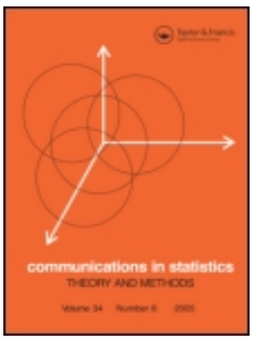

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Construction of uniform designs for mixture experiments with complex constraints

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ABSTRACT
Mixture experiments have attracted increasingly attention due to their great practical value in production and living, while uniform designs over irregular experimental regions have become a hot topic in the area of experimental designs in the past two decades. Noting that the experimental region of a mixture experiment with q components under some constraints is in fact a $(q-1)$-dimensional geometry, this article proposes a new method for searching nearly uniform designs for mixture experiments with any complex constraints. Two examples with some tables and figures are given to illustrate this method.

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1. Introduction

A mixture experiment refers to an experiment that blends some components to form an end product and all properties of the product depend only on the proportions of each component and not on the total amount of the mixture. The extensive application scope and tremendous practical value make the study of mixture experiments much desirable. For accuracy and conciseness, the experimental region of a mixture experiment is usually expressed as:

$$D = \{(x_1, \ldots, x_q) | x_1 + \cdots + x_q = 1, x_i \geq 0, C\text{'s}\}, \tag{1}$$

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 $x_1, \ldots, x_q$. As we see, the conditions $x_1 + \cdots + x_q = 1$ and $x_i \geq 0$ 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. For a given design size n of a mixture experiment with some constraints C's , the more uniformly these n points are scattered in the experimental region, the more reasonably they can represent the whole area, so it is valuable to search uniform designs for a mixture experiment with any complex constraints. Studies on uniform designs for mixture experiments mainly include Wang and Fang (1990, 1996), Fang and Wang (1994), Fang and Yang (2000), Tian and Fang (1999), Borkowski and Piepel (2009), and Ning et al. (2010), most of which discussed about the designs with the C's only being the linear constraints for x_i's, and the methods of constructing uniform designs for mixture experiments with more complex constraints have been little studied.

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The goal of a uniform design is to scatter all the design points in the experimental region as uniformly as possible. But it is difficult to obtain an absolutely uniform design, so most articles on this subject mainly discussed about constructing nearly uniform designs (NUDs) which have relatively good performances under some criteria. Till now, many criteria have been proposed for measuring the uniformity of designs in regular and irregular experimental regions (see, e.g., Fang et al., 2006). As for the case of irregular regions, the mean squared error (MSE) proposed by Fang and Wang (1994), root mean squared distance (RMSD), maximum distance (MD), and average distance (AD) discrepancies proposed by Borkowski and Piepel (2009), and the central composite discrepancy (CCD) proposed by Chuang and Hung (2010) are widely used criteria. In addition to the CCD criterion, a useful algorithm for searching NUDs under the CCD criterion was also recommended by Chuang and Hung (2010), which is called the switching algorithm (SA) and can decrease the burden of search hugely compared with the exhaustive search.

Taking into account that the q-component design region restricted by C's is in fact a $(q-1)$-dimensional geometry, this article proposes an interesting method for searching the NUDs for mixture experiments with any complex constraints C's based on Chuang and Hung (2010)'s method, that is, transforming the experimental region into a $(q-1)$-dimensional coordinate system first, then searching the NUD via the SA, and finally transforming the selected points back into the original coordinate system. The transformation is mainly achieved by the matrix QR decomposition.

The rest of this article is arranged as follows. Section 2 introduces some preliminaries, including the CCD, RMSD, MD, and AD criteria and SA. Section 3 proposes the new method, and provides two examples for illustration and comparison. Some concluding remarks are provided in Sec. 4.

2. Preliminaries

In this section, the CCD, RMSD, MD, and AD criteria and SA will be introduced.

