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Sliced space-filling designs

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SUMMARY

We propose an approach to constructing a new type of design, a sliced space-filling design, intended for computer experiments with qualitative and quantitative factors. The approach starts with constructing a Latin hypercube design based on a special orthogonal array for the quantitative factors and then partitions the design into groups corresponding to different level combinations of the qualitative factors. The points in each group have good space-filling properties. Some illustrative examples are given.

Some key words: Bush's construction; Computer experiment; Design of experiment; Difference matrix; Rao–Hamming construction.

1. INTRODUCTION

The standard framework for computer experiments assumes that the input factors are quantitative (Fang et al., 2005; Koehler & Owen, 1996; Santner et al., 2003). However, some input factors of computer models can be qualitative. For example, a data centre computer experiment can involve qualitative factors like diffuser height and hot-air return-vent location (Schmidt et al., 2005). Computer models in marketing and the social sciences frequently involve qualitative factors such as education level, race and social background. The study of computer experiments with qualitative and quantitative factors involves two aspects: experimental planning and data modelling. Gaussian process models can be used for modelling such experiments. See Qian et al. (2008) for new Gaussian process models with these two types of factors. Related work includes Han et al. (2009) and McMillan et al. (1999). To the best of our knowledge, no systematic study has hitherto been done to address the planning issue. This issue poses new challenges since the existing space-filling designs, such as Latin hypercube types of designs (McKay et al., 1979; Owen, 1992; Tang, 1993), assume that all input factors are quantitative. In this article, a general approach is proposed for constructing a new type of design, called a sliced space-filling design, to accommodate both qualitative and quantitative factors. The approach starts by constructing a Latin hypercube design based on a special orthogonal array for the quantitative factors. The design is then partitioned into groups corresponding to different level combinations of the qualitative factors, each achieving uniformity in low dimensions.

2. SLICED ORTHOGONAL ARRAYS AND SLICED SPACE-FILLING DESIGNS

First we define a special type of orthogonal array. An orthogonal array of size n, m constraints, s levels and strength $t \geqslant 2$ is an $n \times m$ matrix with entries from a set of s levels such that for every $n \times t$ submatrix, the s^t level combinations occur equally often. Such an array is denoted by $\text{OA}(n, m, s, t)$. Let B be an $\text{OA}(n_1, k, s_1, t)$. Suppose the n_1 rows of this array can be partitioned into v subarrays each with n_2 rows, denoted by B_i, and there is a projection δ that collapses the s_1 levels of B into s_2 levels with $s_1 > s_2$. Furthermore, suppose B_i is an $\text{OA}(n_2, k, s_2, t)$ if the s_1 levels of B are collapsed according to δ. Then B, or more precisely $(B_1, \ldots, B_v)$, is a sliced orthogonal array.

Let B be a sliced orthogonal array. The construction of a sliced space-filling design is as follows. The array B is used to generate an orthogonal array-based Latin hypercube design D (Tang, 1993) for the quantitative factors, where the points corresponding to B_i are denoted by D_i. Then the D_is are associated with different level combinations of the qualitative factors. The array D, or more precisely $(\text{D}_1, \ldots, \text{D}_v)$, is a sliced space-filling design. Such designs have some desirable properties. First, for any qualitative factor level combination, the design points for the quantitative factors achieve uniformity in low dimensions. Second, they possess good space-filling properties when collapsed over the qualitative factors. These properties are, to some extent, similar to those of response surface designs with both qualitative and quantitative factors (Box & Draper, 1987; Draper & John, 1988; Wu & Ding, 1998). It is intuitively appealing to use a sliced space-filling design to conduct a computer experiment with qualitative and quantitative factors, where all the factors can affect the response. The effect of the quantitative factors on the response may vary considerably from one level combination of the qualitative factors to another. The first property stated above ensures that, at any qualitative factor level combination, the values of the quantitative factors are spread uniformly in a low-dimensional space. If the effect of the qualitative factors on the response is very small, the second property guarantees that, after these inert factors are fixed at convenient values, the points of the collapsed design for the quantitative factors are uniformly distributed, thus allowing a more thorough exploration of the design space.

