m}(q - p_{q,m})}{qm^2},$$

where $p_{q,m} = \min\{m, \lfloor \frac{q}{2} \rfloor\}$.

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Before proving Theorem 1, we define a dense subset H_m^{q-1} of S^{q-1} and a function $\phi^{(m)} : H_m^{q-1} \to \mathcal{L}\{q,m\}$. Let

$$H_m^{q-1} = \{\mathbf{x} \in S^{q-1} : mx_i - \lfloor mx_i \rfloor, i = 1,\dots,q \text{ are all distinct}\}.$$

Note that H_m^{q-1} is a dense subset of S^{q-1} and can also be expressed as

$$H_m^{q-1} = \left\{\mathbf{x} \in \mathbb{R}_+^q : \mathbf{x} = (\frac{k_1}{m},\dots,\frac{k_q}{m}), \sum_{i=1}^{q} k_i = m, k_1,\dots,k_q \text{ have all different fractional parts}\right\}.$$

For $\mathbf{x} \in H_m^{q-1}$ and $0 \le r \le \frac{1}{m}$, let

$$s_r^{(m)}(\mathbf{x}) = \sum_{i=1}^{q} \frac{\lfloor m(x_i + r) \rfloor}{m}.$$

Then $s_r^{(m)}(\mathbf{x})$ is nondecreasing in r, piecewise constant in r with jump sizes being all $\frac{1}{m}$, and right-continuous in r. Also,

$$s_0^{(m)}(\mathbf{x}) = \frac{\sum_{i=1}^q \lfloor mx_i \rfloor}{m} \le \sum_{i=1}^{q} x_i \le \frac{\sum_{i=1}^q \lfloor mx_i + 1 \rfloor}{m} = s_{\frac{1}{m}}^{(m)}(\mathbf{x}).$$

Since $s_0^{(m)}(\mathbf{x}) \le 1 \le s_{\frac{1}{m}}^{(m)}(\mathbf{x})$, there exists $r^* \in [0, \frac{1}{m}]$ such that $s_{r^*}^{(m)}(\mathbf{x}) = 1$. For $\mathbf{x} \in H_m^{q-1}$, define

$$\phi_i^{(m)}(\mathbf{x}) = \frac{\lfloor m(x_i + r^*) \rfloor}{m}, \quad i = 1,\dots,q,$$

and $\phi^{(m)}(\mathbf{x}) = (\phi_1^{(m)}(\mathbf{x}),\dots,\phi_q^{(m)}(\mathbf{x}))$. Note that $\phi_i^{(m)}(\mathbf{x})$, $i = 1,\dots,q$, is well-defined. This can be verified as follows: If $s_{r_1}^{(m)}(\mathbf{x}) = s_{r_2}^{(m)}(\mathbf{x}) = 1$ and $0 \le r_1 \le r_2 \le \frac{1}{m}$, then $\frac{\lfloor m(x_i+r_1) \rfloor}{m} \le \frac{\lfloor m(x_i+r_2) \rfloor}{m}$, and

$$\sum_{i=1}^{q} \frac{\lfloor m(x_i + r_1) \rfloor}{m} = s_{r_1}^{(m)}(\mathbf{x}) = 1 = s_{r_2}^{(m)}(\mathbf{x}) = \sum_{i=1}^{q} \frac{\lfloor m(x_i + r_2) \rfloor}{m}.$$

Therefore, $\frac{\lfloor m(x_i+r_1) \rfloor}{m} = \frac{\lfloor m(x_i+r_2) \rfloor}{m}$, $i = 1,\dots,q$.

The following lemma shows that for $\mathbf{x} \in H_m^{q-1}$, $\phi^{(m)}(\mathbf{x})$ is the nearest point in S^{q-1} from $\mathbf{x}$. Although this lemma is not directly used in the proof of Theorem 1, it is included for completeness.

Lemma 1. *For* $\mathbf{x} \in H_m^{q-1}$*,*

$$d(\mathbf{x}, \phi^{(m)}(\mathbf{x})) = d(\mathbf{x}, \mathcal{L}\{q,m\}).$$

Proof. Let $\mathbf{y}$ be a point in $\mathcal{L}\{q,m\}$ such that $d(\mathbf{x},\mathbf{y}) = d(\mathbf{x}, \mathcal{L}\{q,m\})$. First, we show

$$x_i - \frac{\lfloor mx_i \rfloor}{m} < x_j - \frac{\lfloor mx_j \rfloor}{m} \quad \text{if } x_i > y_i \text{ and } x_j < y_j. \tag{3}$$

Suppose $x_i > y_i$, $x_j < y_j$ and $x_i - \frac{\lfloor mx_i \rfloor}{m} > x_j - \frac{\lfloor mx_j \rfloor}{m}$. Let

$$\tilde{y}_k = \begin{cases} y_i + \frac{1}{m} & \text{if } k = i, \\ y_j - \frac{1}{m} & \text{if } k = j, \\ y_k & \text{if } k \ne i, k \ne j. \end{cases}$$

Then, $\tilde{\mathbf{y}} \in \mathcal{L}\{q,m\}$ and $d(\mathbf{x},\mathbf{y}) > d(\mathbf{x},\tilde{\mathbf{y}})$, which is a contradiction. Hence, (3) is proved.

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Next, we show

$$|x_i - y_i| < \frac{1}{m}, \quad i = 1, \dots, q. \tag{4}$$

If $x_i \le y_i - \frac{1}{m}$ for some i, then we can choose j such that $x_j > y_j$. Let

$$y'_k = \begin{cases} y_i - \frac{1}{m} & \text{if } k = i, \\ y_j + \frac{1}{m} & \text{if } k = j, \\ y_k & \text{if } k \ne i, k \ne j. \end{cases}$$

Then, $\mathbf{y}' \in \mathcal{L}\{q, m\}$ and $d(\mathbf{x}, \mathbf{y}) > d(\mathbf{x}, \mathbf{y}')$, which is a contradiction. Hence, we have $x_i > y_i - \frac{1}{m}$ for all i. Similarly, we can show $x_i < y_i + \frac{1}{m}$ for all i. Therefore, (4) is proved. By (3) and (4), there exists $r \in [0, \frac{1}{m}]$ such that $\mathbf{y} = s_r^{(m)}(\mathbf{x})$. Since $\phi^{(m)}(\mathbf{x})$ is well-defined, we have $\mathbf{y} = \phi^{(m)}(\mathbf{x})$. □

To prove Theorem 1, we need the following two lemmas. The first lemma is used in the proof of the second lemma. The second lemma is used in the proof of Theorem 1.

Lemma 2. *For $l = 1, \dots, q-1$, let*

$$D_l = \{\mathbf{x} \in \mathbb{R}^q : x_1 \ge 0, \dots, x_l \ge 0, x_{l+1} \le 0, \dots, x_q \le 0, \sum_{i=1}^{q} x_i = 0, \max_{1\le i\le q} x_i - \min_{1\le i\le q} x_i \le 1\}.$$

Then $\max_{\mathbf{x}\in D_l} \|\mathbf{x}\|^2 = \frac{l(q-l)}{q}$.

Proof. Note that D_l is convex and compact. Since $\|\mathbf{x}\|^2$ is a convex function of $\mathbf{x}$, there exists an extreme point $\mathbf{x}^*$ of D_l such that $\max_{\mathbf{x}\in D_l} \|\mathbf{x}\|^2 = \|\mathbf{x}^*\|^2$. If $\mathbf{y} = (y_1, \dots, y_q)$ is a nonzero extreme point of D_l, then (i) $y_i = 0$ or $\max\limits_{1\le j\le l} y_j$ for all $i = 1, \dots, l$, (ii) $y_i = 0$ or $\min\limits_{l+1\le j\le q} y_j$ for all $i = l+1, \dots, q$, and (iii) $\max_{1\le i\le q} x_i - \min_{1\le i\le q} x_i = 1$. Suppose that $\mathbf{y}$ is a nonzero extreme point of D_l. Let l_1 be the number of positive components of $\mathbf{y}$ and let l_2 be the number of negative components of $\mathbf{y}$. Then $\max\limits_{1\le j\le q} y_j = \frac{l_2}{l_1+l_2}$ and $\min\limits_{1\le j\le q} y_j = \frac{-l_1}{l_1+l_2}$. Hence,

$$\|\mathbf{y}\|^2 = \frac{l_1 l_2}{l_1 + l_2} \le \frac{l(q-l)}{q}.$$

Note that $\mathbf{x}^* = (\underbrace{1 - \frac{l}{q}, \dots, 1 - \frac{l}{q}}_{l\text{-tuple}}, \underbrace{\frac{l}{q}, \dots, \frac{l}{q}}_{(q-l)\text{-tuple}})$ is an extreme point with $\|\mathbf{x}^*\|^2 = \frac{l(q-l)}{q}$. Therefore, $\max_{\mathbf{x}\in D_l} \|\mathbf{x}\|^2 = \|\mathbf{x}^*\|^2 = \frac{l(q-l)}{q}$, which completes the proof. □

Lemma 3. *For $\mathbf{x} \in H_m^{q-1}$,*

$$d^2(\mathbf{x}, \phi^{(m)}(\mathbf{x})) \le \frac{p_{q,m}(q - p_{q,m})}{qm^2}.$$

Proof. For $\mathbf{x} \in H_m^{q-1}$, let $\mathbf{y} = m(\mathbf{x} - \phi^{(m)}(\mathbf{x}))$. Since $\sum_{i=1}^{q} y_i = 0$ and $\max\limits_{1\le i\le q} y_i - \min\limits_{1\le i\le q} y_i \le 1$, there exists a permutation $\pi = (\pi_1, \dots, \pi_q)$ on $\{1, \dots, q\}$ such that $(y_{\pi_1}, \dots, y_{\pi_q}) \in D_l$, where l is the number of i's with $y_i > 0$. By Lemma 2,

$$d^2(\mathbf{x}, \phi^{(m)}(\mathbf{x})) = \frac{1}{m^2} \|\mathbf{y}\|^2 \le \frac{l(q-l)}{qm^2}. \tag{5}$$

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Note that $\phi_i^{(m)}(\mathbf{x}) = \frac{\lfloor m(x_i+r^*)\rfloor}{m}$ for some $r^* \in [0, \frac{1}{m}]$. Since $\sum_{i=1}^q \lfloor m(x_i + r^*)\rfloor = m$, we have $l = \sum_{i=1}^q (\lfloor m(x_i + r^*)\rfloor - \lfloor mx_i \rfloor) \leq m$. Hence, $l(q-l) \leq p_{q,m}(q - p_{q,m})$. Therefore, (5) implies the assertion of the lemma. □

Now, we can prove Theorem 1.