2.1. *The CCD criterion*

Suppose D is an irregular geometry in q-dimensional space $\mathcal{R}^q$, which denotes the experimental region of some experiment. For any fixed point $x = (x_1, \ldots, x_q)$ in D, the $(q-1)$-dimensional hyperplane which is perpendicular to the ith axis and gets through point x chops the ith axis into two parts, i.e., $(-\infty, x_i]$ and $(x_i, +\infty)$, where $i = 1, \ldots, q$, then the region D can be divided into 2^q small grids by the q hyperplanes referred to above, denoted by $D_1(x), \ldots, D_{2^q}(x)$, with point x being the center of them. Note that, according to Chuang and Hung (2010), D could be divided into m^q grids surrounding x, and we take $m = 2$ here which will be enough for illustrating the new method. Let $\mathcal{P}$ denote a design with n points from D, and the central composite discrepancy (CCD) used to measure the uniformity of $\mathcal{P}$ can be written as

$$CCD_p(n, \mathcal{P}) = \left\{ \frac{1}{V(D)} \int_D \frac{1}{2^q} \sum_{t=1}^{2^q} \left| \frac{N(D_t(x), \mathcal{P})}{n} - \frac{V(D_t(x))}{V(D)} \right|^p \mathrm{d}x \right\}^{1/p}, \tag{2}$$

where $p > 0, N(D_t(x), \mathcal{P})$ denotes the number of points belonging to $\mathcal{P}$ and falling into $D_t(x)$ at the same time, and $V(D_t(x))$ and $V(D)$ denote the volumes of $D_t(x)$ and D, respectively. In this article, we take $p = 2$ as Chuang and Hung (2010) did in their investigation. Apparently,

a small $CCD_p(n, \mathcal{P})$ value implies a relatively uniform design and the design $\mathcal{P}^*$ with

$$\mathcal{P}^* = \arg \min_{\mathcal{P} \in Z(n)} CCD_p(n, \mathcal{P})$$

is the most uniform design with a given run size n, where $Z(n)$ denotes the set composed of all the designs with n points from D. In a practical application, the region D is often discretized into N points ($N \gg n$), and the $CCD_p(n, \mathcal{P})$ value in Eq. (2) can be approximately calculated through the following expression:

$$CCD_p(n, \mathcal{P}) \approx \left\{ \frac{1}{N} \sum_{i=1}^{N} \frac{1}{2^q} \sum_{t=1}^{2^q} \left| \frac{N(D_t(x_i), \mathcal{P})}{n} - \frac{N(D_t(x_i))}{N} \right|^p \right\}^{1/p}. \tag{3}$$

2.2. *The SA*

The switching algorithm (SA) is an efficient algorithm which has been used in Winker and Fang (1998), Fang et al. (2001), and Chuang and Hung (2010). It could be restated as follows:

Algorithm 2.1. (SA, Chuang and Hung, 2010).

Step 1. Discretize the region D, which means replacing D by N points in it, i.e., $D = \{g_1, \ldots, g_N\}$, where $N \gg n$.
Step 2. Arbitrary choose n points as the initially current design "Cdesign," for example, choose Cdesign $= \{g_1, \ldots, g_n\}$; set the iteration counter $i = 0$ and the next design Ndesign = Cdesign.
Step 3. While $i = 0$ or Ndesign $\neq$ Cdesign
  set $i = i + 1$, Cdesign=Ndesign;
  for $j = 1$ to n do
    let $g^* = \arg \min_{g \in D \setminus \text{Ndesign}} CCD_p(n, \{g\} \bigcup \text{Ndesign} \setminus \{g_j\})$;
    if $CCD_p(n, \{g^*\} \bigcup \text{Ndesign} \setminus \{g_j\}) \leq CCD_p(n, \text{Ndesign})$
      set Ndesign $= \{g^*\} \bigcup \text{Ndesign} \setminus \{g_j\}$;
    end if
  end for
 end while.
Step 4. Export Cdesign, $CCD_p(n, \text{Cdesign})$ and i.

Remark 2.1. Note that N denotes the number of points which we discretize the irregular design area into. The choice of N is arbitrary, of course a larger N means a more uniform final design will be obtained but under a more time-consuming process. The algorithm requires $N \gg n$, and through some simulations we found that the ratio of N to n (the run size of the design) being greater than 5 is enough. Therefore, in the two examples in Sec. 3, we will discretize the corresponding design regions reasonably so that $N/n > 5$.

Chuang and Hung (2010) has shown that the SA has less iteration times, quicker convergence speed and saves time dramatically compared with the exhaustive search, and what is more, the performance of the NUD obtained via the SA is extremely close to the most uniform design.