3. FIELD-TO-FIELD PROJECTIONS

For every prime p and every integer $u \geqslant 1$, there exists a Galois field $\text{GF}(p^u)$ of order p^u. The additive group $\text{GF}(p^u)$ is cyclic, and the multiplicative group $\text{GF}(p^u)/\{0\}$ is cyclic, allowing easy calculations under multiplication. Every Galois field has at least one primitive element. The elements of any Galois field or any subset of a Galois field are arranged in lexicographical order.

Throughout the article, let $s_1 = p^{u_1}$ and $s_2 = p^{u_2}$ be powers of the same prime p with integers $u_1 > u_2 \geqslant 1$ and $q = s_1/s_2 = p^{u_1-u_2}$. Let F denote $\text{GF}(s_1)$ with a primitive polynomial $p_1(x)$. Let $f(x)$ denote the elements of F. Let α be the primitive element x of F, or more precisely the element $[x] \bmod p_1(x)$. In condensed notation, let $\alpha_0, \ldots, \alpha_{s_1-1}$ denote the elements of F with $\alpha_0 = 0$ and $\alpha_i = \alpha^i$ $(i = 1, \ldots, s_1 - 1)$.

Now we present field-to-field projections, which are useful for the construction of sliced orthogonal arrays in §§ 4–6. First, introduce a new projection ϕ by assuming u_2 divides u_1, denoted by $u_2 \mid u_1$. Obtain G as the subfield of F with s_2 elements as follows. The elements of G are identified by using the fact that $\alpha^{s_1-1} = 1$ and taking β to be the primitive element of G given by $\beta = \alpha^{(s_1-1)/(s_2-1)}$. The elements of G are $0, \beta, \beta^2, \ldots, \beta^{s_2-1}$ with $\beta^{s_2-1} = 1$. For $u_2 = 1$, G is reduced to the residue field $\{0, 1, \ldots, p-1\} \bmod p$. The projection ϕ maps the elements of F to those of G. We call it the subfield projection because of the assumed subfield structure. Let $g(x)$ denote the elements of G. In condensed notation, let $\beta_0, \ldots, \beta_{s_2-1}$ denote the same set of elements with $\beta_0 = 0$ and $\beta_i = \beta^i$ $(i = 1, \ldots, s_2 - 1)$. It is known that F can be viewed as a vector space over G with respect to the polynomial basis $\{1, \alpha, \alpha^2, \ldots, \alpha^{\lambda-1}\}$ with $\lambda = u_1/u_2$ (Lidl & Niederreiter, 1997). Any $f(x)$ in F can be uniquely represented as

$$f(x) = b_0 + b_1\alpha + \cdots + b_{\lambda-1}\alpha^{\lambda-1}, \; b_i \in G \quad (i = 0, \ldots, \lambda - 1). \tag{1}$$

For $f(x)$ in (1), define

$$\phi\{f(x)\} = b_0 + b_1\beta + \cdots + b_{\lambda-1}\beta^{\lambda-1}, \; b_i \in G \quad (i = 0, \ldots, \lambda - 1). \tag{2}$$

LEMMA 1. *For the subfield projection* ϕ,

(i) $\phi\{f(x)\} = f(x)$, *for any* $f(x) \in G$;
(ii) $\phi\{f_1(x) + f_2(x)\} = \phi\{f_1(x)\} + \phi\{f(x_2)\}$, *for any* $f_1(x), f_2(x) \in F$;
(iii) $\phi\{f_1(x)f_2(x)\} = \phi\{f_2(x)f_1(x)\}$, *for any* $f_1(x), f_2(x) \in F$;
(iv) $\phi\{f_1(x)f_2(x)\} = \phi\{f_1(x)\}\phi\{f_2(x)\}$, *for any* $f_1(x) \in G$ *and* $f_2(x) \in F$.

Proof. Only (iv) needs a proof. Write any $f_2(x) \in F$ as $f_2(x) = \sum_{i=0}^{\lambda-1} b_i\alpha^i$, $b_i \in G$ $(i = 0, \ldots, \lambda - 1)$. Then, for any $f_1(x) \in G$, $f_1(x)f_2(x) = \sum_{i=0}^{\lambda-1} f_1(x)b_i\alpha^i$ is a polynomial in α of degree at most $\lambda - 1$ and $\phi\{f_1(x)f_2(x)\} = \sum_{i=0}^{\lambda-1} f_1(x)b_i\beta^i$. Thus, $\phi\{f_1(x)f_2(x)\} = \phi\{f_1(x)\}\phi\{f_2(x)\}$ as $\phi\{f_1(x)\} = f_1(x)$ and $\phi\{f_2(x)\} = \sum_{i=0}^{\lambda-1} b_i\beta^i$. □