Proof of Theorem 1. By Lemma 3, if $\mathbf{x} \in H_m^{q-1}$, then

$$d^2(\mathbf{x}, \mathcal{L}\{q,m\}) \leq d^2(\mathbf{x}, \phi^{(m)}(\mathbf{x})) \leq \frac{p_{q,m}(q-p_{q,m})}{qm^2}.$$

Since H_m^{q-1} is dense in S^{q-1} and $d^2(\mathbf{x}, \mathcal{L}\{q,m\})$ is continuous in $\mathbf{x}$ on S^{q-1},

$$MD(\mathcal{L}\{q,m\}) = \sup_{\mathbf{x}\in S^{q-1}} d^2(\mathbf{x}, \mathcal{L}\{q,m\}) = \sup_{\mathbf{x}\in H_m^{q-1}} d^2(\mathbf{x}, \mathcal{L}\{q,m\}) \leq \frac{p_{q,m}(q-p_{q,m})}{qm^2}.$$

For simplicity, we will write $p_{q,m}$ as p for the remainder of this proof. Let $\mathbf{x}_0 = (\frac{1}{q}, \ldots, \frac{1}{q})$. Then there exists $(k_1, \ldots, k_q) \in \mathbb{Z}_+^q$ with $\sum_{i=1}^q k_i = m$ such that

$$d^2\Big(\frac{m-p}{m}\mathbf{e}_1 + \frac{p}{m}\mathbf{x}_0, \mathcal{L}\{q,m\}\Big) = d^2\Big(\frac{m-p}{m}\mathbf{e}_1 + \frac{p}{m}\mathbf{x}_0, (\frac{k_1}{m}, \ldots, \frac{k_q}{m})\Big).$$

Here and subsequently, $\mathbf{e}_i$ is the q-dimensional vector whose ith element is one and all the other elements are zero.

Let $\mathbf{z} = (z_1, \ldots, z_q) = (\frac{k_1}{m}, \ldots, \frac{k_q}{m}) - \frac{m-p}{m}\mathbf{e}_1$. We will show

$$0 \leq z_i \leq \frac{1}{m} \quad \text{for all } i = 1, \ldots, q. \tag{6}$$

Since $z_i \geq 0$ for all $i = 2, \ldots, q$, we first show $z_1 \geq 0$. If $z_1 < 0$, then $k_1 < m - p$. Hence, $\sum_{l=2}^q k_l = m - k_1 > p$. Thus, there exists j such that $k_j \geq 1$, i.e., $z_j \geq \frac{1}{m}$. Then,

$$\begin{aligned}
&d^2\Big(\frac{m-p}{m}\mathbf{e}_1 + \frac{p}{m}\mathbf{x}_0, (\frac{k_1}{m}, \ldots, \frac{k_q}{m})\Big) - d^2\Big(\frac{m-p}{m}\mathbf{e}_1 + \frac{p}{m}\mathbf{x}_0, (\frac{k_1+1}{m}, \frac{k_2}{m}, \ldots, \frac{k_j-1}{m}, \ldots, \frac{k_q}{m})\Big)\\
&= \Big(z_1 - \frac{p}{mq}\Big)^2 + \Big(z_j - \frac{p}{mq}\Big)^2 - \Big[\Big(z_1 + \frac{1}{m} - \frac{p}{mq}\Big)^2 + \Big(z_j - \frac{1}{m} - \frac{p}{mq}\Big)^2\Big]\\
&= \frac{2}{m}\Big(z_j - z_1 - \frac{1}{m}\Big)\\
&> 0,
\end{aligned}$$

which is a contradiction. Therefore, $z_1 \geq 0$. Next, we show $z_i \leq \frac{1}{m}$ for all $i = 1, \ldots, q$. If $z_j \geq \frac{1}{m}$ for all j, then $\sum_{l=1}^q z_l \geq \frac{1}{m}q > \frac{1}{m}p$, which is a contradiction to $\sum_{l=1}^q z_l = \frac{p}{m}$. Therefore, $z_j < \frac{1}{m}$ for some j. Suppose $z_i > \frac{1}{m}$ for some i. Then

$$\begin{aligned}
&d^2\Big(\frac{m-p}{m}\mathbf{e}_1 + \frac{p}{m}\mathbf{x}_0, (\frac{k_1}{m}, \ldots, \frac{k_q}{m})\Big) - d^2\Big(\frac{m-p}{m}\mathbf{e}_1 + \frac{p}{m}\mathbf{x}_0, (\frac{k_1}{m}, \ldots, \frac{k_i-1}{m}, \ldots, \frac{k_j+1}{m}, \ldots, \frac{k_q}{m})\Big)\\
&= \Big(z_i - \frac{p}{mq}\Big)^2 + \Big(z_j - \frac{p}{mq}\Big)^2 - \Big[\Big(z_i - \frac{1}{m} - \frac{p}{mq}\Big)^2 + \Big(z_j + \frac{1}{m} - \frac{p}{mq}\Big)^2\Big]\\
&= \frac{2}{m}\Big(z_i - z_j - \frac{1}{m}\Big).
\end{aligned} \tag{7}$$

Since $z_i > \frac{1}{m}$, $z_j < \frac{1}{m}$ and mz_i and mz_j are integers, we have $z_i \geq \frac{2}{m}$ and $z_j \leq 0$. Thus, the right-hand side of (7) is strictly positive, which is a contradiction. Hence, $z_i \leq \frac{1}{m}$ for all $i = 1, \ldots, q$. Therefore, (6) is proved.

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Since mz_i, $i = 1, \ldots, q$ are integers, (6) implies that $z_i = 0$ or $\frac{1}{m}$ for all $i = 1, \ldots, q$. Since $\sum_{i=1}^{q} z_i = \frac{p}{m}$, $z_i = 0$ for $q - p$ i's and $z_i = \frac{1}{m}$ for p i's. Thus,

$$
\begin{aligned}
d^2\Big(\frac{m-p}{m}\mathbf{e}_1 + \frac{p}{m}\mathbf{x}_0, \mathcal{L}\{q,m\}\Big) &= \sum_{i=1}^{q}\Big(z_i - \frac{p}{mq}\Big)^2 \\
&= p\Big(\frac{1}{m} - \frac{p}{mq}\Big)^2 + (q-p)\Big(\frac{p}{mq}\Big)^2 \\
&= \frac{p(q-p)}{qm^2}.
\end{aligned}
$$

Therefore, $MD(\mathcal{L}\{q,m\}) = \frac{p(q-p)}{qm^2}$. $\square$

4. Derivation for the formula of $MD(\mathcal{Z}(\mathcal{L}\{q,m\}, \mathbf{x}_0, \lambda))$

In this section, we derive the formula for $MD(\mathcal{Z}(\mathcal{L}\{q,m\}, \mathbf{x}_0, \lambda))$, the maximum distance between any point $\mathbf{x}$ in S^{q-1} and the design point of $\mathcal{Z}(\mathcal{L}\{q,m\}, \mathbf{x}_0, \lambda)$ nearest to $\mathbf{x}$. Note that

$$
MD(\mathcal{Z}(\mathcal{L}\{q,m\}, \mathbf{x}_0, \lambda)) = \max\{g_\lambda(q,m),\, h_\lambda(q,m)\}, \tag{8}
$$

where

$$
\begin{aligned}
g_\lambda(q,m) &= \sup_{\mathbf{x} \in \mathcal{Z}(S^{q-1}, \mathbf{x}_0, \lambda)} d^2(\mathbf{x}, \mathcal{Z}(\mathcal{L}\{q,m\}, \mathbf{x}_0, \lambda)), \\
h_\lambda(q,m) &= \sup_{\mathbf{x} \in S^{q-1} \setminus \mathcal{Z}(S^{q-1}, \mathbf{x}_0, \lambda)} d^2(\mathbf{x}, \mathcal{Z}(\mathcal{L}\{q,m\}, \mathbf{x}_0, \lambda)).
\end{aligned}
$$

Hence, in order to obtain the formula for $MD(\mathcal{Z}(\mathcal{L}\{q,m\}, \mathbf{x}_0, \lambda))$, we have to find the expressions for $g_\lambda(q,m)$ and $h_\lambda(q,m)$. To do this, we need the following three lemmas. The first lemma is for $g_\lambda(q,m)$, while the other two lemmas are for $h_\lambda(q,m)$.