2.3. The RMSD, MD, and AD criteria

We now introduce three commonly used criteria for measuring the uniformity of designs, which will assist us to understand the CCD criterion. Suppose $\mathcal{P} = \{p_1, \ldots, p_n\}$ denotes a design composed of n points in irregular region $D \subseteq \mathcal{R}^q$, and the distance between a point $x = (x_1, \ldots, x_q)$ in D and the design $\mathcal{P}$ is defined as

$$d(x, \mathcal{P}) = \min_{1 \le i \le n} d(x, p_i), \quad 1 \le i \le n, \text{ where}$$
$$d(x, p_i) = [(x - p_i)(x - p_i)']^{1/2},$$

then the root of mean squared distance (RMSD), maximum distance (MD), and average distance (AD) discrepancies are defined as

$$RMSD(\mathcal{P}) = \sqrt{E[(d(x, \mathcal{P}))^2]}, \quad MD(\mathcal{P}) = \max_{x \in D}[d(x, \mathcal{P})], \text{ and}$$
$$AD(\mathcal{P}) = E[d(x, \mathcal{P})],$$

respectively, where $E[f(x)] = \int_D f(x)dx$. If the region D is discretized into N points $\{u_1, \ldots, u_N\}$, then the RMSD, MD, and AD values can be approximated by

$$RMSD(\mathcal{P}) \approx \sqrt{\frac{1}{N}\sum_{m=1}^{N}(d(u_m, \mathcal{P}))^2}, \quad MD(\mathcal{P}) \approx \max_{m=1,\ldots,N} d(u_m, \mathcal{P}), \text{ and}$$
$$AD(\mathcal{P}) \approx \frac{1}{N}\sum_{m=1}^{N} d(u_m, \mathcal{P}),$$

respectively. Apparently, using this three criteria to evaluate the uniformity of designs is reasonable but searching the optimal or nearly optimal design under some of these three criteria is difficult because of the tremendous computing burden.

3. The new method

This section devotes to the new method for finding NUDs for mixture experiments under the CCD criterion. Let us see the principle of the mapping used in the method.

Theorem 3.1. *The simplex* $H = \{(x_1, \ldots, x_q) | \sum_{i=1}^{q} x_i = 1, x_i \ge 0\}$ *can be transformed into the hyperplane* $H_1 = \{(z_1, \ldots, z_q) | z_q = 0\}$ *with its shape and size invariant via the mapping* $T : z = [x - (1, 0, \ldots, 0)]Q$, *where* $x \in H$, $z \in H_1$ *and* Q *is the orthogonal matrix coming from the matrix QR decomposition* $\begin{pmatrix} -1,\ldots,-1 \\ I_{q-1} \end{pmatrix} = Q \begin{pmatrix} R_{(q-1)\times(q-1)} \\ 0_{1\times(q-1)} \end{pmatrix}$, *with* I_{q-1} *being a unity matrix of order* $q - 1$, $R_{(q-1)\times(q-1)}$ *being an upper triangular matrix and* $0_{1\times(q-1)}$ *being a* $(q - 1)$*-dimensional zero vector. And the inverse mapping of* T *can be written as* $T^{-1} : x = zQ' + (1, 0, \ldots, 0)$, *where* z *is in the image of* H, *i.e.,* $z \in T(H)$, *and* $x \in H$.

Proof. The theory of the matrix QR decomposition says that: for any real matrix A with n rows, m columns and rank m, where $n > m$, it can be decomposed as $A = B_{n\times n} \begin{pmatrix} C_{m\times m} \\ 0_{(n-m)\times m} \end{pmatrix}$, where $B_{n\times n}$ represents an orthogonal matrix, $C_{m\times m}$ denotes an upper triangular matrix and $0_{(n-m)\times m}$ is a matrix with all entries zero.