Next we present another projection φ, taken from Qian et al. (2009) for constructing nested space-filling designs. Let F_0 denote the subset $\{a_0 + a_1x + \cdots + a_{u_2-1}x^{u_2-1} \mid a_j \in \mathrm{GF}(p)\}$ of F. Clearly, F_0 has s_2 elements. Here we use G to denote the Galois field $\mathrm{GF}(s_2)$ with a primitive polynomial $p_2(x)$. Let $g(x)$ denote the elements of G. In condensed notation, let $\beta_0, \ldots, \beta_{s_2-1}$ denote the same set of elements, where $\beta_0 = 0$, $\beta_i = \beta^i$ $(i = 1, \ldots, s_2 - 1)$ and β is the primitive element x of G. This projection maps the elements of F to those of G. For any element $\beta_i = a_0 + a_1x + \cdots + a_{u_2-1}x^{u_2-1}$ in G, or more precisely the element $[\beta_i]$ mod $p_2(x)$, let $\tilde{\beta}_i$ denote the corresponding element $[a_0 + a_1x + \cdots + a_{u_2-1}x^{u_2-1}]$ mod $p_1(x)$ in F_0. Whenever necessary, we use the symbol ˜ to denote polynomials with coefficients from F_0, and vectors and matrices based on F_0. For $u_2 > 1$ and any $f(x) \in F$, $\varphi\{f(x)\}$ is defined by

$$\varphi\{f(x)\} = f(x)\{\mathrm{mod}\ p_2(x)\}. \tag{3}$$

For $u_2 = 1$, take $\varphi\{f(x)\} = a_0$ for any $f(x) = a_0 + a_1x + \cdots + a_{u_1-1}x^{u_1-1}$. Because φ works by taking modulus residues, we call it the modulus projection.

LEMMA 2. *For the modulus projection* φ,

(i) $\varphi(\tilde{\beta}_i) = \beta_i$, *for any* $\tilde{\beta}_i \in F_0$;
(ii) $\varphi(\alpha_i + \alpha_j) = \varphi(\alpha_i) + \varphi(\alpha_j)$, *for any* $\alpha_i, \alpha_j \in F$;
(iii) $\varphi(\prod_{j=1}^{t} \tilde{\beta}_{ij}) = \prod_{j=1}^{t} \beta_{ij}$, *for any* $\tilde{\beta}_{i1}, \ldots, \tilde{\beta}_{it} \in F_0$ *and* $tu_2 \leqslant u_1 + t - 1$.

Only (iii) needs a proof. It can be readily verified following the definition of φ.

We now introduce some useful notation. For a matrix A, A' denotes the transpose of A, $a + A$ denotes the elementwise sum of A and a scalar a, and $A(:, j)$ denotes the jth column, $A(i, :)$ denotes the ith row and $A(i, j)$ denotes the (i, j)th entry of A. Let δ be either of the projections described above. For a vector a based on F, $\delta(a)$ denotes the vector obtained from a after the levels of its entries are collapsed according to δ. Similarly, define $\delta(\mathrm{D})$ for an array D based on F. For any $B \subseteq F$, let $\delta(B) = [\delta\{f(x)\} : f(x) \in B]$. For any $g(x) \in G$, let $\delta^{-1}\{g(x)\} = \{f(x) \in$

$F : \delta\{f(x)\} = g(x)\}$. For $D \subseteq G$, let $\delta^{-1}(D) = [f(x) \in F : \delta\{f(x)\} \in D]$. Define Γ to be the $s_2 \times q$ kernel matrix of δ, given as

$$\Gamma = \begin{pmatrix} \delta^{-1}(\beta_0) \\ \delta^{-1}(\beta_1) \\ \vdots \\ \delta^{-1}(\beta_{s_2-1}) \end{pmatrix}, \tag{4}$$

where the entries in each row are arranged in lexicographical order; each element of F appears precisely once; and $\delta\{\Gamma(:, j)\} = G$. Define $c_1(x) = 0$. For the modulus projection φ, $\Gamma(:, 1)$ is F_0 and

$$\Gamma(:, j) = \Gamma(:, 1) + c_j(x) \quad (j \geqslant 2), \tag{5}$$

where $c_j(x)$ is a multiple of $p_2(x)$ for $u_2 > 1$ and is a polynomial in x of degree at most $u_1 - 1$ and zero constant coefficient for $u_2 = 1$.