Lemma 4. *We have*

$$
g_\lambda(q,m) = \Big(\frac{\lambda}{1+\lambda}\Big)^2 \frac{p_{q,m}(q - p_{q,m})}{qm^2}, \quad m \geq 1, q \geq 1.
$$

Proof. Note that

$$
g_\lambda(q,m) = \sup_{\mathbf{x} \in \mathcal{Z}(S^{q-1}, \mathbf{x}_0, \lambda)} d^2(\mathbf{x}, \mathcal{Z}(\mathcal{L}\{q,m\}, \mathbf{x}_0, \lambda)) = \Big(\frac{\lambda}{1+\lambda}\Big)^2 \sup_{\mathbf{x} \in S^{q-1}} d^2(\mathbf{x}, \mathcal{L}\{q,m\}).
$$

Since $\sup_{\mathbf{x} \in S^{q-1}} d^2(\mathbf{x}, \mathcal{L}\{q,m\}) = MD(\mathcal{L}\{q,m\})$, we obtain the lemma by Theorem 1. $\square$

Lemma 5. *Let* $S_0^{q-1} = \{\mathbf{x} \in S^{q-1} : x_q = 0\}$. *Then,*

$$
h_\lambda(q,m) = \sup_{\mathbf{x} \in S_0^{q-1}} d^2(\mathbf{x}, \mathcal{Z}(\mathcal{L}\{q,m\}, \mathbf{x}_0, \lambda)).
$$

Proof. Let $\mathbf{x} \in S^{q-1} \setminus \mathcal{Z}(S^{q-1}, \mathbf{x}_0, \lambda)$. We will show that there exists $\tilde{\mathbf{x}} \in S_0^{q-1}$ such that

$$
d(\mathbf{x}, \mathcal{Z}(\mathcal{L}(q,m), \mathbf{x}_0, \lambda)) \leq d(\tilde{\mathbf{x}}, \mathcal{Z}(\mathcal{L}(q,m), \mathbf{x}_0, \lambda)). \tag{9}
$$

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Since $\mathbf{x} \in S^{q-1} \setminus \mathcal{Z}(S^{q-1}, \mathbf{x}_0, \lambda)$, $x_i < \frac{1}{1+\lambda}\frac{1}{q}$ for some i. Without loss of generality, we may assume $x_q < \frac{1}{1+\lambda}\frac{1}{q}$. Let

$$\tilde{\mathbf{x}} = \mathbf{x} + \frac{qx_q}{q-1}(\mathbf{x}_0 - \mathbf{e}_q).$$

Then, $\tilde{\mathbf{x}} \in S_0^{q-1}$. For any $\mathbf{y} \in \mathcal{Z}(\mathcal{L}(q,m), \mathbf{x}_0, \lambda)$,

$$\|\tilde{\mathbf{x}} - \mathbf{y}\|^2 = \|\mathbf{x} - \mathbf{y}\|^2 + \frac{2qx_q}{q-1}(\mathbf{x} - \mathbf{y}) \cdot (\mathbf{x}_0 - \mathbf{e}_q) + \left(\frac{qx_q}{q-1}\right)^2 \|\mathbf{x}_0 - \mathbf{e}_q\|^2. \tag{10}$$

Since the qth component of $\mathbf{x} - \mathbf{y} + \frac{q(x_q - y_q)}{q-1}(\mathbf{x}_0 - \mathbf{e}_q)$ is zero and the sum of all components is also zero, we have

$$\left(\mathbf{x} - \mathbf{y} + \frac{q(x_q - y_q)}{q-1}(\mathbf{x}_0 - \mathbf{e}_q)\right) \cdot (\mathbf{x}_0 - \mathbf{e}_q) = 0.$$

Therefore,

$$(\mathbf{x} - \mathbf{y}) \cdot (\mathbf{x}_0 - \mathbf{e}_q) = \frac{-q(x_q - y_q)}{q-1} \|\mathbf{x}_0 - \mathbf{e}_q\|^2.$$

Since $\mathbf{y} \in \mathcal{Z}(\mathcal{L}(q,m), \mathbf{x}_0, \lambda)$, $y_q \geq \frac{1}{1+\lambda}\frac{1}{q}$. Thus, $y_q > x_q$ and so $(\mathbf{x} - \mathbf{y}) \cdot (\mathbf{x}_0 - \mathbf{e}_q) > 0$. Hence, (10) yields $\|\tilde{\mathbf{x}} - \mathbf{y}\|^2 \geq \|\mathbf{x} - \mathbf{y}\|^2$, and (9) is obtained. □

Lemma 6. *We have*

$$h_\lambda(q,m) = \max_{1 \leq l \leq q-1} \left\{ \left(\frac{\lambda}{1+\lambda}\right)^2 \frac{1}{m^2} \frac{p_{l,m}(l - p_{l,m})}{l} + \frac{q-l}{(1+\lambda)^2 ql} \right\}, \quad m \geq 1, q \geq 2.$$

Proof. First, we prove by induction on q that

$$h_\lambda(q,m) \leq \max_{1 \leq l \leq q-1} \left\{ \left(\frac{\lambda}{1+\lambda}\right)^2 \frac{1}{m^2} \frac{p_{l,m}(l - p_{l,m})}{l} + \frac{q-l}{(1+\lambda)^2 ql} \right\}, \quad m \geq 1, q \geq 2. \tag{11}$$

For $q = 2$,

$$\begin{aligned} h_\lambda(2,m) &= \min_{0 \leq k \leq m} \left\{ \left\| (1,0) - \left(\frac{\lambda}{\lambda+1}\left(\frac{k}{m}, \frac{m-k}{m}\right) + \frac{1}{\lambda+1}\left(\frac{1}{2}, \frac{1}{2}\right) \right) \right\|^2 \right\} \\ &= \left\| (1,0) - \left(\frac{\lambda}{\lambda+1} + \frac{1}{2}\frac{1}{\lambda+1}, \frac{1}{2}\frac{1}{\lambda+1} \right) \right\|^2 \\ &= \frac{1}{2(\lambda+1)^2}. \end{aligned}$$

Since the right-hand side of (11) for $q = 2$ is $\frac{1}{2(\lambda+1)^2}$, (11) holds for $q = 2$. Consider $q \geq 3$. Suppose that

$$h_\lambda(q',m) \leq \max_{1 \leq l \leq q'-1} \left\{ \left(\frac{\lambda}{1+\lambda}\right)^2 \frac{1}{m^2} \frac{p_{l,m}(l - p_{l,m})}{l} + \frac{q'-l}{(1+\lambda)^2 q'l} \right\}$$

holds for $q' < q$. Let $\mathbf{x} \in S_0^{q-1}$ be arbitrary. The proof of (11) is complete if we show

$$d^2(\mathbf{x}, \mathcal{Z}(\mathcal{L}\{q,m\}, \mathbf{x}_0, \lambda)) \leq \max_{1 \leq l \leq q-1} \left\{ \left(\frac{\lambda}{1+\lambda}\right)^2 \frac{1}{m^2} \frac{p_{l,m}(l - p_{l,m})}{l} + \frac{q-l}{(1+\lambda)^2 ql} \right\}, \tag{12}$$

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by Lemma 5. Let l be the number of j's such that $x_j > \frac{1}{1+\lambda}\frac{1}{q}$. If $l = 0$, then $\sum_{j=1}^{q} x_j \leq \sum_{j=1}^{q} \frac{1}{1+\lambda}\frac{1}{q} < 1$, which is a contradiction. Hence, $l \geq 1$. Also, $l \leq q-1$, since $x_q = 0$. Hence, $1 \leq l \leq q-1$. Without loss of generality, we assume

$$x_j > \frac{1}{1+\lambda}\frac{1}{q}, \quad j = 1, \ldots, l,$$
$$x_j \leq \frac{1}{1+\lambda}\frac{1}{q}, \quad j = l+1, \ldots, q.$$