This theory guarantees the existence of matrix Q mentioned in the theorem. Then we have $\begin{pmatrix} -1,\ldots,-1 \\ I_{q-1} \end{pmatrix} = Q \begin{pmatrix} R_{(q-1)\times(q-1)} \\ 0_{1\times(q-1)} \end{pmatrix}$ and it is easily to prove that:

(i) for any point $x \in H$, its image $T(x)$ really falls into the hyperplane H_1 and for any $z \in T(H)$, its preimage $T^{-1}(z) \in H$;

(ii) the mappings T and T^{-1} keep the Euclid distance invariant, which means $d(x_1, x_2) = d(T(x_1), T(x_2))$ and $d(z_1, z_2) = d(T^{-1}(z_1), T^{-1}(z_2))$, where $x_1, x_2 \in H$, $z_1, z_2 \in T(H)$, and $d(a, b) = [(a-b)(a-b)']^{1/2}$.

So the image $T(H)$ is a subset of H_1 and has the identical shape with the simplex H; and vice versa. □

Furthermore, from this theorem, we can easily show the following.

Corollary 3.1.

(i) The geometry formed by any subset of the simplex H is identical with its image in H_1 after the mapping T.

(ii) If $R_{(q-1)\times(q-1)} = (r_{ij})$, then the points $(0, \ldots, 0)$, $(r_{11}, \ldots, r_{q-1,1}, 0)$, $\ldots$, $(r_{1,q-1}, \ldots, r_{q-1,q-1}, 0)$ are the images of the vertices of the simplex H successively;

(iii) T and T^{-1} can also be viewed as one-to-one mappings between the hyperplane $H_0 = \{(x_1, \ldots, x_q) | \sum_{i=1}^{q} x_i = 1\}$ in $\mathcal{R}^q$ and the $(q-1)$-dimensional space $\mathcal{R}^{q-1}$ but their formulae should be changed a little. Let M and M^{-1} denote the changed ones and they can be expressed as $M : y = [x - (1, 0, \ldots, 0)]Q\binom{I_{q-1}}{0}$ and $M^{-1} : x = y(I_{q-1}, 0)Q' + (1, 0, \ldots, 0)$, respectively, where $x \in H_0$ and $y \in \mathcal{R}^{q-1}$.

Now, let us present the new method for finding NUDs for mixture experiments under the CCD criterion.

Algorithm 3.1.

Step 1. Let D denote the experimental region of a mixture experiment with some constraints, as defined in (1).

Step 2. Transform D into $\mathcal{R}^{q-1}$ through the mapping M proposed in Corollary 3.1, i.e., $y = [x - (1, 0, \ldots, 0)]Q\binom{I_{q-1}}{0}$, $x \in H$. Denote the image after the transformation as D_1.

Step 3. Give the run size n, and search the NUD in D_1 under the CCD criterion by the SA in Algorithm 2.1.

Step 4. Transform the points of the NUD back into the simplex H, by the inverse mapping $M^{-1} : x = y(I_{q-1}, 0)Q' + (1, 0, \ldots, 0)$, $y \in \mathcal{R}^{q-1}$, then we obtain the final NUD in D.

The mappings M and M^{-1} used in the algorithm can also be replaced by the T and T^{-1} provided in Theorem 3.1, respectively, and the result will be the same.

Next, two examples are presented for illustrating this new method.

Example 3.1. Now, we revisit the problem considered in Borkowski and Piepel (2009). Three components x_1, x_2, and x_3 are needed for generating some product, and they have constraints:

$$0.1 \le x_1 \le 0.7,\ 0 \le x_2 \le 0.8,\ 0.1 \le x_3 \le 0.6 \text{ and } x_1 - x_2 \ge 0.$$

We denote the experimental region as S, which could be seen in Fig. 1a, i.e., the area formed by sequentially linking the points C, D, E, F, G, and the equilateral triangle with the vertices $(1, 0, 0)$, $(0, 1, 0)$, and $(0, 0, 1)$ refers to the simplex $H = \{(x_1, x_2, x_3) | x_1 + x_2 + x_3 = 1, x_i \ge 0\}$.