Example 1. Let $p = 2, u_1 = 2$ and $u_2 = 1$ with $s_1 = 4$ and $s_2 = 2$. Use $p_1(x) = x^2 + x + 1$ for $F = \mathrm{GF}(4)$ with $\alpha = x$. Take G to be the subfield $\{0, 1\}$ of F with $\beta = 1$. Here ϕ is $\{0, x + 1\} \to 0$, $\{1, x\} \to 1$, and

$$\Gamma = \begin{pmatrix} 0 & x+1 \\ 1 & x \end{pmatrix}.$$

Example 2. Let $p = 2$, $u_1 = 4$ and $u_2 = 2$ with $s_1 = 16$ and $s_2 = 4$. Use $p_1(x) = x^4 + x + 1$ for $F = \mathrm{GF}(16)$ with $\alpha = x$. Let G be the subfield $\{0, x^2 + x, x^2 + x + 1, 1\}$ of F, where $\beta = x^2 + x$ and $\beta^2 = x^2 + x + 1$. Here ϕ is $\{0, x^2, x^3 + x + 1, x^3 + x^2 + x + 1\} \to 0$, $\{1, x^2 + 1, x^3 + x, x^3 + x^2 + x\} \to 1$, $\{x, x^2 + x, x^3 + 1, x^3 + x^2 + 1\} \to x^2 + x$, $\{x + 1, x^2 + x + 1, x^3, x^3 + x^2\} \to x^2 + x + 1$, and

$$\Gamma = \begin{pmatrix} 0 & x^2 & x^3+x+1 & x^3+x^2+x+1 \\ 1 & x^2+1 & x^3+x & x^3+x^2+x \\ x & x^2+x & x^3+1 & x^3+x^2+1 \\ x+1 & x^2+x+1 & x^3 & x^3+x^2 \end{pmatrix}.$$

Example 3. Let $p = 2$, $u_1 = 3$ and $u_2 = 2$ with $s_1 = 8$ and $s_2 = 4$. Use $p_1(x) = x^3 + x + 1$ for $F = \mathrm{GF}(8)$ and $p_2(x) = x^2 + x + 1$ for $G = \mathrm{GF}(4)$. Here φ is $\{0, x^2 + x + 1\} \to 0$, $\{1, x^2 + x\} \to 1$,$\{x, x^2 + 1\} \to x$, $\{x + 1, x^2\} \to x + 1$, and

$$\Gamma' = \begin{pmatrix} 0 & 1 & x & x+1 \\ x^2+x+1 & x^2+x & x^2+1 & x^2 \end{pmatrix}.$$

4. CONSTRUCTION OF SLICED ORTHOGONAL ARRAYS USING BUSH'S METHOD

4·1. *Construction with subfield projection*

This construction assumes $u_2 \mid u_1$ and uses the projection ϕ in (2) and the relevant notation in § 3. We first use Bush's method (Hedayat et al., 1999) to obtain an orthogonal array. For $s_2 \geqslant 2$ and $s_2 \geqslant t - 1 \geqslant 0$ with $n_1 = s_1^t$, construct an $n_1 \times (s_1 + 1)$ empty array, whose first s_1 columns are labelled with the elements of F and whose rows are labelled by the n_1 polynomials over F of degree at most $t - 1$ in the variable Y, denoted by $\psi_1, \ldots, \psi_{n_1}$. Hereinafter we call a column labelled with α_i, column α_i, and a row labelled with ψ_j, row ψ_j. Next, the entry in column

α_i and row ψ_j is defined to be $\psi_j(\alpha_i)$, i.e. the value of the polynomial ψ_j at the point α_i. In the last column of the array, the entry in row ψ_j is taken to be the coefficient of Y^{t-1} in ψ_j. After all entries are filled in, let B_0 denote the resulting array, which is an $\mathrm{OA}(n_1, m_1, s_1, t)$ with $m_1 = s_1 + 1$.