Let $\mathcal{L}^l\{q,m\} = \{\mathbf{y} \in \mathcal{L}\{q,m\} : y_{l+1} = \cdots = y_q = 0\}$. Note that if $\mathbf{y} \in \mathcal{L}^l\{q,m\}$, then $\mathbf{y} = (y_1, \ldots, y_l, \mathbf{0}_{q-l})$, where $(y_1, \ldots, y_l) \in \mathcal{L}\{l,m\}$. Here and subsequently, $\mathbf{0}_k$ and $\mathbf{1}_k$ denote the k-dimensional vectors with all components equal to 0 and 1, respectively. Then,

$$\begin{aligned}
d^2(\mathbf{x}, \mathcal{Z}(\mathcal{L}\{q,m\}, \mathbf{x}_0, \lambda)) &= \min_{\mathbf{y}\in\mathcal{L}\{q,m\}} d^2\Big(\mathbf{x}, \frac{\lambda}{\lambda+1}\mathbf{y} + \frac{1}{\lambda+1}\mathbf{x}_0\Big) \\
&\leq \min_{\mathbf{y}\in\mathcal{L}^l\{q,m\}} d^2\Big(\mathbf{x}, \frac{\lambda}{\lambda+1}\mathbf{y} + \frac{1}{\lambda+1}\mathbf{x}_0\Big) \\
&= \min_{\mathbf{z}\in\mathcal{L}\{l,m\}} d^2\Big(\mathbf{x}, \frac{\lambda}{\lambda+1}(\mathbf{z}, \mathbf{0}_{q-l}) + \frac{1}{\lambda+1}\mathbf{x}_0\Big) \\
&= \min_{\mathbf{z}\in\mathcal{L}\{l,m\}} \Big\{ \sum_{j=1}^{l} \Big(\big(x_j - \frac{1}{\lambda+1}\frac{1}{q}\big) - \frac{\lambda}{\lambda+1} z_j\Big)^2 + \sum_{j=l+1}^{q} \Big(x_j - \frac{1}{\lambda+1}\frac{1}{q}\Big)^2 \Big\} \\
&= \sum_{j=l+1}^{q} \Big(x_j - \frac{1}{\lambda+1}\frac{1}{q}\Big)^2 + \min_{\mathbf{z}\in\mathcal{L}\{l,m\}} \Big\| \mathbf{x}' - \frac{\lambda}{\lambda+1}\mathbf{z} \Big\|^2, \qquad (13)
\end{aligned}$$

where $\mathbf{x}' = (x_1, \ldots, x_l) - \frac{1}{\lambda+1}\frac{1}{q}\mathbf{1}_l$. Note that $\mathbf{x}' \geq \mathbf{0}_l$, where the inequality between the vectors must be interpreted componentwise. Let

$$\sum_{j=1}^{l} x'_j = 1 - \sum_{j=l+1}^{q} x_j - \frac{1}{\lambda+1}\frac{l}{q} \equiv a. \qquad (14)$$

Then, (13) becomes

$$d^2(\mathbf{x}, \mathcal{Z}(\mathcal{L}\{q,m\}, \mathbf{x}_0, \lambda)) \leq \sum_{j=l+1}^{q} \Big(x_j - \frac{1}{\lambda+1}\frac{1}{q}\Big)^2 + a^2 \min_{\mathbf{z}\in\mathcal{L}\{l,m\}} \Big\| \frac{1}{a}\mathbf{x}' - \frac{\lambda}{a(\lambda+1)}\mathbf{z} \Big\|^2. \qquad (15)$$

Note that $a > \frac{\lambda}{\lambda+1}$, $\sum_{j=1}^{l} \frac{1}{a} x'_j = 1$ and $\sum_{j=1}^{l} \frac{\lambda}{a(\lambda+1)} z_j = \frac{\lambda}{a(\lambda+1)} < 1$. We investigate $\Big\| \frac{1}{a}\mathbf{x}' - \frac{\lambda}{a(\lambda+1)}\mathbf{z} \Big\|^2$ in (15). If $\mathbf{x}_0^l = (\frac{1}{l}, \ldots, \frac{1}{l})$, then

$$\begin{aligned}
\Big\| \frac{1}{a}\mathbf{x}' - \frac{\lambda}{a(\lambda+1)}\mathbf{z} \Big\|^2 &= \Big\| \frac{1}{a}\mathbf{x}' - \Big(\frac{\lambda}{a(\lambda+1)}\mathbf{z} + \frac{a(\lambda+1)-\lambda}{a(\lambda+1)}\mathbf{x}_0^l\Big) + \frac{a(\lambda+1)-\lambda}{a(\lambda+1)}\mathbf{x}_0^l \Big\|^2 \\
&= \Big\| \frac{1}{a}\mathbf{x}' - \Big(\frac{\lambda}{a(\lambda+1)}\mathbf{z} + \frac{a(\lambda+1)-\lambda}{a(\lambda+1)}\mathbf{x}_0^l\Big) \Big\|^2 + \Big(\frac{a(\lambda+1)-\lambda}{a(\lambda+1)}\Big)^2 \frac{1}{l}.
\end{aligned}$$

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If we substitute this into (15), then we obtain

$$\begin{aligned}
&d^2(\mathbf{x}, \mathcal{Z}(\mathcal{L}\{q,m\}, \mathbf{x}_0, \lambda)) \\
&\leq \sum_{j=l+1}^{q} \left(x_j - \frac{1}{\lambda+1}\frac{1}{q}\right)^2 + \left(\frac{a(\lambda+1)-\lambda}{\lambda+1}\right)^2 \frac{1}{l} + a^2 \min_{\mathbf{w}\in\mathcal{Z}(\mathcal{L}\{l,m\},\mathbf{x}_0^l,\lambda')} \left\| \frac{1}{a}\mathbf{x}' - \mathbf{w} \right\|^2 \\
&\leq \sum_{j=l+1}^{q} \left(x_j - \frac{1}{\lambda+1}\frac{1}{q}\right)^2 + \left(\frac{a(\lambda+1)-\lambda}{\lambda+1}\right)^2 \frac{1}{l} + a^2 \max\{g_{\lambda'}(l,m), h_{\lambda'}(l,m)\}, \qquad (16)
\end{aligned}$$

where λ' satisfies $\frac{a(\lambda+1)-\lambda}{a(\lambda+1)} = \frac{1}{\lambda'+1}$, i.e., $\lambda' = \frac{\lambda}{a(\lambda+1)-\lambda}$ and the last inequality follows from (8). Now, we get an upper bound of the right-hand side of (16). Note that $a \leq 1 - \frac{1}{\lambda+1}\frac{l}{q}$ by (14) and $0 \leq \frac{1}{\lambda+1}\frac{1}{q} - x_j \leq \frac{1}{\lambda+1}\frac{1}{q}$ for $j = l+1, \ldots, q$. Hence,

$$\begin{aligned}
&\sum_{j=l+1}^{q} \left(x_j - \frac{1}{\lambda+1}\frac{1}{q}\right)^2 + \left(\frac{a(\lambda+1)-\lambda}{\lambda+1}\right)^2 \frac{1}{l} + a^2 g_{\lambda'}(l,m) \\
&= \sum_{j=l+1}^{q} \left(x_j - \frac{1}{\lambda+1}\frac{1}{q}\right)^2 + \left(\frac{a(\lambda+1)-\lambda}{\lambda+1}\right)^2 \frac{1}{l} + \left(\frac{a\lambda'}{1+\lambda'}\right)^2 \frac{p_{l,m}(l-p_{l,m})}{m^2 l} \\
&= \sum_{j=l+1}^{q} \left(x_j - \frac{1}{\lambda+1}\frac{1}{q}\right)^2 + \left(\frac{a(\lambda+1)-\lambda}{\lambda+1}\right)^2 \frac{1}{l} + \left(\frac{\lambda}{\lambda+1}\right)^2 \frac{p_{l,m}(l-p_{l,m})}{m^2 l} \\
&\leq \frac{q-l}{(\lambda+1)^2 q^2} + \left(\frac{q-l}{q(\lambda+1)}\right)^2 \frac{1}{l} + \left(\frac{\lambda}{\lambda+1}\right)^2 \frac{p_{l,m}(l-p_{l,m})}{l m^2} \\
&= \frac{q-l}{(\lambda+1)^2 q l} + \left(\frac{\lambda}{\lambda+1}\right)^2 \frac{p_{l,m}(l-p_{l,m})}{l m^2}. \qquad (17)
\end{aligned}$$

On the other hand,

$$\begin{aligned}
&\sum_{j=l+1}^{q} \left(x_j - \frac{1}{\lambda+1}\frac{1}{q}\right)^2 + \left(\frac{a(\lambda+1)-\lambda}{\lambda+1}\right)^2 \frac{1}{l} + a^2 h_{\lambda'}(l,m) \\
&= \sum_{j=l+1}^{q} \left(x_j - \frac{1}{\lambda+1}\frac{1}{q}\right)^2 + \left(\frac{a(\lambda+1)-\lambda}{\lambda+1}\right)^2 \frac{1}{l} \\
&\quad + a^2 \max_{1\leq l'\leq l-1} \left\{ \left(\frac{\lambda'}{1+\lambda'}\right)^2 \frac{1}{m^2} \frac{p_{l',m}(l'-p_{l',m})}{l'} + \frac{1}{(\lambda'+1)^2} \frac{l-l'}{ll'} \right\} \\
&= \sum_{j=l+1}^{q} \left(x_j - \frac{1}{\lambda+1}\frac{1}{q}\right)^2 + \left(\frac{a(\lambda+1)-\lambda}{\lambda+1}\right)^2 \frac{1}{l} \\
&\quad + \max_{1\leq l'\leq l-1} \left\{ \left(\frac{\lambda}{\lambda+1}\right)^2 \frac{1}{m^2} \frac{p_{l',m}(l'-p_{l',m})}{l'} + \left(\frac{a(\lambda+1)-\lambda}{\lambda+1}\right)^2 \frac{l-l'}{ll'} \right\},
\end{aligned}$$

