

Lattice point partition designs for experiments with mixture

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Abstract. The upper bound on the model error will be decreased when the mean square error and the maximum distance deviation are sufficiently small in the uniform designs for mixture experiments and the design is more robust for the model. However, the analytical expressions of MSED and MD are currently only available in the hypercube, but both types of deviations in other studies are just approximations. Although it can obtain good approximations in the low-dimensional case, the calculation will be more complicated for an experiment with more variables. Therefore, in this paper, an algorithm based on lattice point partitioning design is proposed to obtain the analytical expression of the MSED and MD in the region covered by the lattice points. Furthermore, the design's optimality is considered and illustrated by examples under the same uniformity.

§1 Introduction

The experimenter is mainly interested in obtaining a quality product or an effective experimental scheme in engineering, food, agriculture, and medicine. However, for practical considerations, such as time constraints or resources, the experimenter needs to consider how to choose an excellent experimental design with a minimum number of experiments to obtain complete information about the product and how to choose experimental points on the domain when the underlying model is unknown. Therefore, the researcher proposed various practical design methods for this purpose, such as orthogonal experimental design, uniform experimental design, simplex-lattice design, and simplex-centroid design in mixture experimental (see Ryan[1], Fang et al.[2], Scheffé[3], and Silvey[4]). The main interest in this paper is the design for experiments with the mixture and the uniform design.

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For a mixture experiment, the product's response is only related to the proportion of each component in the mixture and not to its total amount. For example, in considering photostability studies of photographic film coating materials, Cornell [5] found that stability was only related to the relative proportions of two coupling agents, two coupling agent solvents, and three stabilizers. The response in mixture experiment designs is commonly associated with factors by an underlying linear model for parameters. Therefore, the computation of optimal designs aims to choose the combination of experiments that are combinations of proportions of components to maximize the information gathered from the complete set of experiments. The use of optimality criteria is a strategy grounded on the statistical theory where the main goal is finding a design with maximum information, i.e., guaranteeing the minimization of the confidence region of the parameters. The scholars proposed various optimality criteria for these purpose considerations, such as D -, A -, E - and R -optimality criteria, see Atkinson et al. [6] and Dette [7]. Moreover, under these optimality criteria, an optimal design is the best design if the underlying model is known. Optimal designs have many attractive properties. However, as pointed out by Fang and Wang [8], Borkowski and Piepel [9], the optimal design has the following two drawbacks: (i) The optimal design distributes too many experimental points on or near the boundary of the experimental region, especially when the dimensionality of factors is high; (ii) The optimal design depends on the models' assumptions, and it is not a robust design. When the underlying model is unknown, optimal designs may have a poor performance.

As for the uniform design method (Fang and Wang [8]; Fang [10]; Wang and Fang [11]) in analyzing the experimental data, it is not based on maximizing the experiment information and is also not depends on the underlying model but tries to spread the design points uniformly over the experimental region and does not allow repetition. The uniform design is robust to the model specification, which is also an optimal space-filling criterion. Many authors have studied uniform designs for mixture experiments and proposed some methods to measure the uniformity of dispersion of experimental points in the mixture experimental region. Fang and Wang [8] proposed the mean squared error deviation (MSED) and root mean squared error (RMSD) criteria. Borkowski and Piepel [9] presented the average distance (AD) and maximum distance deviation (MD) criteria. Moreover, as Fang et al. [2] mentioned, the star discrepancy is a popularly used measure of uniformity in quasi-Monte Carlo methods. The lower the star discrepancy, the better the uniformity of the set of points under consideration will be. From Koksma-Hlawka inequality, the star deviation controls the upper bound of the model's error. Hence, for a mixture uniform experiment design, it is sufficient that the values of MSED and MD be small enough to result in fewer upper bounds on the model deviations and more robustness. However, it is noted that the MSED and MD values were obtained using approximate formulas in the available literature. Theoretically, both approximate values converge to the actual value in probability. Nevertheless, we note that the approximate values depend on the number of random mixture points in NT-net and also on the structure of the mixture region. Therefore, it is difficult to obtain analytical expressions of these deviations mentioned above for an irregular experimental region or more components. Ning et al. [13] proposed DM_2 -deviations and obtained analytical

expression of DM_2 -deviations on regular simplex by using the regenerative kernel Hilbert space tools. To calculate the deviation by constructing an efficient algorithm, Chuang and Hung [14] constructed a switching algorithm. Ning et al. [15] presented a new method for producing a uniform design of mixture experiments based on the number-theoretic LBG algorithm. Chen et al. [16] presented a discrete particle swarm optimization algorithm. Liu and Liu [17] proposed a new algorithm using the central composite discrepancy (CCD) criterion to obtain a uniform design for mixture experiments with constraints. However, the approximation's accuracy is insufficient to meet our requirements. Therefore, obtaining analytical expressions for both deviations or approximate solutions with controlled errors is necessary.

The uniform design considers how to uniformly distribute the points in the experimental region when the underlying model is unknown, and it is the design related to space-filling. And there is various literature to investigate the approach for space-filling experimental design when the underlying model is unknown, see Pronzato [18, 19]. The development of mixture experimental design has also significantly contributed to the development of irregular region filling experimental design. This paper mainly wants to obtain the analytical expressions for the deviations by using the lattice point partition design when the model is unknown. However, as the number of components of mixture experiments increases, the methods mentioned above shall result in numerous computations or obtain an approximate value of the deviation. The lattice point set is an essential tool for experiment design and has the following properties: (i) The designs constructed by lattice point sets are uniformly dispersed in the experimental region; (ii) Transformation or rotation does not change the self-similar structure of the lattice point set; (iii) The deviations in sub-simplexes obtained by lattice point division are fixed, which is favorable to the calculation of MSE. Much literature studied space-filling design by using lattice point sets, such as Zhou and Xu [20] proved that the linear transformations of a good lattice point set could improve its space-filling performance. He [21, 22] studied the design of interlaced lattices with minimax distances and sliced space-filling. Li et al. [23] discussed the properties of the mixture lattice point set and gave its application to both nonparametric modeling and uniformity tests on a simplex experimental region. Therefore, we propose an approach to obtain the analytic expressions of MSED and MD for a regular-simplex experimental region. For the method, using a lattice point set, we first divide the experimental region to obtain several standard congruent sub-simplexes without common interior points. Secondly, take all vertices of the sub-simplexes as design points.