Let B be the submatrix of B_0 consisting of the columns labelled by the elements of G and the last column. Clearly, B is an $\mathrm{OA}(n_1, m_2, s_1, t)$ with $m_2 = s_2 + 1$. Now partition B into groups. Let Q^t denote the set of all possible t-tuples from $Q = \{1, \ldots, q\}$ with $q = s_1/s_2$. Pick an arbitrary t-tuple $(l_0, \ldots, l_{t-1}) \in Q^t$. Consider all s_2^t polynomials in Y of degree at most $t-1$ with coefficient b_i taking values in $\Gamma(:, l_i)$ in (4), denoted by $\varphi_1, \ldots, \varphi_{n_2}$ with $n_2 = s_2^t$. Obtain $B_{l_0,\ldots,l_{t-1}}$ as the submatrix of B consisting of rows $\varphi_1, \ldots, \varphi_{n_2}$. Repeat the above procedure for all possible t-tuples in Q^t.

THEOREM 1. *For $s_2 \geqslant t-1 > 0$ and $u_2 \mid u_1$,*

(i) *the matrix B is an $\mathrm{OA}(n_1, m_2, s_1, t)$;*
(ii) *the submatrices $B_{l_0,\ldots,l_{t-1}}$ form a partition of B and $\phi(B_{l_0,\ldots,l_{t-1}})$ is an $\mathrm{OA}(n_2, m_2, s_2, t)$.*

Proof. Only part (ii) needs a proof. Pick an arbitrary t-tuple $(l_0, \ldots, l_{t-1}) \in Q^t$. From Lemma 1, for any j, the entry $\phi(\sum_{i=0}^{t-1} b_i \beta_j^i)$ of $\phi(B_{l_0,\ldots,l_{t-1}})$ in row $b_0 + b_1 Y + \cdots + b_{t-1} Y^{t-1}$ with $b_i \in \Gamma(:, l_i)$ and column β_j equals $\sum_{i=0}^{t-1} \phi(b_i)\beta_j^i$. From (4), $\phi\{\Gamma(:, l_i)\} = G$ $(i = 0, \ldots, t-1)$. This implies that the polynomials $\phi(b_0) + \phi(b_1)Y + \cdots + \phi(b_{t-1})Y^{t-1}$ with $b_i \in \Gamma(:, l_i)$ constitute all polynomials in Y over G of degree at most $t-1$. Denote these polynomials by $\psi_1, \ldots, \psi_{n_2}$. Since $s_2 \geqslant t-1$, $\phi(B_{l_0,\ldots,l_{t-1}})$ is essentially obtained by using Bush's construction with a generator matrix, whose first s_2 columns are labelled with the elements of G and whose rows are labelled by $\psi_1, \ldots, \psi_{n_2}$. Thus, $\phi(B_{l_0,\ldots,l_{t-1}})$ is an $\mathrm{OA}(n_2, m_2, s_2, t)$. □

Example 4. Let $p = 2$, $t = 2$, $u_1 = 2$ and $u_2 = 1$ with $s_1 = 4$ and $s_2 = 2$. Use $p_1(x) = x^2 + x + 1$ for $F = \mathrm{GF}(4)$ with $\alpha = x$. Let G be the subfield $\{0, 1\}$ of F with $\beta = 1$. Here the projection ϕ is $\{0, x+1\} \to 0$, $\{1, x\} \to 1$. From Theorem 1, the transpose of B is

$$\begin{pmatrix} 0 & 1 & x & x+1 & 0 & 1 & x & x+1 & 0 & 1 & x & x+1 & 0 & 1 & x & x+1 \\ 0 & 1 & x & x+1 & 1 & 0 & x+1 & x & x & x+1 & 0 & 1 & x+1 & x & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & x & x & x & x & x+1 & x+1 & x+1 & x+1 \end{pmatrix},$$

which is partitioned into B_{11} with rows 1, 2, 5, 6, B_{12} with rows 9, 10, 13, 14, B_{21} with rows 3, 4, 7, 8 and B_{22} with rows 11, 12, 15, 16. Each $\phi(B_{ij})$ is an OA(4, 3, 2, 2), given as

$$\begin{pmatrix} 1 & 1 & 0 \\ 0 & 0 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 1 \end{pmatrix}.$$

4·2. *Construction with modulus projection*

This construction modifies the previous one by replacing ϕ with φ, and G with F_0 in obtaining the matrix B. The relevant notation in § 3 is used. For B and $B_{l_0,\ldots,l_{t-1}}$ obtained from this construction, we have the following theorem.