First of all, according to the QR decomposition, we have

$$\begin{pmatrix} -1 & -1 \\ 1 & 0 \\ 0 & 1 \end{pmatrix} = Q_{3\times 3} \begin{pmatrix} R_{2\times 2} \\ 0_{1\times 2} \end{pmatrix} = \begin{pmatrix} -\sqrt{2}/2 & -\sqrt{6}/6 & \sqrt{3}/3 \\ \sqrt{2}/2 & -\sqrt{6}/6 & \sqrt{3}/3 \\ 0 & \sqrt{6}/3 & \sqrt{3}/3 \end{pmatrix} \begin{pmatrix} \sqrt{2} & \sqrt{2}/2 \\ 0 & \sqrt{6}/2 \\ 0 & 0 \end{pmatrix},$$

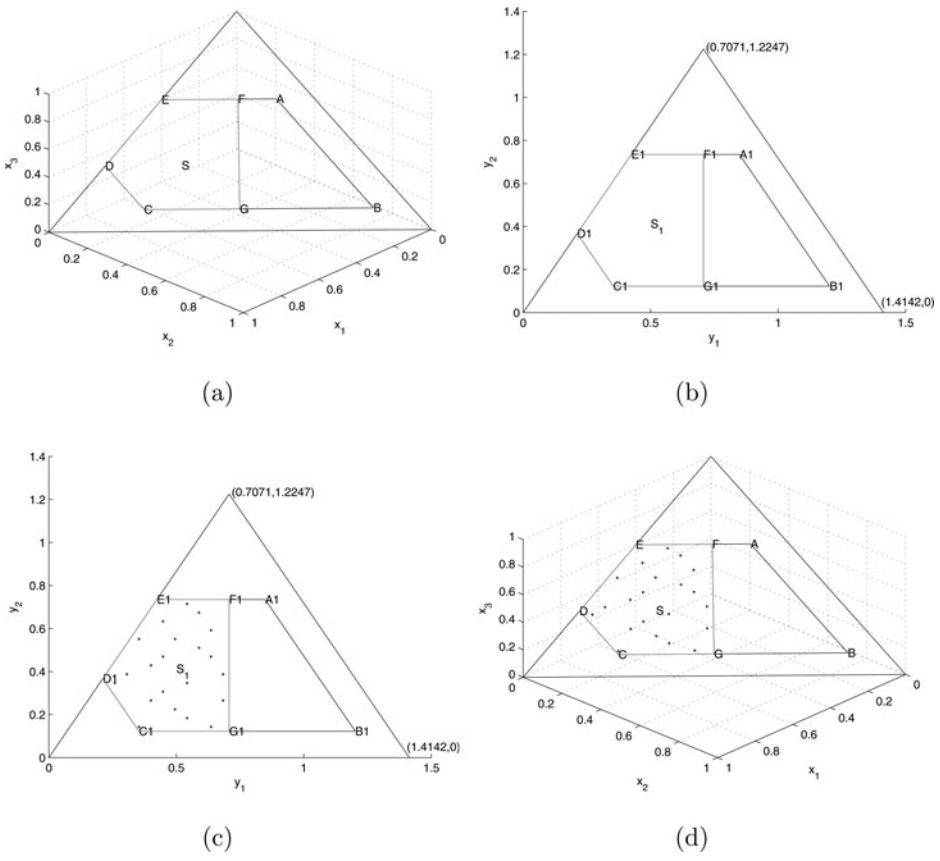

Figure 1. Illustration for Example 3.1: (a) the experimental region S (i.e., the region enclosed by points C, D, E, F, G); (b) the image of S after the mapping (i.e., the region enclosed by points C_1, D_1, E_1, F_1, G_1); (c) the NUD with $n = 21$ in the image of S; and (d) the final NUD with $n = 21$ in S. The points are: $A = (0.1, 0.3, 0.6)$, $B = (0.1, 0.8, 0.1)$, $C = (0.7, 0.2, 0.1)$, $D = (0.7, 0, 0.3)$, $E = (0.4, 0, 0.6)$, $F = (0.2, 0.2, 0.6)$, $G = (0.45, 0.45, 0.1)$, $A_1 = (0.8485, 0.7348)$, $B_1 = (1.2021, 0.1225)$, $C_1 = (0.3536, 0.1225)$, $D_1 = (0.2121, 0.3674)$, $E_1 = (0.4243, 0.7348)$, $F_1 = (0.7071, 0.7348)$, and $G_1 = (0.7071, 0.1225)$.