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where the first equality follows from the induction hypothesis. Since $a \leq 1 - \frac{1}{\lambda+1}\frac{l}{q}$ and $0 \leq \frac{1}{\lambda+1}\frac{1}{q} - x_j \leq \frac{1}{\lambda+1}\frac{1}{q}$ for $j = l+1, \ldots, q$, we obtain

$$\begin{aligned}
&\sum_{j=l+1}^{q}\left(x_j - \frac{1}{\lambda+1}\frac{1}{q}\right)^2 + \left(\frac{a(\lambda+1)-\lambda}{\lambda+1}\right)^2\frac{1}{l} + a^2 h_{\lambda'}(l,m) \\
\leq& \frac{q-l}{(\lambda+1)^2q^2} + \left(\frac{q-l}{q(\lambda+1)}\right)^2\frac{1}{l} + \max_{1\leq l'\leq l-1}\left\{\left(\frac{\lambda}{\lambda+1}\right)^2\frac{1}{m^2}\frac{p_{l',m}(l'-p_{l',m})}{l'} + \left(\frac{q-l}{q(\lambda+1)}\right)^2\frac{l-l'}{ll'}\right\} \\
=& \frac{q-l}{(\lambda+1)^2ql} + \max_{1\leq l'\leq l-1}\left\{\left(\frac{\lambda}{\lambda+1}\right)^2\frac{1}{m^2}\frac{p_{l',m}(l'-p_{l',m})}{l'} + \left(\frac{q-l}{q(\lambda+1)}\right)^2\frac{l-l'}{ll'}\right\} \\
=& \max_{1\leq l'\leq l-1}\left\{\left(\frac{\lambda}{\lambda+1}\right)^2\frac{1}{m^2}\frac{p_{l',m}(l'-p_{l',m})}{l'} + \frac{q-l}{(\lambda+1)^2ql} + \frac{(q-l)^2(l-l')}{q^2(\lambda+1)^2ll'}\right\}. \qquad (18)
\end{aligned}$$

It can be easily checked that

$$\frac{q-l}{(\lambda+1)^2ql} + \frac{(q-l)^2(l-l')}{q^2(\lambda+1)^2ll'} < \frac{q-l'}{(1+\lambda)^2ql'}.$$

Hence, (18) becomes

$$\begin{aligned}
&\sum_{j=l+1}^{q}\left(x_j - \frac{1}{\lambda+1}\frac{1}{q}\right)^2 + \left(\frac{a(\lambda+1)-\lambda}{\lambda+1}\right)^2\frac{1}{l} + a^2 h_{\lambda'}(l,m) \\
<& \max_{1\leq l'\leq l-1}\left\{\left(\frac{\lambda}{\lambda+1}\right)^2\frac{1}{m^2}\frac{p_{l',m}(l'-p_{l',m})}{l'} + \frac{q-l'}{(1+\lambda)^2ql'}\right\}. \qquad (19)
\end{aligned}$$

By (17) and (19), (16) becomes

$$d^2(\mathbf{x}, \mathcal{Z}(\mathcal{L}\{q,m\},\mathbf{x}_0,\lambda)) \leq \max_{1\leq l'\leq l}\left\{\left(\frac{\lambda}{\lambda+1}\right)^2\frac{1}{m^2}\frac{p_{l',m}(l'-p_{l',m})}{l'} + \frac{q-l'}{(1+\lambda)^2ql'}\right\}.$$

88 Therefore, (12) holds and so (11) is proved.

Next, we prove

$$h_\lambda(q,m) \geq \max_{1\leq l\leq q-1}\left\{\left(\frac{\lambda}{1+\lambda}\right)^2\frac{1}{m^2}\frac{p_{l,m}(l-p_{l,m})}{l} + \frac{q-l}{(1+\lambda)^2ql}\right\}, \quad m \geq 1, q \geq 2. \qquad (20)$$

Suppose $m \geq 1$ and $q \geq 2$. For $l = 1, 2, \ldots, q-1$, we will show

$$h_\lambda(q,m) \geq \left(\frac{\lambda}{1+\lambda}\right)^2\frac{1}{m^2}\frac{p_{l,m}(l-p_{l,m})}{l} + \frac{q-l}{(1+\lambda)^2ql}.$$

Let $\mathbf{x} = (x_1, \ldots, x_q)$, where

$$x_i = \begin{cases} \frac{\lambda}{1+\lambda}\left(\frac{m-p_{l,m}}{m} + \frac{p_{l,m}}{m}\frac{1}{l}\right) + \frac{1}{1+\lambda}\frac{1}{l} & \text{if } i = 1, \\ \frac{\lambda}{1+\lambda}\frac{p_{l,m}}{m}\frac{1}{l} + \frac{1}{1+\lambda}\frac{1}{l} & \text{if } i = 2, \ldots, l, \\ 0 & \text{if } i = l+1, \ldots, q. \end{cases}$$

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If $\mathbf{y} \in \mathcal{L}\{q,m\}$ and $y_j > 0$ for some $j \in \{l+1,\dots,q\}$, then there exists $i \in \{1,\dots,l\}$ such that $x_i > y_i$. Let

$$y'_k = \begin{cases} y_i + \frac{1}{m} & \text{if } k = i, \\ y_j - \frac{1}{m} & \text{if } k = j, \\ y_k & \text{if } k \neq i, k \neq j. \end{cases}$$

Then $d^2(\mathbf{x},\mathbf{y}) > d^2(\mathbf{x},\mathbf{y}')$. Hence,

$$\begin{aligned} d^2(\mathbf{x}, \mathcal{Z}(\mathcal{L}\{q,m\},\mathbf{x}_0,\lambda)) &= \min_{\mathbf{y}\in\mathcal{L}\{q,m\}} d^2\Big(\mathbf{x}, \frac{\lambda}{1+\lambda}\mathbf{y} + \frac{1}{1+\lambda}\mathbf{x}_0\Big) \\ &= \min_{\mathbf{y}\in\mathcal{L}^l\{q,m\}} d^2\Big(\mathbf{x}, \frac{\lambda}{1+\lambda}\mathbf{y} + \frac{1}{1+\lambda}\mathbf{x}_0\Big) \\ &= \min_{\mathbf{y}\in\mathcal{L}^l\{q,m\}} \sum_{j=1}^{l}\Big(x_j - \frac{\lambda}{1+\lambda}y_j - \frac{1}{1+\lambda}\frac{1}{q}\Big)^2 + \frac{q-l}{(1+\lambda)^2q^2} \\ &= \min_{\mathbf{y}'\in\mathcal{L}\{l,m\}} \Big\|\mathbf{x}' - \Big(\frac{\lambda}{1+\lambda}\mathbf{y}' + \frac{1}{1+\lambda}\frac{1}{q}\mathbf{1}_l\Big)\Big\|^2 + \frac{q-l}{(1+\lambda)^2q^2}, \end{aligned} \tag{21}$$

where $\mathbf{x}' = (x_1,\dots,x_l)$. Let $\mathbf{x}_0^l = \frac{1}{l}\mathbf{1}_l$. Then,

$$\begin{aligned} &\min_{\mathbf{y}'\in\mathcal{L}\{l,m\}} \Big\|\mathbf{x}' - \Big(\frac{\lambda}{1+\lambda}\mathbf{y}' + \frac{1}{1+\lambda}\frac{1}{q}\mathbf{1}_l\Big)\Big\|^2 + \frac{q-l}{(1+\lambda)^2q^2} \\ &= \min_{\mathbf{y}'\in\mathcal{L}\{l,m\}} \Big\|\mathbf{x}' - \Big(\frac{\lambda}{1+\lambda}\mathbf{y}' + \frac{1}{1+\lambda}\mathbf{x}_0^l - \frac{1}{1+\lambda}\frac{q-l}{lq}\mathbf{1}_l\Big)\Big\|^2 + \frac{q-l}{(1+\lambda)^2q^2} \\ &= \min_{\mathbf{y}'\in\mathcal{L}\{l,m\}} \Big\|\mathbf{x}' - \Big(\frac{\lambda}{1+\lambda}\mathbf{y}' + \frac{1}{1+\lambda}\mathbf{x}_0^l\Big)\Big\|^2 + \frac{(q-l)^2}{(1+\lambda)^2lq^2} + \frac{q-l}{(1+\lambda)^2q^2} \\ &= \Big(\frac{\lambda}{1+\lambda}\Big)^2 \min_{\mathbf{y}'\in\mathcal{L}\{l,m\}} \|\mathbf{x}'' - \mathbf{y}'\|^2 + \frac{q-l}{(1+\lambda)^2ql}, \end{aligned} \tag{22}$$

where $\mathbf{x}'' = (x''_1,\dots,x''_l)$ with

$$x''_i = \begin{cases} \frac{m-p_{l,m}}{m} + \frac{p_{l,m}}{m}\frac{1}{l} & \text{if } i = 1, \\ \frac{p_{l,m}}{m}\frac{1}{l} & \text{if } i = 2,\dots,l. \end{cases}$$

Hence, by (21) and (22), we have

$$d^2(\mathbf{x}, \mathcal{Z}(\mathcal{L}\{q,m\},\mathbf{x}_0,\lambda)) = \Big(\frac{\lambda}{1+\lambda}\Big)^2 \min_{\mathbf{y}'\in\mathcal{L}\{l,m\}} \|\mathbf{x}'' - \mathbf{y}'\|^2 + \frac{q-l}{(1+\lambda)^2ql}. \tag{23}$$

If $\mathbf{z} \in \mathcal{L}\{l,m\}$ and $z_j \geq \frac{2}{m}$ for some $j = 2,\dots,l$, then

$$\min_{\mathbf{y}'\in\mathcal{L}\{l,m\}} \|\mathbf{x}'' - \mathbf{y}'\|^2 < \|\mathbf{x}'' - \mathbf{z}\|^2 . \tag{24}$$