This paper mainly proposes a lattice point partition algorithm for the mixture region based on the underlying model is unknown. Under the lattice point partition design, we obtained the analytical expressions of the MSED and the MD in a standard sub-simplex. The rest of the paper is organized as follows. In Section 2, the preliminaries and notations for the mixture experiments and the uniform design are given. Section 3 introduces the partition method for a standard mixture region. Based on the lattice point partition designs, the analytical expressions of MD and MSED are obtained in Section 4. Section 5 shows that the MSED and MD are valid by two examples and give the problems that can be studied further.

§2 Preliminaries

2.1 Experimental region

For a mixture experiment with q components, $x_1, x_2, \dots, x_q$ are the proportions of each component, which satisfy $\sum_{i=1}^q x_i = 1, x_i \geq 0, i = 1, 2, \dots, q$, and construct a $(q-1)$ -dimensional regular simplex given by

$$S^{q-1} = \left\{ \mathbf{x} = (x_1, x_2, \dots, x_q)^T : 0 \leq x_i \leq 1, i = 1, 2, \dots, q, \sum_{i=1}^q x_i = 1 \right\}. \quad (1)$$

However, for the practical considerations, additional constraints exist on the mixture components, and the typical restrictions include as follows.

(i) Single component constraints (SSCs)

$$0 \leq a_i \leq x_i \leq b_i \leq 1, i = 1, 2, \dots, q, \quad (2)$$

(ii) Multiple component constraints (MCCs)

$$l_j \leq \sum_{i=1}^q M_{ji} x_i \leq u_j, j = 1, 2, \dots, Q,$$

where Q is numbers of MCCs.

Furthermore, if the experiments with additional constraints mentioned above, and then the experimental region will be a sub-simplex of S^{q-1} , denotes as

$$\mathcal{X} = \left\{ \mathbf{x} = (x_1, x_2, \dots, x_q)^T : \sum_{i=1}^q x_i = 1, x_i \geq 0, i = 1, 2, \dots, q, C's \right\}, \quad (3)$$

where $C's$ is a set of additional constraints, such as SSCs and MCCs.

2.2 Models and optimal designs

In a mixture experimental design, the response is usually related to the factors by the underlying model. However, the optimal design aims to find the design with the maximum amount of information and minimize the confidence region of the parameter, which usually needs to assume that the form of the underlying model is known and obtain an optimal experimental solution for a specific optimal criterion. Due to the restrictions of the experimental region S^{q-1} , the general regression models cannot be directly applied to the mixture experiments. Therefore, various mixture models have been proposed including mixture polynomial models, Becker's mixture models, and additive mixture models ([3, 4, 5, 6, 24, 25]). In this paper, we are mainly interested in linear models, assuming that the response y at $\mathbf{x}$ is written as

$$y = \theta^T f(\mathbf{x}) + \varepsilon, \quad (4)$$

where $\theta = (\theta_1, \theta_2, \dots, \theta_s)^T$ is a s -dimensional vector of unknown parameters, $f(\mathbf{x}) = (f_1(\mathbf{x}), f_2(\mathbf{x}), \dots, f_s(\mathbf{x}))^T$ is a given functional vector, ε is a random error with zero mean and variance σ^2 .

The optimal design for model (4) is a probability distribution with finite supporting points

$\mathbf{x}_i \in S^{q-1}$, $i = 1, 2, \dots, n$, and can be given by

$$\xi = \begin{pmatrix} \mathbf{x}_1 & \mathbf{x}_2 & \cdots & \mathbf{x}_n \\ \omega_1 & \omega_2 & \cdots & \omega_n \end{pmatrix}, \quad (5)$$

where ω_i , $i = 1, 2, \dots, n$ is a weight for each design point, which are nonnegative and sum to 1, and such that $\xi(\mathbf{x}_i) = \omega_i$, $i = 1, 2, \dots, n$.

In addition, we have the information matrix of design ξ for model (4) defined as

$$M(\xi) = \int_{S^{q-1}} f(\mathbf{x}) f^T(\mathbf{x}) \xi(d\mathbf{x}). \quad (6)$$

From the definition of the information matrix, it follows that the information matrix does not depend on the observations of the experiment. Moreover, an essential property of linear models is that the information matrix does not depend on the values of the unknown parameters either. It only depends on design ξ . According to Fedorov and Leonov [26], if the information matrix is non-singular, then the least squares estimate $\hat{\theta}$ of the parameter θ is also uniquely determined, and we have

$$\text{Var}(\hat{\theta}) \propto M^{-1}(\xi), \quad (7)$$

where $M^{-1}(\xi)$ is the inverse matrix of $M(\xi)$.

The above equation (7) suggests addressing the following optimization problem, that is, to find the optimal design.

$$\xi^* = \arg \min_{\xi \in \Xi} \Phi(M^{-1}(\xi)),$$

where Φ is a scalar functional that is usually called an optimality criterion, Ξ be the set of all competing designs.

The commonly optimality criteria, such as D -, A -, and R -optimality criteria, are based on the above matrix $M^{-1}(\xi)$. For model (4), we have

(i) a design ξ^* is said to be D -optimal if $\xi^* = \arg \min_{\xi \in \Xi} \det(M^{-1}(\xi))$,

(ii) a design ξ^* is said to be A -optimal if $\xi^* = \arg \min_{\xi \in \Xi} \text{tr}(M^{-1}(\xi))$,

(iii) a design ξ^* is said to be R -optimal if $\xi^* = \arg \min_{\xi \in \Xi} \prod_{i=1}^s (M^{-1}(\xi))_{ii}$,

where $\det(\cdot)$ and $\text{tr}(\cdot)$ denote the determinant and trace of matrix, respectively.

2.3 Lattice point sets and measures of uniformity

Optimal design is an efficient method to obtain the best design scheme under the optimality criterion when the underlying model is known. For practical cases, however, the underlying model is often unknown, and the optimal design approach has a poor performance. Therefore, in this section, we consider the uniformity of the design point in the experimental region when the underlying model is unknown. For the convenience of discussing lattice point partition designs on the regular simplex, we first define two types of point sets below.