so the mapping and its inverse mapping can be expressed as

$$M: \quad y = [x - (1,0,0)] \begin{pmatrix} -\sqrt{2}/2 & -\sqrt{6}/6 & \sqrt{3}/3 \\ \sqrt{2}/2 & -\sqrt{6}/6 & \sqrt{3}/3 \\ 0 & \sqrt{6}/3 & \sqrt{3}/3 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 0 \end{pmatrix}, \text{ and}$$

$$M^{-1}: \quad x = y \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} -\sqrt{2}/2 & \sqrt{2}/2 & 0 \\ -\sqrt{6}/6 & -\sqrt{6}/6 & \sqrt{6}/3 \\ \sqrt{3}/3 & \sqrt{3}/3 & \sqrt{3}/3 \end{pmatrix} + (1,0,0),$$

respectively. Figure 1b shows the image of S, denoted by S_1, i.e., the region enclosed by the points C_1, D_1, E_1, F_1, G_1, and the vertices of the simplex H after the mapping, i.e., $(0, 0)$, $(\sqrt{2}, 0)$ and $(\sqrt{2}/2, \sqrt{6}/2)$.

Next we discretize the region S_1 into 128 points, the process of this discretization proceeds in this way: the range intervals of the equilateral triangle in Fig. 1b are $[0, \sqrt{2}]$ on the axis y_1 and $[0, \sqrt{6}/2]$ on the axis y_2, respectively, then we divide the rectangle $[0, \sqrt{2}] \times [0, \sqrt{6}/2]$ into 30×30 small grids with the same size, take all the center points of these grids and keep

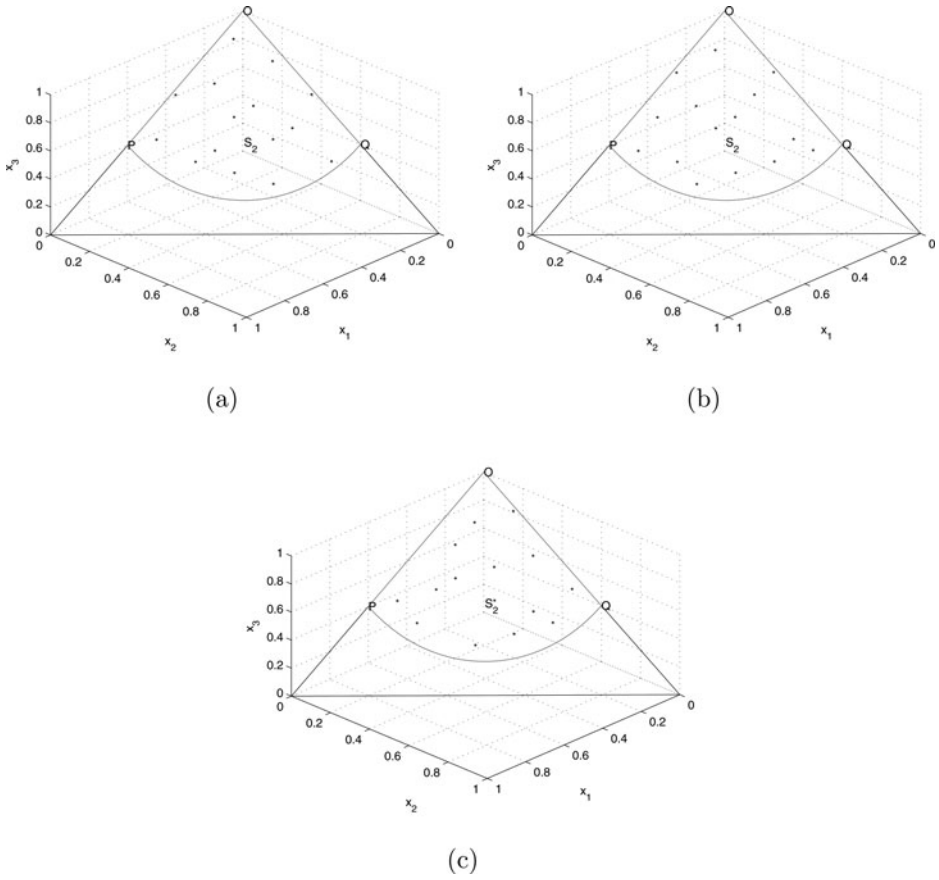

Figure 2. Illustration for Example 3.2: (a), (b), and (c) display three different NUDs with $n = 15$ in the sector region obtained by repeatedly run the program three times. The coordinates of the vertices of the sector are: $O = (0, 0, 1)$, $P = (0.6, 0, 0.4)$, and $Q = (0, 0.6, 0.4)$.

the ones just falling into S_1, finally, 128 points are kept and will be used as a substitute for the continuous region S_1.