This can be proved as follows: Since $z_j \geq \frac{2}{m}$ for some $j = 2,\dots,l$, there are two cases to consider: (i) $z_j \geq \frac{2}{m}$ for some $j = 2,\dots,l$ and $z_k = 0$ for some $k = 2,\dots,l$, and (ii) $z_j \geq \frac{2}{m}$ for some $j = 2,\dots,l$ and $z_k \geq \frac{1}{m}$ for all $k = 2,\dots,l$. In case (i), if we let

$$z'_i = \begin{cases} z_j - \frac{1}{m} & \text{if } i = j, \\ z_k + \frac{1}{m} & \text{if } i = k, \\ z_i & \text{if } i \neq j, i \neq k, \end{cases}$$

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then $\|\mathbf{x}''-\mathbf{z}\|^2 > \|\mathbf{x}''-\mathbf{z}'\|^2$. In case (ii), $z_1 = 1-\sum_{i=2}^{l} z_i \leq 1-\frac{l}{m} < x_1''$ and if we let

$$z_i'' = \begin{cases} z_1 + \frac{1}{m} & \text{if } i = 1, \\ z_j - \frac{1}{m} & \text{if } i = j, \\ z_i & \text{if } i \neq 1, i \neq j, \end{cases}$$

then $\|\mathbf{x}''-\mathbf{z}\|^2 > \|\mathbf{x}''-\mathbf{z}''\|^2$. Hence, (24) holds if $z_j \geq \frac{2}{m}$ for some $j = 2,\ldots,l$. Therefore, (23) becomes

$$d^2(\mathbf{x}, \mathcal{Z}(\mathcal{L}\{q,m\},\mathbf{x}_0,\lambda)) = \Big(\frac{\lambda}{1+\lambda}\Big)^2 \min_{\mathbf{y}\in\mathcal{L}^*\{l,m\}} \|\mathbf{x}''-\mathbf{y}\|^2 + \frac{q-l}{(1+\lambda)^2 ql}, \tag{25}$$

where $\mathcal{L}^*\{l,m\} = \{\mathbf{y} \in \mathcal{L}\{l,m\} : y_j = 0 \text{ or } \frac{1}{m} \text{ for all } j = 2,\ldots,l\}$. For $\mathbf{y} \in \mathcal{L}^*\{l,m\}$, let l' be the number of j's such that $y_j = \frac{1}{m}$, $j = 2,\ldots,l$. Then $y_1 = 1-\frac{l'}{m}$ and

$$\|\mathbf{x}''-\mathbf{y}\|^2 = \Big(\big(\frac{m-p_{l,m}}{m} + \frac{p_{l,m}}{m}\frac{1}{l}\big) - \big(1-\frac{l'}{m}\big)\Big)^2 + \Big(\frac{p_{l,m}}{m}\frac{1}{l} - \frac{1}{m}\Big)^2 l' + \Big(\frac{p_{l,m}}{m}\frac{1}{l}\Big)^2 (l-l'-1).$$

Hence,

$$\begin{aligned} \min_{\mathbf{y}\in\mathcal{L}^*\{l,m\}} \|\mathbf{x}''-\mathbf{y}\|^2 &= \min_{0\leq l'\leq l-1} \left\{ \Big(\frac{l'+(\frac{1}{l}-1)p_{l,m}}{m}\Big)^2 + \Big(\frac{p_{l,m}}{m}\frac{1}{l} - \frac{1}{m}\Big)^2 l' + \Big(\frac{p_{l,m}}{m}\frac{1}{l}\Big)^2 (l-l'-1) \right\} \\ &= \Big(\frac{p_{l,m}}{ml}\Big)^2 + \Big(\frac{p_{l,m}}{ml} - \frac{1}{m}\Big)^2 p_{l,m} + \Big(\frac{p_{l,m}}{ml}\Big)^2 (l-p_{l,m}-1) \\ &= \frac{p_{l,m}(l-p_{l,m})}{m^2 l}, \end{aligned}$$

where the second equality follows from the fact that the function in the braces takes the minimum at $l' = p_{l,m}$. Hence, by (25), we obtain

$$d^2(\mathbf{x}, \mathcal{Z}(\mathcal{L}\{q,m\},\mathbf{x}_0,\lambda)) = \Big(\frac{\lambda}{1+\lambda}\Big)^2 \frac{p_{l,m}(l-p_{l,m})}{m^2 l} + \frac{q-l}{(1+\lambda)^2 ql}.$$

Therefore, (20) is proved. By (11) and (20), we complete the proof. □

In summary, (8) together with Lemmas 4 and 6 give the formula for $MD(\mathcal{Z}(\mathcal{L}\{q,m\},\mathbf{x}_0,\lambda))$, as shown below in Theorem 2.

Theorem 2. *$MD(\mathcal{Z}(\mathcal{L}\{q,m\},\mathbf{x}_0,\lambda))$ is given by*

$$MD(\mathcal{Z}(\mathcal{L}\{q,m\},\mathbf{x}_0,\lambda)) = \max\{g_\lambda(q,m),\, h_\lambda(q,m)\},$$

where

$$\begin{aligned} g_\lambda(q,m) &= \Big(\frac{\lambda}{1+\lambda}\Big)^2 \frac{p_{q,m}(q-p_{q,m})}{qm^2}, \quad m \geq 1, q \geq 1, \\ h_\lambda(q,m) &= \max_{1\leq l\leq q-1} \left\{ \Big(\frac{\lambda}{1+\lambda}\Big)^2 \frac{1}{m^2} \frac{p_{l,m}(l-p_{l,m})}{l} + \frac{q-l}{(1+\lambda)^2 ql} \right\}, \quad m \geq 1, q \geq 2. \end{aligned}$$

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92 ## 5. Refinement of the conjecture

In this section, we refine Conjecture 1 by using the formulas for $MD(\mathcal{L}\{q,m\})$ and $MD(\mathcal{Z}(\mathcal{L}\{q,m\},\mathbf{x}_0,\lambda))$ given in Theorem 1 and Theorem 2, respectively. For convenience, we repeat the theorems here:

$$MD(\mathcal{L}\{q,m\}) = \frac{p_{q,m}(q-p_{q,m})}{qm^2},$$
$$MD(\mathcal{Z}(\mathcal{L}\{q,m\},\mathbf{x}_0,\lambda)) = \max\{g_\lambda(q,m),\, h_\lambda(q,m)\},$$

where

$$g_\lambda(q,m) = \left(\frac{\lambda}{1+\lambda}\right)^2 \frac{p_{q,m}(q-p_{q,m})}{qm^2}, \quad m \geq 1, q \geq 1,$$
$$h_\lambda(q,m) = \max_{1\leq l\leq q-1} \left\{ \left(\frac{\lambda}{1+\lambda}\right)^2 \frac{p_{l,m}(l-p_{l,m})}{m^2 l} + \frac{1}{(1+\lambda)^2}\left(\frac{1}{l}-\frac{1}{q}\right) \right\}, \quad m \geq 1, q \geq 2,$$

93 with $p_{q,m} = \min\{m, \lfloor \frac{q}{2} \rfloor\}$.

Let

$$h_\lambda^{(l)}(q,m) = \left(\frac{\lambda}{1+\lambda}\right)^2 \frac{p_{l,m}(l-p_{l,m})}{m^2 l} + \frac{1}{(1+\lambda)^2}\left(\frac{1}{l}-\frac{1}{q}\right).$$

Then, for $1 \leq l \leq \min\{2m, q-1\}$,

$$h_\lambda^{(l)}(q,m) = \begin{cases} \left(\frac{\lambda}{1+\lambda}\right)^2 \frac{l}{4m^2} + \frac{1}{(1+\lambda)^2}\left(\frac{1}{l}-\frac{1}{q}\right) & \text{if } l \text{ is even and } l < 2m, \\ \left(\frac{\lambda}{1+\lambda}\right)^2 \frac{l^2-1}{4m^2 l} + \frac{1}{(1+\lambda)^2}\left(\frac{1}{l}-\frac{1}{q}\right) & \text{if } l \text{ is odd and } l < 2m, \\ \left(\frac{\lambda}{1+\lambda}\right)^2 \frac{l-m}{ml} + \frac{1}{(1+\lambda)^2}\left(\frac{1}{l}-\frac{1}{q}\right) & \text{if } l \geq 2m. \end{cases}$$

94 Note that $h_\lambda(q,m) = \max_{1\leq l\leq q-1} h_\lambda^{(l)}(q,m)$. The following lemma gives another expression for
95 $h_\lambda(q,m)$, which will be used in the proof of Theorem 3.