Definition 2.1. For an arbitrary design point $\mathbf{x} \in S^{q-1}$, let $i_1, i_2, \dots, i_q$ be a permutation of $1, 2, \dots, q$, then the permutation point set generated by $\mathbf{x}$ can be defined as

$$\mathcal{P}(\mathbf{x}) = \{\mathbf{x}, \mathbf{x}_{i_1}, \mathbf{x}_{i_2}, \dots, \mathbf{x}_{i_p}\},$$

where $\mathbf{x}_i = (x_{i_1}, x_{i_2}, \dots, x_{i_q})^T, i = 1, 2, \dots, p$.

Definition 2.2. For any positive integers m and q , if there exists $\alpha_i \in \mathbb{Z}^+, i = 1, 2, \dots, q$, such that $\sum_{i=1}^q \alpha_i = m$, then the set of q -component m -order lattice points consisting of all possible combination of the point $(\frac{\alpha_1}{m}, \frac{\alpha_2}{m}, \dots, \frac{\alpha_q}{m})$ can be defined as

$$\mathcal{L}\{q, m\} = \left\{ \left(\frac{\alpha_1}{m}, \frac{\alpha_2}{m}, \dots, \frac{\alpha_q}{m} \right)^T : \alpha_i \in \mathbb{Z}^+, i = 1, 2, \dots, q, \sum_{i=1}^q \alpha_i = m \right\}. \quad (8)$$

Furthermore, the q -component m -order centroid point sets can be defined as

$$\mathcal{C}\{q, m\} = \bigcup_{i=1}^m \mathcal{P}(\mathbf{x}_i), \quad (9)$$

where $\mathbf{x}_i = \frac{1}{i} \sum_{j=1}^i \mathbf{e}_q(j), i = 1, 2, \dots, q, m \leq q$, $\mathbf{e}_q(j)$ is a q -dimensional column vector with j th element being 1 and other elements being 0 and denote $\mathcal{C}\{q\} = \mathcal{C}\{q, q\}$.

However, when the underlying model is unknown, the experimenter is interested in the dispersion of the design points in the experimental domain. The uniform design is proposed for such a purpose. However, how to measure the degree of uniformity of the distribution of a design is worth considering and studying. Therefore, scholars have proposed various deviation criteria for measuring the uniformity of a design based on the consideration of different criteria. We give two common deviations in the following, as seen in Fang and Wang [8], Borkowski and Piepel [9].

Definition 2.3. Suppose $\mathcal{D}_n = \{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n\}$ is a design with n support points in $\mathcal{X}$. Then, the distance between $\mathbf{x} = (x_1, x_2, \dots, x_q)^T \in \mathcal{X}$ and $\mathcal{D}_n$ are defined as

$$d^2(\mathbf{x}, \mathcal{D}_n) = \min_{1 \leq i \leq n} \{d^2(\mathbf{x}, \mathbf{x}_i)\},$$

where $d^2(\mathbf{x}, \mathbf{x}_i) = \|\mathbf{x} - \mathbf{x}_i\|^2$ is Euclidean distance.

Furthermore, we have the definition MSED and MD for $\mathcal{D}_n$ as follows

$$\text{MSED}(\mathcal{D}_n) = E(d^2(\mathbf{x}, \mathcal{D}_n)) = \frac{1}{\int_{\mathcal{X}} d\mathbf{x}} \int_{\mathcal{X}} d^2(\mathbf{x}, \mathcal{D}_n) d\mathbf{x}, \quad (10)$$

$$\text{MD}(\mathcal{D}_n) = \max_{\mathbf{x} \in \mathcal{X}} d^2(\mathbf{x}, \mathcal{D}_n). \quad (11)$$

As mentioned above, the robustness of the model depends on the uniformity of the design. In a mixture experiments, if the MSED and MD are both sufficiently small, the upper bound of the model error can be reduced to achieve robustness. From the above definition of deviations, it is obvious that these deviations have a common problem that is complicated to calculate. Therefore, we use their numerical theoretical to estimate approximate true value in practical problems.

Definition 2.4. Let $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N \in \mathcal{X}$ are N random mixture experimental points with uniform distribution, then the MSED and MD values for the design $\mathcal{D}_n$ can be approximated by

$$msed(\mathcal{D}_n) = \frac{1}{N} \sum_{k=1}^N d^2(\mathbf{x}_k, \mathcal{D}_n), \quad md(\mathcal{D}_n) = \max_{1 \leq k \leq N} \{d^2(\mathbf{x}_k, \mathcal{D}_n)\}, \quad (12)$$

respectively.

We can note that m_{sd} and m_d are respectively finite actual values of MSED and MD. When the NT-net generated by the experimental domain contains a sufficient number of randomly mixture experimental points, m_{sd} and m_d will theoretically converge to MSED and MD in probability. However, the accuracy of the approximation does not satisfy the needs of many situations. So, it often aims to obtain the analytic expressions of MSED and MD, or the approximate solutions with controlled errors. Ning et al. [13] constructed the analytic expressions of DM_2 - deviation based on the regenerated Hilbert space over the regular simplex region. As for the mixture experimental region with constraints, the analytic expressions of MSED and MD are still not obtained. Therefore, we consider the use of lattice points partition to construct the analytic expressions of MSED and MD on the constrained region.

§3 Partitioning method of mixture experimental region

This section mainly presents partitioning methods for two specific types of mixture experimental regions. Firstly, we introduce the partitioning method for convex polyhedral mixture experimental regions proposed by Guan[27]. Then, we give another partitioning method for the mixture experimental region with both upper and lower bound constraints.

3.1 Partitioning of the regular simplex S^{q-1}

Let $\mathcal{X}_i^k$ be i -th k -dimensional cell composed by the vertices of the regular experimental region S^{q-1} . For example, $\mathcal{X}_i^0$ is the i -th vertex of S^{q-1} , $\mathcal{X}_j^1$ is the j -th edge of S^{q-1} , $\dots$, and $\mathcal{X}_p^{q-1}$ is the p -th sub-simplex of S^{q-1} . Then, from the result in Guan [27], the p -th sub-simplex of S^{q-1} can be given by

$$\mathcal{X}_p^{q-1} = V\{\mathbf{x}_{p1}, \mathbf{x}_{p2}, \dots, \mathbf{x}_{pq}\},$$

where $\mathbf{x}_{p1}, \mathbf{x}_{p2}, \dots, \mathbf{x}_{pq}$ be the q vertices of $\mathcal{X}_p^{q-1}$.