THEOREM 2. *For $tu_2 \leqslant u_1 + t - 1$ and $s_2 \geqslant t-1 \geqslant 0$,*

(i) *the matrix B is an $\mathrm{OA}(n_1, m_2, s_1, t)$;*
(ii) *the submatrices $B_{l_0,\ldots,l_{t-1}}$ form a partition of B and $\varphi(B_{l_0,\ldots,l_{t-1}})$ is an $\mathrm{OA}(n_2, m_2, s_2, t)$.*

Proof. First consider $B_{1,\dots,1}$, the submatrix of B consisting of the rows labelled by all s_2^t polynomials in Y over F_0 of degree at most $t-1$. Let $\tilde{h}_1, \dots, \tilde{h}_{n_2}$ denote these polynomials with $n_2 = s_2^t$. Identify h_i for every $\tilde{h}_i$; see § 1 for the definition of $\tilde{\ }$. Since $\varphi(F_0) = G$, $h_1, \dots, h_{n_2}$ constitute all polynomials in Y over G of degree at most $t-1$. Since $tu_2 \leqslant u_1 + t - 1$, Lemma 2 implies that the entry $\varphi\{\tilde{h}_k(\tilde{\beta}_j)\}$ of $\varphi(B_{1,\dots,1})$ in row $\tilde{h}_k$ and column $\tilde{\beta}_j$ equals $h_k(\beta_j)$, and $\varphi(B_{1,\dots,1})$ is essentially obtained by using Bush's construction with a generating matrix, whose first s_2 columns are labelled with the elements of G and whose rows are labelled by $h_1, \dots, h_{n_2}$. Thus, $\varphi(B_{1,\dots,1})$ is an OA(n_2, m_2, s_2, t).

Now pick an arbitrary t-tuple $(l_0, \dots, l_{t-1})$ in Q^t. Consider all polynomials in Y of degree at most $t-1$ with coefficient b_i taking values in $\Gamma(:, l_i)$. Denote them by $\psi_1, \dots, \psi_{n_2}$. From (5),

$$\psi_k(\tilde{\beta}_j) = \tilde{h}_k(\tilde{\beta}_j) + \tau(\tilde{\beta}_j) \tag{6}$$

with the same polynomial $\tau = \sum_{i=0}^{t-1} c_{l_i}(x) Y^i$ used for all ψ_ks. From Lemma 2, projecting (6) by φ gives $\varphi\{\psi_k(\tilde{\beta}_j)\} = h_k(\beta_j) + \eta_j$ with $\eta_j = \varphi\{\tau(\tilde{\beta}_j)\} \in G$. It follows that the jth column of $\varphi(B_{l_0,\dots,l_{t-1}})$ equals that of $\varphi(B_{1,\dots,1})$ plus η_j. If $\eta_j = 0$, the two are the same. Otherwise, the latter can be obtained by permuting some factor levels of the former as G is a cyclic additive group. Because permuting the levels of some factors in an orthogonal array yields another orthogonal array with the same parameters, $\varphi(B_{l_0,\dots,l_{t-1}})$ is an OA(n_2, m_2, s_2, t). □

Example 5. Let $p = 2, u_1 = 3, u_2 = 2$ and $t = 2$ with $s_1 = 8$ and $s_2 = 4$. The condition $tu_2 \leqslant u_1 + t - 1$ in Theorem 2 is satisfied. Use $p_1(x) = x^3 + x + 1$ for $F = \mathrm{GF}(8)$ and $p_2(x) = x^2 + x + 1$ for $G = \mathrm{GF}(4)$. Here φ is $\{0, x^2+x+1\} \to 0, \{1, x^2+x\} \to 1, \{x, x^2+1\} \to x, \{x+1, x^2\} \to x+1$. We have

$$\Gamma' = \begin{pmatrix} 0 & 1 & x & x+1 \\ x^2+x+1 & x^2+x & x^2+1 & x^2 \end{pmatrix}.$$