Lemma 7. *If $q \geq 3$ and $\frac{m}{\sqrt{p_{q,m}}} \leq \lambda \leq m$, then*

$$h_\lambda(q,m) = \max\{h_\lambda^{(1)}(q,m), h_\lambda^{(q-1)}(q,m)\}.$$

Proof. We divide the proof into two cases: $2m \leq q-1$ and $2m > q-1$. First, we consider the case of $2m \leq q-1$. Note that

$$\max\{h_\lambda^{(l)}(q,m) : 1 \leq l \leq 2m, l \text{ is even}\} = \max\{h_\lambda^{(2)}(q,m), h_\lambda^{(2m)}(q,m)\},$$
$$\max\{h_\lambda^{(l)}(q,m) : 1 \leq l \leq 2m, l \text{ is odd}\} = \max\{h_\lambda^{(1)}(q,m), h_\lambda^{(2m-1)}(q,m)\}.$$

Hence,

$$\max_{1\leq l\leq 2m} h_\lambda^{(l)}(q,m) = \max\{h_\lambda^{(1)}(q,m), h_\lambda^{(2)}(q,m), h_\lambda^{(2m-1)}(q,m), h_\lambda^{(2m)}(q,m)\}.$$

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Note that $h_\lambda^{(1)}(q,m) = \frac{1}{(1+\lambda)^2}\big(1-\frac{1}{q}\big)$ and $h_\lambda^{(2)}(q,m) = \frac{1}{(1+\lambda)^2}\big(\frac{1}{2}\big(\frac{\lambda}{m}\big)^2 + \frac{1}{2} - \frac{1}{q}\big)$. Since $\lambda \le m$, we have $h_\lambda^{(1)}(q,m) \ge h_\lambda^{(2)}(q,m)$. Thus,

$$\max_{1\le l\le 2m} h_\lambda^{(l)}(q,m) = \max\{h_\lambda^{(1)}(q,m), h_\lambda^{(2m-1)}(q,m), h_\lambda^{(2m)}(q,m)\}.$$

Since $p_{q,m} = m$, $\lambda \ge \sqrt{m}$. Then,

$$\begin{aligned} h_\lambda^{(2m)}(q,m) - h_\lambda^{(2m-1)}(q,m) &= \frac{1}{(\lambda+1)^2}\Big(\Big(\frac{\lambda}{m}\Big)^2\Big(\frac{m}{2} - \frac{m(m-1)}{2m-1}\Big) + \frac{1}{2m} - \frac{1}{2m-1}\Big) \\ &\ge \frac{1}{(\lambda+1)^2}\Big(\frac{1}{2} - \frac{m-1}{2m-1} + \frac{1}{2m} - \frac{1}{2m-1}\Big) \\ &> 0. \end{aligned}$$

Hence

$$\max_{1\le l\le 2m} h_\lambda^{(l)}(q,m) = \max\{h_\lambda^{(1)}(q,m), h_\lambda^{(2m)}(q,m)\}.$$

Note that for $l = 2m, \ldots, q-1$,

$$\begin{aligned} h_\lambda^{(l)}(q,m) &= \Big(\frac{\lambda}{1+\lambda}\Big)^2 \frac{m(l-m)}{m^2 l} + \frac{1}{(1+\lambda)^2}\Big(\frac{1}{l} - \frac{1}{q}\Big) \\ &= -\frac{1}{(1+\lambda)^2}(\lambda^2-1)\frac{1}{l} + \Big(\frac{\lambda}{1+\lambda}\Big)^2 \frac{1}{m} - \frac{1}{(1+\lambda)^2 q} \end{aligned}$$

is increasing in l. Hence

$$\max_{1\le l\le q-1} h_\lambda^{(l)}(q,m) = \max\{h_\lambda^{(1)}(q,m), h_\lambda^{(q-1)}(q,m)\},$$

96 which is the desired result.

Next, we consider the case of $2m > q-1$. Note that

$$\max\{h_\lambda^{(l)}(q,m) : 1 \le l \le q-1, l \text{ is even}\} = \begin{cases} \max\{h_\lambda^{(2)}(q,m), h_\lambda^{(q-2)}(q,m)\} & \text{if } q \text{ is even,} \\ \max\{h_\lambda^{(2)}(q,m), h_\lambda^{(q-1)}(q,m)\} & \text{if } q \text{ is odd,} \end{cases}$$

$$\max\{h_\lambda^{(l)}(q,m) : 1 \le l \le q-1, l \text{ is odd}\} = \begin{cases} \max\{h_\lambda^{(1)}(q,m), h_\lambda^{(q-1)}(q,m)\} & \text{if } q \text{ is even,} \\ \max\{h_\lambda^{(1)}(q,m), h_\lambda^{(q-2)}(q,m)\} & \text{if } q \text{ is odd.} \end{cases}$$

Since $h_\lambda^{(1)}(q,m) \ge h_\lambda^{(2)}(q,m)$, we have

$$\max_{1\le l\le q-1} h_\lambda^{(l)}(q,m) = \max\{h_\lambda^{(1)}(q,m), h_\lambda^{(q-2)}(q,m), h_\lambda^{(q-1)}(q,m)\}.$$

Note that

$$\begin{aligned} h_\lambda^{(q-1)}(q,m) - h_\lambda^{(q-2)}(q,m) =& \frac{1}{(\lambda+1)^2}\Big\{\Big(\frac{\lambda}{m}\Big)^2\Big(\frac{p_{q-1,m}(q-1-p_{q-1,m})}{q-1} - \frac{p_{q-2,m}(q-2-p_{q-2,m})}{q-2}\Big)\Big\} \\ &- \frac{1}{(\lambda+1)^2}\Big(\frac{1}{q-1} - \frac{1}{q-2}\Big). \end{aligned} \tag{26}$$

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If q is even, then $p_{q-1,m} = \frac{q-2}{2}$ and $p_{q-2,m} = \frac{q-2}{2}$. In this case, (26) becomes

$$\begin{aligned} h_\lambda^{(q-1)}(q,m) - h_\lambda^{(q-2)}(q,m) &= \frac{1}{(\lambda+1)^2}\Big\{\Big(\frac{\lambda}{m}\Big)^2\Big(\frac{(q-2)q}{4(q-1)} - \frac{q-2}{4}\Big) - \frac{1}{q-1} + \frac{1}{q-2}\Big\} \\ &\geq \frac{1}{(\lambda+1)^2}\Big(\frac{q-2}{2(q-1)} - \frac{q-2}{2q} - \frac{1}{q-1} + \frac{1}{q-2}\Big) \\ &> 0, \end{aligned}$$

where the second inequality follows from $\frac{\lambda}{m} \geq \frac{1}{\sqrt{p_{q,m}}} \geq \sqrt{\frac{2}{q}}$ since $\lambda \geq \frac{m}{\sqrt{p_{q,m}}}$. If q is odd, then $p_{q-1,m} = \frac{q-1}{2}$ and $p_{q-2,m} = \frac{q-3}{2}$. In this case, (26) becomes

$$\begin{aligned} h_\lambda^{(q-1)}(q,m) - h_\lambda^{(q-2)}(q,m) &= \frac{1}{(\lambda+1)^2}\Big\{\Big(\frac{\lambda}{m}\Big)^2\Big(\frac{q-1}{4} - \frac{(q-3)(q-1)}{4(q-2)}\Big) - \frac{1}{q-1} + \frac{1}{q-2}\Big\} \\ &\geq \frac{1}{(\lambda+1)^2}\Big(\frac{1}{2} - \frac{q-3}{2(q-2)} - \frac{1}{q-1} + \frac{1}{q-2}\Big) \\ &> 0, \end{aligned}$$

where the second inequality follows from $\frac{\lambda}{m} \geq \frac{1}{\sqrt{p_{q,m}}} \geq \sqrt{\frac{2}{q-1}}$ since $\lambda \geq \frac{m}{\sqrt{p_{q,m}}}$. Hence

$$\max_{1\leq l\leq q-1} h_\lambda^{(l)}(q,m) = \max\{h_\lambda^{(1)}(q,m), h_\lambda^{(q-1)}(q,m)\},$$

97 which completes the proof. □

98 Finally, we have the following theorem, which is a refinement of Conjecture 1.

Theorem 3. *$MD(\mathcal{Z}(\mathcal{L}\{q,m\},\mathbf{x}_0,\lambda))$ has a minimum at $\lambda = \lambda^*$, where $\lambda^* = m\sqrt{\frac{q-1}{p_{q,m}(q-p_{q,m})}}$. Furthermore,*

$$MD(\mathcal{Z}(\mathcal{L}\{q,m\},\mathbf{x}_0,\lambda)) > MD(\mathcal{Z}(\mathcal{L}\{q,m\},\mathbf{x}_0,\lambda^*)) \quad \text{for all } \lambda \in [0,\infty)\setminus\{\lambda^*\}. \tag{27}$$

Moreover,

$$\min_{\lambda\in[0,\infty)} MD(\mathcal{Z}(\mathcal{L}\{q,m\},\mathbf{x}_0,\lambda)) = \frac{q-1}{q(1+\lambda^*)^2} \tag{28}$$

99 **Proof.** When $q = 2$, $g_\lambda(2,m) = \big(\frac{\lambda}{1+\lambda}\big)^2\frac{1}{2m^2}$ and $h_\lambda(2,m) = \frac{1}{2(1+\lambda)^2}$. Since $g_\lambda(2,m)$ is strictly increasing
100 in λ and $h_\lambda(q,m)$ is strictly decreasing in λ, $MD(\mathcal{Z}(\mathcal{L}\{q,m\},\mathbf{x}_0,\lambda))$ has a minimum at $\lambda = m$. Note
101 that $p_{q,m} = 1$ and $\lambda^* = m$ when $q = 2$. Thus, the theorem holds when $q = 2$.