Moreover, we have the sub-simplex of S^{q-1} without common interior points by the partitioning of the regular experimental region as follows.

- (i) under the lattice point sets (8), S^{q-1} can be partitioned into m^{q-1} sub-simplex;
- (ii) under the central point sets (9), S^{q-1} can be partitioned into $q!$ sub-simplex.

Taking three-component simplex as example, using the central point set $\mathcal{C}\{3\}$, the S^{3-1} can be partitioned into 6 sub-simplex, as shown in Fig.1(a), and can be partitioned into 16 sub-simplex by using lattice point set $\mathcal{L}\{3, 4\}$, as shown in Fig.1(b).

3.2 Partitioning of the SSCs

For the mixture experimental region (3) with SSCs, denotes as

$$\mathcal{X}_{[a,b]} = \left\{ \mathbf{x} = (x_1, \dots, x_q)^T : 0 \leq a_i \leq x_i \leq b_i \leq 1, i = 1, \dots, q, \sum_{i=1}^q x_i = 1 \right\}, \quad (13)$$

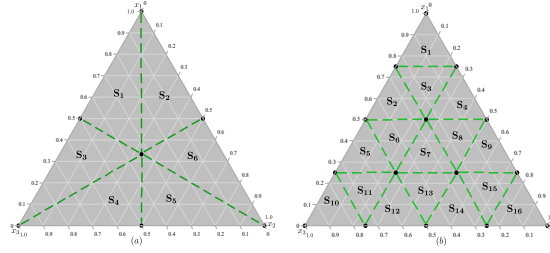


Figure 1. (a) Partitioning of the regular simplex S^{q-1} under $\mathcal{C}\{3\}$, (b) Partitioning of the regular simplex S^{q-1} under $\mathcal{L}\{3,4\}$.

where $\mathbf{a} = (a_1, a_2, \dots, a_q)^T$, $\mathbf{b} = (b_1, b_2, \dots, b_q)^T$ are the lower and upper bound constraint vectors, respectively.

Now in order to construct the partitioning of the SSCs, we first note that a design point $\mathbf{x} = (x_1, x_2, \dots, x_q)^T \in \mathcal{X}_{[\mathbf{a}, \mathbf{b}]} \subseteq S^{q-1}$ can be mapped to an experimental region with only upper bound constraints by a linear transformation

$$z_i = \frac{x_i - a_i}{1 - \mathbf{a}^T \mathbf{1}_q}, i = 1, 2, \dots, q,$$

where $\mathbf{1}_q$ is q -dimensional column vector with all elements being 1. So, here we mainly consider the experimental region with only the upper bound constraints and denote it as $\mathcal{X}_{\mathbf{b}} = \mathcal{X}_{[\mathbf{0}_q, \mathbf{b}]}$.

Without loss of generality, let

$$b_i = \frac{m_i}{m}, i = 1, 2, \dots, q,$$

where $m_1, m_2, \dots, m_q \in \mathbb{Z}^+$, and satisfies $\sum_{i=1}^q m_i > m$. c denotes the greatest common divisor of $m_1, m_2, \dots, m_q, m - m_1, m - m_2, \dots, m - m_q$.

Now, we give the method of the partitioning of $\mathcal{X}_{\mathbf{b}}$ as follows.

Step 1. Let $\delta_0 = \frac{c}{m}$, the upper bound constraints can be written as $(k_i - 1)\delta_0 = b_i, i = 1, 2, \dots, q$, where $k_i, i = 1, 2, \dots, q$ are positive integers.

Step 2. Construct a matrix $R'_{\mathcal{X}_{\mathbf{b}}}(\delta_0) = (R_1, R_2, \dots, R_{q-1})$, where $R_1 = \mathbf{d}_1 \otimes \mathbf{1}_{k_2 k_3 \dots k_{q-1}}$, $R_2 = \mathbf{1}_{k_1} \otimes \mathbf{d}_2 \otimes \mathbf{1}_{k_3 k_4 \dots k_{q-1}}, \dots, R_{q-1} = \mathbf{1}_{k_1 k_2 \dots k_{q-2}} \otimes \mathbf{d}_{q-1}$, $\otimes$ is the Kronecker product, $\mathbf{d}_i^T = (0, \delta_0, 2\delta_0, \dots, (k_i - 1)\delta_0), i = 1, 2, \dots, q - 1$.

Step 3. Let $\mathbf{h} = \mathbf{1}_K - R'_{\mathcal{X}_{\mathbf{b}}}(\delta_0) \mathbf{1}_{q-1} = (h_1, h_2, \dots, h_K)^T$, where $K = k_1 k_2 \dots k_{q-1}$.

Step 4. Construct a matrix $R_{\mathcal{X}_{\mathbf{b}}}(\delta_0) = (\mathbf{e}_K(i_1), \mathbf{e}_K(i_2), \dots, \mathbf{e}_K(i_r)) (R'_{\mathcal{X}_{\mathbf{b}}}(\delta_0), \mathbf{h})$, where $\{i_1, i_2, \dots, i_r\}$ is a index set and satisfy $0 \leq h_{i_j} \leq b_q$.

Step 5. Take each row of elements of the matrix $R_{\mathcal{X}_{\mathbf{b}}}(\delta_0)$ to obtain a complete covered lattice point set $\mathcal{L}_{\mathcal{X}_{\mathbf{b}}}(\delta_0)$.

Now, from the method above, the region $\mathcal{X}_{\mathbf{b}}$ can be partitioned into several sub-simplices without common interior points. For example, Fig.2 shows that the experimental region $\mathcal{X}_{\mathbf{b}}$ with upper bound-constrained $\mathbf{b} = (\frac{1}{2}, \frac{3}{4}, \frac{3}{4})^T$ for three-component mixture system can be partitioned into 10 sub-simplices.