For a given run size $n = 21$, an NUD can be constructed according to the new method and its points are drawn in Fig. 1d. The CCD value of this final NUD ends in 0.0201, which indicts that this NUD is a fairly uniform design. The corresponding values of RMSD, MD and AD are 0.0506, 0.1027, and 0.0466, respectively, which are close to but slightly larger than that of Borkowshi and Piepel (2009), which are 0.0469, 0.0878, and 0.0433, respectively. This means that the uniformity of the design obtained through the new method is almost the same but a little worse than that of Borkowshi and Piepel (2009), but the advantage of the new method lies in that it can deal with mixture experiments with any complex constraints and Borkowshi and Piepel's (2009) can only handle the case with linear constraints.

Example 3.2 will construct NUDs for a mixture experiment with non-linear constraints which cannot be solved by the method of Borkowshi and Piepel (2009).

Example 3.2. Consider the design region

$$S_2 = \{(x_1, x_2, x_3) | x_1 + x_2 + x_3 = 1, x_1^2 + x_2^2 \leq 0.36, x_i \geq 0\}$$

Table 1. The values of CCD, RMSD, MD, and AD of the three NUDs in Example 3.2.

	CCD	RMSD	MD	AD
Figure 2 (a)‡	0.0282	0.0840	0.1414	0.0752
Figure 2 (b)	0.0290	0.0841	0.1541	0.0748
Figure 2 (c)	0.0283	0.0833	0.1837	0.0740

‡: Figure 2a denotes the design drawn in Fig. 2a and so on.

with $n = 15$ points. Similarly as we do in Example 3.1, obtain the image of S_2 through the mapping, denoted by S_3, discretize S_3 into 112 points, i.e., dividing the rectangle $[0, \sqrt{2}] \times [0, \sqrt{6}/2]$ into 20×20 small grids with the same size and keeping the corresponding center points that falling into S_3, where among the 400 center points, there are just 112 such points. Then use the new method to construct NUDs. Repeatedly run the program for three times, we get three different designs just as Fig. 2 shows. The corresponding values of CCD, RMSD, MD, and AD are listed in Table 1. It can be seen from Fig. 2 that all these three designs have good uniformity, and Table 1 shows that these three NUDs have similar values under each of these four criteria, which means that the NUDs constructed by the new method have stable quality.

Remark 3.1. Because the initial design in the SA (i.e., Algorithm 2.1) is arbitrary, the resulting design will not be exclusive. However, Chuang and Hung (2010) showed that all the resulting designs from the SA approximate very well the optimal design (based on exhaustive search) and have a very small standard deviation of the CCD values through a trail of 100 times simulations on a unit square input domain, which means the SA is a stable algorithm and each resulting design from the SA is very close to the optimal design (based on exhaustive search). Of course the CPU time for finding the NUD based on the SA is far less than that of finding the optimal design.

4. Concluding remarks

This article proposes a new method to handle the problem of constructing NUDs for mixture experiments with complex constraints, based on the CCD criterion for irregular experimental regions and the SA used in Chuang and Hung (2010). And what is more, the experimental region of a q-component mixture experiment with any constraints is essentially a $(q-1)$-dimensional irregular geometry and both of them come to the same thing, so the uniform designs for irregular regions and mixture experiments can be constructed by the same methods under the same criteria, and it is not necessary to treat them separately as in the past. This will greatly broaden the ways of coping with these two problems.

One more point to be noted is that both examples consider the case when there are $q = 3$ components involved in each mixture experiment, and hence the CCD value of each design in the SA (i.e., Algorithm 2.1) is calculated by taking the "q in Eq. (3)" equal to 2. As for the case when there are $q > 5$ (a larger q) components, both Algorithms 2.1 and 3.1 can be carried out the same as $q = 3$. In particular, the CCD value of each design can also be calculated using Eq. (3). However, for this case, for any point x, the region D is no longer divided into $2^2 = 4$ small grids around x, but 2^{q-1} ones, thus the computation of Eq. (3) would be more complex.

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