From Theorem 2, B is an OA(64, 5, 8, 2), which is partitioned into B_{11}, B_{12}, B_{21} and B_{22}, and each $\varphi(B_{ij})$ is an OA(16, 5, 4, 2). For example, B_{21} is

$$\begin{pmatrix}
x^2+x+1 & x^2+x+1 & x^2+x+1 & x^2+x+1 & 0 \\
x^2+x & x^2+x & x^2+x & x^2+x & 0 \\
x^2+1 & x^2+1 & x^2+1 & x^2+1 & 0 \\
x^2 & x^2 & x^2 & x^2 & 0 \\
x^2+x+1 & x^2+x & x^2+1 & x^2 & 1 \\
x^2+x & x^2+x+1 & x^2 & x^2+1 & 1 \\
x^2+1 & x^2 & x^2+x+1 & x^2+x & 1 \\
x^2 & x^2+1 & x^2+x & x^2+x+1 & 1 \\
x^2+x+1 & x^2+1 & x+1 & 1 & x \\
x^2+x & x^2 & x & 0 & x \\
x^2+1 & x^2+x+1 & 1 & x+1 & x \\
x^2 & x^2+x & 0 & x & x \\
x^2+x+1 & x^2 & 1 & x & x+1 \\
x^2+x & x^2+1 & 0 & x+1 & x+1 \\
x^2+1 & x^2+x & x+1 & 0 & x+1 \\
x^2 & x^2+x+1 & x & 1 & x+1
\end{pmatrix},$$

and the transpose of $\varphi(B_{21})$ is

$$\begin{pmatrix} 0 & 1 & x & x+1 & 0 & 1 & x & x+1 & 0 & 1 & x & x+1 & 0 & 1 & x & x+1 \\ 0 & 1 & x & x+1 & 1 & 0 & x+1 & x & x & x+1 & 0 & 1 & x+1 & x & 1 & 0 \\ 0 & 1 & x & x+1 & x & x+1 & 0 & 1 & x+1 & x & 1 & 0 & 1 & 0 & x+1 & x \\ 0 & 1 & x & x+1 & x+1 & x & 1 & 0 & 1 & 0 & x+1 & x & x & x+1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & x & x & x & x & x+1 & x+1 & x+1 & x+1 \end{pmatrix}.$$

The constructed sliced orthogonal arrays in §§ 4·1 and 4·2 have different sets of parameters and complement each other. For $t = 3$ and $2 \leqslant u_1 \leqslant 10$, we can only use ϕ for constructing those with $(u_1, u_2) = (6, 3), (8, 4), (10, 5)$ and only φ for those with $(u_1, u_2) = (5, 2), (7, 2), (7, 3), (8, 3), (9, 2), (10, 3), (10, 4)$.

5. Construction of sliced orthogonal arrays using the Rao–Hamming method

In this section we present a method for constructing sliced orthogonal arrays using the Rao–Hamming method. This construction uses the modulus projection φ and relevant notation from § 3. It is inspired by the method in Qian et al. (2009) for constructing nested space-filling designs.

We first use the Rao–Hamming method to construct an orthogonal array (Hedayat et al., 1999). For any integer $k \geqslant 2$, obtain a $k \times m_1$ matrix Z with $m_1 = (s_1^k - 1)/(s_1 - 1)$ by collecting all column vectors $(c_1, \ldots, c_k)$, where $c_j \in F$ and the first nonzero entry is one. By taking all linear combinations of the row vectors of Z with coefficients from F, obtain a matrix B_0. Clearly, B_0 is an $\mathrm{OA}(n_1, m_1, s_1, 2)$ with $n_1 = s_1^k$. Let $\tilde{U}$ be the submatrix of Z consisting of all columns whose nonzero entries take values in F_0 only. Denote by $\tilde{u}_1, \ldots, \tilde{u}_k$ the rows of $\tilde{U}$. Then obtain a submatrix B of B_0 by taking all linear combinations $\xi_1\tilde{u}_1 + \cdots + \xi_k\tilde{u}_k$ with coefficient $\xi_i \in F$.

Now partition B into groups. Pick an arbitrary k-tuple $(l_1, \ldots, l_k) \in Q^k$ with $Q = \{1, \ldots, q\}$ and $q = s_1/s_2$. Obtain a matrix $B_{l_1,\ldots,l_k}$ by taking the rows of B corresponding to the linear combinations $\xi_1\tilde{u}_1 + \cdots + \xi_k\tilde{u}_k$ with $\xi_i \in \Gamma(:, l_i)$, $i = 1, \ldots, k$. The matrix $B_{l_1,\ldots,l_k}$ has n_2 rows with $n_2 = s_2^k$. Repeat the above procedure for all possible k-tuples in Q^k.