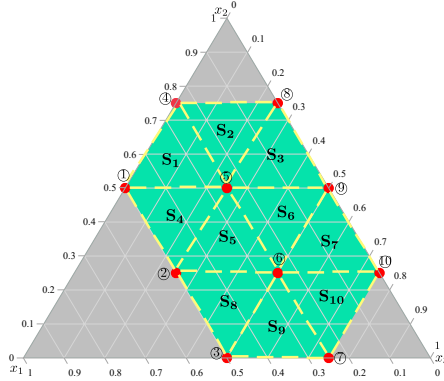


Figure 2. Partitioning of the three-component mixture system with upper bound-constrained $\mathbf{b} = \left(\frac{1}{2}, \frac{3}{4}, \frac{3}{4}\right)^T$.

§4 Uniformity measures for the lattice point partition designs in the mixture region

Based on the partitioning method of the mixture region presented in Section 3, we can obtain several sub-simplices without common interior points. This section will construct the lattice point partitioning designs for the mixture experiments based on these sub-simplices and provide the analytic expressions for MSED and MD under the lattice point partitioning designs. Now in order to construct the design we need, we first present the definition of the congruence of the two sub-simplices.

Definition 4.1. Let $\mathcal{X}_1^{q-1} = V\{\mathbf{x}_{11}, \mathbf{x}_{12}, \dots, \mathbf{x}_{1q}\}$ and $\mathcal{X}_2^{q-1} = V\{\mathbf{x}_{21}, \mathbf{x}_{22}, \dots, \mathbf{x}_{2q}\}$ denote two sub-simplices. The simplex $\mathcal{X}_1^{q-1}$ and $\mathcal{X}_2^{q-1}$ are called congruent if for any design points $\mathbf{x}_{1i}, \mathbf{x}_{1j} \in \mathcal{X}_1^{q-1}$ and $\mathbf{x}_{2i}, \mathbf{x}_{2j} \in \mathcal{X}_2^{q-1}$ satisfies

$$d^2(\mathbf{x}_{1i}, \mathbf{x}_{1j}) = d^2(\mathbf{x}_{2i}, \mathbf{x}_{2j}), 1 \leq i < j \leq q.$$

From Definition 4.1, we can find that the corresponding edge length of two sub-simplices are equal and both of them can be obtained by the point transformation on S^{q-1} . That is, if we assume that the matrix $H_i = (\mathbf{x}_{i1}, \mathbf{x}_{i2}, \dots, \mathbf{x}_{iq}), i = 1, 2$ and two design points $\mathbf{s}_1 = H_1 \mathbf{y} \in \mathcal{X}_1^{q-1}$, $\mathbf{s}_{01} = H_1 \mathbf{y}_0 \in \mathcal{X}_1^{q-1}$, then there are two corresponding points $\mathbf{s}_2 = H_2 \mathbf{y} \in \mathcal{X}_2^{q-1}$, $\mathbf{s}_{02} = H_2 \mathbf{y}_0 \in \mathcal{X}_2^{q-1}$, respectively, and satisfy

$$\begin{aligned} d^2(\mathbf{s}_1, \mathbf{s}_{01}) &= (\mathbf{y} - \mathbf{y}_0)^T H_1^T H_1 (\mathbf{y} - \mathbf{y}_0)^T \\ &= (\mathbf{y} - \mathbf{y}_0)^T H_2^T H_2 (\mathbf{y} - \mathbf{y}_0)^T \\ &= d^2(\mathbf{s}_2, \mathbf{s}_{02}), \end{aligned}$$

where $\mathbf{y}$ and $\mathbf{y}_0$ are any two points of the regular simplex S^{q-1} . It shows that the distance between two points corresponding to two congruent simplices is equal, and further, the simplex $\mathcal{X}^{q-1}$ is called a standard sub-simplex if the lengths of the edges of the sub-simplices are equal.

The theorem below shows the distance between any two points of the sub-simplex $\mathcal{X}^{q-1}$.

Theorem 4.1. Suppose $\mathcal{X}^{q-1} = V\{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_q\}$ is a sub-simplex of S^{q-1} and let $H = (\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_q)$ is a matrix defined in $\mathbb{R}^{q \times q}$, then for any one point $\mathbf{t}_0 \in \mathcal{X}^{q-1}$

$$E(d^2(\mathbf{x}, \mathbf{t}_0)) = \frac{1}{q(q+1)} \mathbf{1}_q^T M_0 \mathbf{1}_q - \frac{2}{q} \mathbf{t}_0^T H \mathbf{1}_q + \mathbf{t}_0^T \mathbf{t}_0, \quad (14)$$

$$\max_{\mathbf{x} \in \mathcal{X}^{q-1}} d^2(\mathbf{x}, \mathbf{t}_0) = \max_{\mathbf{x} \in \mathcal{D}_q} d^2(\mathbf{x}, \mathbf{t}_0), \quad (15)$$

where $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_q$ are q vertices of $\mathcal{X}^{q-1}$, $M_0 = (\mathbf{I}_q + \mathbf{J}_q) \odot H^T H$, $\odot$ is the Hadamard product, and $\mathcal{D}_q = \{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_q\}$ is a design consisting of q vertices.

Proof. Let $\mathbf{t}_0^T H = (c_1, c_2, \dots, c_q)$. For any design point $\mathbf{x} \in \mathcal{X}^{q-1}$, there exists a point $\mathbf{y} = (y_1, y_2, \dots, y_q)^T \in S^{q-1}$ and satisfies $\mathbf{x} = H\mathbf{y}$, then