Assume $q \geq 3$. By Lemma 7, for $\frac{m}{\sqrt{p_{q,m}}} \leq \lambda \leq m$,

$$MD(\mathcal{Z}(\mathcal{L}\{q,m\},\mathbf{x}_0,\lambda)) = \max\{g_\lambda(q,m), h_\lambda^{(1)}(q,m), h_\lambda^{(q-1)}(q,m)\}.$$

We will show that $g_\lambda(q,m) \geq h_\lambda^{(q-1)}(q,m)$ for $\frac{m}{\sqrt{p_{q,m}}} \leq \lambda \leq m$. Note that

$$\begin{aligned} g_\lambda(q,m) - h_\lambda^{(q-1)}(q,m) =& \Big(\frac{\lambda}{1+\lambda}\Big)^2\Big(\frac{p_{q,m}(q-p_{q,m})}{m^2 q} - \frac{p_{q-1,m}(q-1-p_{q-1,m})}{m^2(q-1)}\Big) \\ &+ \frac{1}{(1+\lambda)^2}\Big(\frac{1}{q} - \frac{1}{q-1}\Big). \end{aligned} \tag{29}$$

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If $m \leq \frac{q-1}{2}$, then $p_{q-1,m} = m$. In this case, (29) becomes

$$\begin{aligned} g_\lambda(q,m) - h_\lambda^{(q-1)}(q,m) &= \left(\frac{\lambda}{1+\lambda}\right)^2 \frac{1}{m}\left(\frac{q-m}{q} - \frac{q-1-m}{q-1}\right) + \frac{1}{(1+\lambda)^2}\left(\frac{1}{q} - \frac{1}{q-1}\right) \\ &= \left(\frac{\lambda}{1+\lambda}\right)^2 \frac{1}{m}\left(\frac{1}{q-1} - \frac{1}{q}\right) - \frac{1}{(1+\lambda)^2}\left(\frac{1}{q-1} - \frac{1}{q}\right) \\ &\geq 0 \end{aligned}$$

since $\lambda \geq \frac{m}{\sqrt{p_{q,m}}} = \sqrt{m}$. Next, suppose $m > \frac{q-1}{2}$. We divide the proof into two cases, according to whether q is even or q is odd. If q is even, then $p_{q,m} = \frac{q}{2}$ and $p_{q-1,m} = \frac{q-2}{2}$. In this case, (29) becomes

$$\begin{aligned} g_\lambda(q,m) - h_\lambda^{(q-1)}(q,m) &= \frac{1}{(\lambda+1)^2}\left\{\left(\frac{\lambda}{m}\right)^2\left(\frac{q}{4} - \frac{(q-2)q}{4(q-1)}\right) + \frac{1}{q} - \frac{1}{q-1}\right\} \\ &= \frac{1}{(\lambda+1)^2}\left\{\left(\frac{\lambda}{m}\right)^2 \frac{q}{4(q-1)} + \frac{1}{q} - \frac{1}{q-1}\right\} \\ &\geq \frac{1}{(\lambda+1)^2}\left(\frac{q}{4p_{q,m}(q-1)} + \frac{1}{q} - \frac{1}{q-1}\right) \\ &= \frac{1}{(\lambda+1)^2}\left(\frac{1}{2(q-1)} + \frac{1}{q} - \frac{1}{q-1}\right) \\ &> 0, \end{aligned}$$

where the third inequality follows from $\frac{\lambda}{m} \geq \frac{1}{\sqrt{p_{q,m}}}$. If q is odd, then $p_{q,m} = p_{q-1,m} = \frac{q-1}{2}$. In this case, (29) becomes

$$\begin{aligned} g_\lambda(q,m) - h_\lambda^{(q-1)}(q,m) &= \frac{1}{(\lambda+1)^2}\left\{\left(\frac{\lambda}{m}\right)^2\left(\frac{q^2-1}{4q} - \frac{q-1}{4}\right) + \frac{1}{q} - \frac{1}{q-1}\right\} \\ &\geq \frac{1}{(\lambda+1)^2}\left(\frac{2}{q-1}\left(\frac{q^2-1}{4q} - \frac{q-1}{4}\right) + \frac{1}{q} - \frac{1}{q-1}\right) \\ &= \frac{1}{(\lambda+1)^2}\left(\frac{1}{2q} + \frac{1}{q} - \frac{1}{q-1}\right) \\ &> 0, \end{aligned}$$

where the second inequality follows from $\frac{\lambda}{m} \geq \frac{1}{\sqrt{p_{q,m}}} = \sqrt{\frac{2}{q-1}}$. Hence, for $\frac{m}{\sqrt{p_{q,m}}} \leq \lambda \leq m$, $g_\lambda(q,m) \geq h_\lambda^{(q-1)}(q,m)$. Therefore, for $\frac{m}{\sqrt{p_{q,m}}} \leq \lambda \leq m$,

$$MD(\mathcal{Z}(\mathcal{L}\{q,m\}, \mathbf{x}_0, \lambda)) = \max\{g_\lambda(q,m), h_\lambda^{(1)}(q,m)\}.$$

Since $\frac{m}{\sqrt{p_{q,m}}} \leq \lambda^* = m\sqrt{\frac{q-1}{p_{q,m}(q-p_{q,m})}}$ and $g_{\lambda^*}(q,m) = h_{\lambda^*}^{(1)}(q,m)$, we have

$$MD(\mathcal{Z}(\mathcal{L}\{q,m\}, \mathbf{x}_0, \lambda^*)) = g_{\lambda^*}(q,m) = h_{\lambda^*}^{(1)}(q,m).$$

Since $g_\lambda(q,m)$ is strictly increasing in λ,

$$MD(\mathcal{Z}(\mathcal{L}\{q,m\}, \mathbf{x}_0, \lambda)) \geq g_m(q,m) > g_{\lambda^*}(q,m) = MD(\mathcal{Z}(\mathcal{L}\{q,m\}, \mathbf{x}_0, \lambda^*)) \quad \text{for all } \lambda > \lambda^*.$$

Since $h_\lambda^{(1)}(q,m)$ is strictly decreasing in λ,

$$MD(\mathcal{Z}(\mathcal{L}\{q,m\}, \mathbf{x}_0, \lambda)) \geq h_\lambda^{(1)}(q,m) > h_{\lambda^*}(q,m) = MD(\mathcal{Z}(\mathcal{L}\{q,m\}, \mathbf{x}_0, \lambda^*)) \quad \text{for all } \lambda < \lambda^*.$$

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Therefore,

$$MD(\mathcal{Z}(\mathcal{L}\{q,m\},\mathbf{x}_0,\lambda^*)) < MD(\mathcal{Z}(\mathcal{L}\{q,m\},\mathbf{x}_0,\lambda)) \quad \text{for all } \lambda \neq \lambda^*,$$

which proves (27). Moreover,

$$MD(\mathcal{Z}(\mathcal{L}\{q,m\},\mathbf{x}_0,\lambda^*)) = g_{\lambda^*}(q,m) = h^{(1)}_{\lambda^*}(q,m) = \frac{q-1}{q(1+\lambda^*)^2},$$

which is (28). □

Remark 2. Conjecture 1(i) says that $MD(\mathcal{Z}(\mathcal{L}\{q,m\},\mathbf{x}_0,\lambda))$ has a minimum at $\lambda = m$. Therefore, Conjecture 1(i) is true when $p_{q,m} = 1$, i.e., when either $q \leq 3$ or $m = 1$. Conjecture 1(ii) says that

$$MD(\mathcal{Z}(\mathcal{L}\{q,m\},\mathbf{x}_0,m)) = MD(\mathcal{L}\{q,m+1\}) = \frac{q-1}{q(m+1)^2}. \tag{30}$$

However, note from our results that

$$MD(\mathcal{L}\{q,m+1\}) = \frac{p_{q,m+1}(q-p_{q,m+1})}{q(m+1)^2},$$
$$MD(\mathcal{Z}(\mathcal{L}\{q,m\},\mathbf{x}_0,m)) = \frac{p_{q,m}(q-p_{q,m})}{q(1+m)^2}.$$

Hence, $MD(\mathcal{Z}(\mathcal{L}\{q,m\},\mathbf{x}_0,m)) = MD(\mathcal{L}\{q,m+1\})$ if and only if $p_{q,m} = p_{q,m+1}$. That is, the first equality in (30) holds if and only if $m \geq \lfloor \frac{q}{2} \rfloor$, i.e., $q \leq 2m+1$. Also, $MD(\mathcal{L}\{q,m+1\}) = \frac{q-1}{q(m+1)^2}$ if and only if $p_{q,m+1} = 1$ if and only if $q \leq 3$. Hence, the second equality in (30) holds if and only if $q \leq 3$. Note that $MD(\mathcal{Z}(\mathcal{L}\{q,m\},\mathbf{x}_0,m)) = \frac{q-1}{q(m+1)^2}$ if and only if $p_{q,m} = 1$ if and only if either $q \leq 3$ or $m = 1$. Therefore, Conjecture 1(ii) is true only when $q \leq 3$.

6. Conclusions

This paper is inspired by the conjecture, made by Li and Zhang [5], on the pseudo component transformation of the lattice points in the simplex. Specifically, they made the conjecture that the two maximum distances $MD(\mathcal{L}\{q,m\})$ and $MD(\mathcal{Z}(\mathcal{L}\{q,m\},\mathbf{x}_0,\lambda))$ have a special property. In general, it is difficult to calculate the maximum distance in most practical problems. We have derived the formulas for $MD(\mathcal{L}\{q,m\})$ and $MD(\mathcal{Z}(\mathcal{L}\{q,m\},\mathbf{x}_0,\lambda))$. By using these formulas, we have shown that the conjecture of Li and Zhang [5] is not true in general. Also, we have refined the conjecture of Li and Zhang [5] and have proved the refined conjecture.

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