$$\begin{aligned} & \int_{\mathcal{X}^{q-1}} d^2(\mathbf{x}, \mathbf{t}_0) d\mathbf{x} \\ &= \int_{\mathcal{X}^{q-1}} (\mathbf{x} - \mathbf{t}_0)^T (\mathbf{x} - \mathbf{t}_0) d\mathbf{x} = \int_{S^{q-1}} (H\mathbf{y} - \mathbf{t}_0)^T (H\mathbf{y} - \mathbf{t}_0) |H| d\mathbf{y} \\ &= |H| \left(\sum_{i=1}^q g_{ii} \int_{S^{q-1}} y_i^2 d\mathbf{y} + 2 \sum_{i < j} g_{ij} \int_{S^{q-1}} y_i y_j d\mathbf{y} - 2 \sum_{i=1}^q c_i \int_{S^{q-1}} y_i d\mathbf{y} + c_0 \right) \\ &= |H| \left(\frac{1}{\Gamma(q+2)} \mathbf{1}_q^T [\text{diag}(g_{11}, g_{22}, \dots, g_{qq}) + G] \mathbf{1}_q - \frac{2}{\Gamma(q+1)} \mathbf{t}_0^T H \mathbf{1}_q + c_0 \right) \\ &= |H| \left(\frac{1}{\Gamma(q+2)} \mathbf{1}_q^T M_0 \mathbf{1}_q - \frac{2}{\Gamma(q+1)} \mathbf{t}_0^T H \mathbf{1}_q + c_0 \right), \end{aligned}$$

where $c_0 = \frac{\mathbf{t}_0^T \mathbf{t}_0}{\Gamma(q)}$, $\Gamma(\cdot)$ is Gamma function, $G = H^T H$, $g_{11}, g_{22}, \dots, g_{qq}$ are the diagonal elements of matrix G .

Since

$$\int_{\mathcal{X}^{q-1}} d\mathbf{x} = \int_{S^{q-1}} |H| d\mathbf{y} = \frac{|H|}{\Gamma(q)},$$

and from (10), we know that

$$E(d^2(\mathbf{x}, \mathbf{t}_0)) = \frac{1}{\int_{\mathcal{X}^{q-1}} d\mathbf{x}} \int_{\mathcal{X}^{q-1}} d^2(\mathbf{x}, \mathbf{t}_0) d\mathbf{x} = \frac{1}{q(q+1)} \mathbf{1}_q^T M_0 \mathbf{1}_q - \frac{2}{q} \mathbf{t}_0^T H \mathbf{1}_q + \mathbf{t}_0^T \mathbf{t}_0.$$

Because the maximum of the distances between a single design point $\mathcal{D}_1 = \{\mathbf{x}\}$ of the interior of the sub-simplex $\mathcal{X}^{q-1}$ and a point $\mathbf{t}_0$ must be obtained at the vertices of the sub-simplex, then $\mathbf{x} \in \mathcal{D}_q$, so that equation (14) and (15) holds. $\square$

Theorem 4.1 provide the distance between any two points of the sub-simplex $\mathcal{X}^{q-1}$. The following theorem can be established to obtain the analytic expressions of the MSED and MD in a standard sub-simplex.

Theorem 4.2. Let $\mathcal{X}^{q-1} = V\{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_q\}$ is a standard sub-simplex of S^{q-1} , $\mathcal{D}_q = \{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_q\}$ is a design consisting of q vertices of the $\mathcal{X}^{q-1}$ and $H = (\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_q)$, then

$$\text{MSED}(\mathcal{D}_q) = \frac{1}{q(q+1)} \mathbf{1}_q^T M_{11} \mathbf{1}_q - \frac{2}{q} \mathbf{x}_1^T H F_{11}^T \mathbf{1}_q + \mathbf{x}_1^T \mathbf{x}_1, \quad (16)$$

$$\text{MD}(\mathcal{D}_q) = d^2(\mathbf{x}_0, \mathbf{x}_1). \quad (17)$$

where $M_{11} = (\mathbf{I}_q + \mathbf{J}_q) \odot (F_{11}H^T H F_{11}^T)$, $F_{11} = (\mathbf{f}_1, \mathbf{f}_2, \dots, \mathbf{f}_q)$ and $\mathbf{f}_1^T = \left(1, \frac{1}{2}, \frac{1}{3}, \dots, \frac{1}{q}\right)$, $\mathbf{f}_2^T = \left(0, \frac{1}{2}, \frac{1}{3}, \dots, \frac{1}{q}\right)$, $\dots$, $\mathbf{f}_q^T = \left(0, 0, \dots, 0, \frac{1}{q}\right)$, $\mathbf{x}_0 = \frac{1}{q}H\mathbf{1}_q$.

Proof. Denote

$$H F_{ji}^T = (\mathbf{x}_{ji_1}, \mathbf{x}_{ji_2}, \dots, \mathbf{x}_{ji_q}), j = 1, 2, \dots, q, i = 1, 2, \dots, (q-1)!,$$

where $F_{ji}^T = (\mathbf{f}_{i_1}, \dots, \mathbf{f}_{i_{j-1}}, \mathbf{f}_1, \mathbf{f}_{i_{j+1}}, \dots, \mathbf{f}_{i_{q-1}})$, $i_1, i_2, \dots, i_{q-1}$ is a permutation of $2, 3, \dots, q$.

From the result in Section 3.1, under the central point sets $\mathcal{C}\{q\}$, the simplex $\mathcal{X}^{q-1}$ can be partitioned into $q!$ sub-simplex with no common interior point, that is

$$\mathcal{X}^{q-1} = \bigcup_{j=1}^q \bigcup_{i=1}^{(q-1)!} V\{\mathbf{x}_{ji_1}, \mathbf{x}_{ji_2}, \dots, \mathbf{x}_{ji_q}\}.$$

Let $\mathcal{X}_{ji}^{q-1} = V\{\mathbf{x}_{ji_1}, \mathbf{x}_{ji_2}, \dots, \mathbf{x}_{ji_q}\}$ is the j th sub-simplex of $\mathcal{X}^{q-1}$. Since $\mathcal{X}^{q-1}$ is a standard sub-simplex, then each of the sub-simplex $\mathcal{X}_{ji}^{q-1}$ are congruent.

It shows that $d^2(\mathbf{x}, \mathcal{D}_q) = d^2(\mathbf{x}, \mathbf{x}_j)$ when $\mathbf{x} \in \mathcal{X}_{ji}^{q-1}$. Furthermore, for any one point $\mathbf{y} \in S^{q-1}$,

$$d^2(H F_{ji}^T \mathbf{y}, \mathbf{x}_j) = d^2(H F_{ki}^T \mathbf{y}, \mathbf{x}_k),$$

where $\mathbf{x}_j, \mathbf{x}_k \in \mathcal{D}_q, j, k = 1, 2, \dots, q, j \neq k$.

From Theorem 4.1, results in (14) and (15), then

$$\begin{aligned} & \int_{\mathcal{X}^{q-1}} d^2(\mathbf{x}, \mathcal{D}_q) d\mathbf{x} \\ &= \sum_{j=1}^q \sum_{i=1}^{(q-1)!} \int_{\mathcal{X}_{ji}^{q-1}} d^2(\mathbf{x}, \mathbf{x}_j) d\mathbf{x} \\ &= \sum_{j=1}^q \sum_{i=1}^{(q-1)!} \int_{S^{q-1}} d^2(H F_{ji}^T \mathbf{y}, \mathbf{x}_j) |H F_{ji}^T| d\mathbf{y} \\ &= \sum_{j=1}^q \sum_{i=1}^{(q-1)!} |H F_{ji}^T| \left\{ \frac{1}{\Gamma(q+2)} \mathbf{1}_q^T M_{ji} \mathbf{1}_q - \frac{2}{\Gamma(q+1)} \mathbf{x}_i^T H F_{ji}^T \mathbf{1}_q + \frac{\mathbf{x}_i^T \mathbf{x}_i}{\Gamma(q)} \right\} \\ &= |H| \left\{ \frac{1}{(q+1)!} \mathbf{1}_q^T M_{11} \mathbf{1}_q - \frac{2}{q!} \mathbf{x}_1^T H F_{11}^T \mathbf{1}_q + \frac{\mathbf{x}_1^T \mathbf{x}_1}{(q-1)!} \right\}, \end{aligned}$$

where $M_{ji} = \text{diag}(p_{ji,1}, p_{ji,2}, \dots, p_{ji,q}) + P_{ji}$, $P_{ji} = F_{ji}H^T H F_{ji}^T$, $p_{ji,l}, l = 1, 2, \dots, q$ is the l th element on the diagonal of P_{ji} .

Since

$$\int_{\mathcal{X}^{q-1}} d\mathbf{x} = \frac{|H|}{(q-1)!}.$$

Then, we have

$$\text{MSED}(\mathcal{D}_q) = \frac{1}{q(q+1)} \mathbf{1}_q^T M_{11} \mathbf{1}_q - \frac{2}{q} \mathbf{x}_1^T H F_{11}^T \mathbf{1}_q + \mathbf{x}_1^T \mathbf{x}_1,$$

and

$$\text{MD}(\mathcal{D}_q) = \max_{\mathbf{x} \in S^{q-1}} d^2(\mathbf{x}, \mathcal{D}_q) = \max_{\mathbf{x} \in \mathcal{X}_1^{q-1}} d^2(\mathbf{x}, \mathbf{x}_1) = d^2(\mathbf{x}_0, \mathbf{x}_1).$$

□

Corollary 4.1. Suppose $\mathcal{X}$ is a mixture region that can be partitioned by a lattice point set

$\mathcal{L}_{\mathcal{X}}(\delta_0)$ into N sub-simplex with no common interior points, that is

$$\mathcal{X} = \bigcup_{i=1}^N \mathcal{X}_i^{q-1} = \bigcup_{i=1}^N V\{\mathbf{x}_{i1}, \mathbf{x}_{i2}, \dots, \mathbf{x}_{iq}\}.$$

Let $\mathcal{D}_{iq} = \{\mathbf{x}_{i1}, \mathbf{x}_{i2}, \dots, \mathbf{x}_{iq}\}$ be a vertex design on the i th sub-simplex $\mathcal{X}_i^{q-1}$, then

$$\text{MSED}(\mathcal{L}_{\mathcal{X}}(\delta_0)) = \text{MSED}(\mathcal{D}_{1q}), \quad \text{MD}(\mathcal{D}_{iq}) = d^2(\mathbf{x}_{11}, \mathbf{x}_{10}),$$

where $\mathbf{x}_{10} = \frac{1}{q} \sum_{j=1}^q \mathbf{x}_{1j}$, $\mathbf{x}_{ij} \in \mathcal{L}_{\mathcal{X}}(\delta_0)$, $i = 1, 2, \dots, N$, $j = 1, 2, \dots, q$.

Proof. Denote $\text{MSED}(\mathcal{D}_{iq})$, $i = 1, 2, \dots, N$ be the MSED for the design $\mathcal{D}_{iq}$. Then

$$\begin{aligned} \text{MSED}(\mathcal{L}_{\mathcal{X}}(\delta_0)) &= \frac{1}{\int_{\mathcal{X}} d\mathbf{x}} \int_{\mathcal{X}} d^2(\mathbf{x}, \mathcal{L}_{\mathcal{X}}(\delta_0)) d\mathbf{x} \\ &= \left[\sum_{i=1}^k \left(\int_{\mathcal{X}_i^{q-1}} d\mathbf{x} \right) \right]^{-1} \left(\sum_{i=1}^k \int_{\mathcal{X}_i^{q-1}} d\mathbf{x} \right) \text{MSED}(\mathcal{D}_{1q}) \\ &= \text{MSED}(\mathcal{D}_{1q}). \end{aligned}$$

From Theorems 4.1 and 4.2, result MD can be obtained similarly. $\square$

§5 Special cases

In this section, we present two examples that indicate that our method of lattice point partition design is effective for obtaining MSED and MD in an experiment with mixture while consider the D -optimality of different lattice point partitioning designs under the same uniformity.

Example 1. Consider three components x_1 , x_2 , and x_3 are needed for generating some product in an experiment with mixture, and they have constraints as follows

$$0 \leq x_1 \leq \frac{1}{2}, 0 \leq x_2 \leq \frac{3}{4} \text{ and } 0 \leq x_3 \leq \frac{3}{4}.$$

Now, the mixture experimental region with above constraints can be denoted by $\mathcal{X}_{\mathbf{b}}$, $\mathbf{b} = (\frac{1}{2}, \frac{3}{4}, \frac{3}{4})^T$. Following, we divide the experimental domain $\mathcal{X}_{\mathbf{b}}$ with an upper bound constrain by using the lattice point set $\mathcal{L}_{\mathcal{X}_{\mathbf{b}}}(\delta_0)$ into 10 standard sub-simplexes with no common interior point, and obtain 10 vertices, as shown in Fig 2. Then, we construct a lattice point partition design $\mathcal{D}_1$ with these 10 design points, as shown in Table 1. Moreover, we divide the region $\mathcal{X}_{\mathbf{b}}$ into 30 standard sub-simplexes, as shown in Fig 3, and we obtain lattice point partition design $\mathcal{D}_2$ with twenty design points, as shown in Table 1. Furthermore, from the results of above Theorem 4.2 and Corollary 4.1, the values of MSED and MD can be obtained, as shown in Table 1.

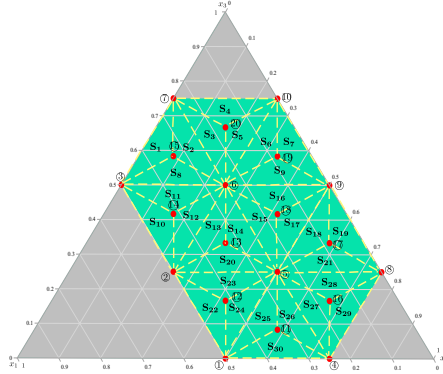


Figure 3. Lattice point partition design for three-component with twenty vertex points.

Table 1. The design points and values of MSED and MD for $q = 3$.

Design	$\mathcal{D}_1$				$\mathcal{D}_2$			
	NO.	x_1	x_2	x_3	NO.	x_1	x_2	x_3
Points	1	$\frac{1}{2}$	$\frac{1}{2}$	0	11	$\frac{1}{3}$	$\frac{7}{12}$	$\frac{1}{12}$
	2	$\frac{1}{2}$	$\frac{1}{4}$	$\frac{1}{4}$	12	$\frac{5}{12}$	$\frac{5}{12}$	$\frac{1}{6}$
	3	$\frac{1}{2}$	0	$\frac{1}{2}$	13	$\frac{1}{3}$	$\frac{1}{3}$	$\frac{1}{3}$
	4	$\frac{1}{4}$	$\frac{3}{4}$	0	14	$\frac{5}{12}$	$\frac{1}{6}$	$\frac{5}{12}$
	5	$\frac{1}{4}$	$\frac{1}{2}$	$\frac{1}{4}$	15	$\frac{1}{3}$	$\frac{1}{12}$	$\frac{7}{12}$
	6	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{2}$	16	$\frac{1}{6}$	$\frac{2}{3}$	$\frac{1}{6}$
	7	$\frac{1}{4}$	0	$\frac{3}{4}$	17	$\frac{1}{12}$	$\frac{7}{12}$	$\frac{1}{3}$
	8	0	$\frac{3}{4}$	$\frac{1}{4}$	18	$\frac{1}{6}$	$\frac{5}{12}$	$\frac{5}{12}$
	9	0	$\frac{1}{2}$	$\frac{1}{2}$	19	$\frac{1}{12}$	$\frac{1}{3}$	$\frac{7}{12}$
	10	0	$\frac{1}{4}$	$\frac{3}{4}$	20	$\frac{1}{6}$	$\frac{1}{6}$	$\frac{2}{3}$
MSED	0.08539				0.04775			
MD	0.53033				0.53033			

Note: the design $\mathcal{D}_2$ contains 20 points, here we only provide the points 11 to 20, and the points 1 to 10 are the same as design $\mathcal{D}_1$.

Note that the uniformity of design $\mathcal{D}_2$ is optimal under the MSED criterion, but both designs have the same MD value, and the number of design points of $\mathcal{D}_2$ are twice as $\mathcal{D}_1$. Therefore, in the following example, we will consider the case where the MD is the same and use the D -optimality of the design to determine which lattice point partition design is optimum.

Example 2. Consider the D -optimality of these lattice point partition designs $\mathcal{D}_i, i = 1, 2$, where the points of $\mathcal{D}_i$ as shown in Table 1.

As discussed in Section 1, the optimal design depends on an underlying model. So, for

3-component mixture experiments, we first suppose the response y at $\mathbf{x}$ can be written as

$$E(y) = \sum_{i=1}^3 \beta_i x_i + \sum_{1 \leq i < j \leq 3} \beta_{ij} x_i x_j. \quad (18)$$

Then, from the results of Section 2.2, a design $\mathcal{D}_i$ is D -optimal if it minimizes the determinant of the matrix $M^{-1}(\xi)$ for the model (18). The design points of two design are shown in Table 1, it is easy to calculate that the determinant of information matrix for $\mathcal{D}_i$, and shown in Table 2. Then, under the MD and the results of Table 2, $\mathcal{D}_1$ is an optimal design.

Table 2. The values of $\det(M(\mathcal{D}_i))$.

Designs	$\mathcal{D}_1$	$\mathcal{D}_2$
$\det(M(\mathcal{D}_i))$	6.427×10^{-12}	1.163×10^{-12}

§6 Discussion

Mixture experimental design and uniform design are two essential experimental design methods. The response in the mixture experiment design is commonly related to factors by an underlying model of the parameters. Therefore, the computation of optimal designs aims to obtain optimum combinations proportions of components with the minimum number of experiments. Furthermore, maximizing the information gathered from the complete set of experiments and estimating the parameters effectively. However, the optimal design poorly performs when the underlying model is unknown and brings a significant bias. In contrast, the uniform design is an experimental method that only considers the uniform distribution of experimental points within the experimental region, which is not dependent on the model and is more robust.

The MSED and MD are two desirable criteria for uniform designs. Obtaining the analytical expressions of two criteria is a challenging task, especially when the experiments relate to more components. In this paper, we first present the partition method for two different mixture regions and obtain a series of sub-simplex with no common interior points. Furthermore, the constructed lattice point partition design and standard sub-simplex are used to construct the analytical expressions of MSED and MD. Finally, it is shown that the MSED and MD obtained from the lattice point partition design are effective to determine the uniformity measure of the design points in the mixture region. In addition, it is feasible to use the D -optimal to choose an optimal design when the deviations are the same.

In further studies, we shall plan to discuss the analytical expressions of the MSED and MD criteria for the irregular experimental regions, or also construct an efficient algorithm for approximation. Moreover, it is also attractive for us to construct a compound design by using the connection between the uniformity and optimality criteria. We hope to report these results in our paper soon.

Declarations

Conflict of interest The authors declare no conflict of interest.

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