Theorem 3. *For $2u_2 \leqslant u_1 + 1$,*

(i) *the matrix B is an $\mathrm{OA}(n_1, m_2, s_1, 2)$ with $m_2 = (s_2^k - 1)/(s_2 - 1)$;*
(ii) *the submatrices $B_{l_1,\ldots,l_k}$ form a partition of B and $\varphi(B_{l_1,\ldots,l_k})$ is an $\mathrm{OA}(n_2, m_2, s_2, 2)$.*

Proof. Only part (ii) needs a proof. First consider $B_{1,\ldots,1}$, the submatrix whose rows are obtained as all linear combinations $\tilde{\eta}_1\tilde{u}_1 + \cdots + \tilde{\eta}_k\tilde{u}_k$ with $\tilde{\eta}_i \in \Gamma(:, 1)$. We can view $B_{1,\ldots,1} \subset B$ as a nested orthogonal array used in Qian et al. (2009) for constructing nested space-filling designs. It follows from Theorem 1 in Qian et al. (2009) that $\varphi(B_{1,\ldots,1})$ is an $\mathrm{OA}(n_2, m_2, s_2, 2)$. This can also be directly verified using Lemma 2.

Now pick an arbitrary k-tuple $(l_1, \ldots, l_k)$ of Q^k. From (5), any row $\xi_1\tilde{u}_1 + \cdots + \xi_k\tilde{u}_k$ in $B_{l_1,\ldots,l_k}$ can be expressed as

$$\tilde{\eta}_1\tilde{u}_1 + \cdots + \tilde{\eta}_k\tilde{u}_k + \tau, \quad (7)$$

where $\tilde{\eta}_1\tilde{u}_1 + \cdots + \tilde{\eta}_k\tilde{u}_k$ is a row in $B_{1,\ldots,1}$ and the row vector $\tau = \sum_{i=1}^k c_{l_i}(x)\tilde{u}_i$ does not depend on $\xi_1, \ldots, \xi_k$. From Lemma 2, projecting (7) by φ gives $\varphi(\xi_1\tilde{u}_1 + \cdots + \xi_k\tilde{u}_k) = \varphi(\tilde{\eta}_1\tilde{u}_1 + \cdots + \tilde{\eta}_k\tilde{u}_k) + \varphi(\tau)$, where the elements of $\varphi(\tau)$ are denoted by $\epsilon_1, \ldots, \epsilon_{m_2}$. It follows that the jth column of $\varphi(B_{l_1,\ldots,l_k})$ equals that of $\varphi(B_{1,\ldots,1})$ plus $\epsilon_j \in G$. If $\epsilon_j = 0$, the two are the same. Otherwise, the latter can be obtained by permuting some factor levels of the former because G is a cyclic additive group. Since permuting the levels of some factors in an orthogonal array yields another orthogonal array with the same parameters, $\varphi(B_{l_1,\ldots,l_k})$ is an OA$(n_2, m_2, s_2, 2)$. □

Although this construction can be modified by replacing φ with ϕ, this modification does not give any new sliced orthogonal arrays since $u_2 \mid u_1$ implies $2u_2 \leqslant u_1 + 1$.

Example 6. Let $k = 2, p = 2, u_1 = 3$ and $u_2 = 2$ with $s_1 = 8$ and $s_2 = 4$. The condition $2u_2 \leqslant u_1 + 1$ in Theorem 3 is satisfied. Use $p_1(x) = x^3 + x + 1$ for $F = \text{GF}(8)$ and $p_2(x) = x^2 + x + 1$ for $G = \text{GF}(4)$. Here φ is $\{0, x^2 + x + 1\} \to 0, \{1, x^2 + x\} \to 1, \{x, x^2 + 1\} \to x, \{x + 1, x^2\} \to x + 1$, and

$$\Gamma' = \begin{pmatrix} 0 & 1 & x & x+1 \\ x^2+x+1 & x^2+x & x^2+1 & x^2 \end{pmatrix}.$$

From Theorem 3, B is an OA(64, 5, 8, 2), which is partitioned into B_{11}, B_{12}, B_{21} and B_{22}, and each $\varphi(B_{ij})$ is an OA(16, 5, 4, 2).

6. CONSTRUCTION OF SLICED ORTHOGONAL ARRAYS USING DIFFERENCE MATRICES

In this section we provide a procedure for constructing sliced orthogonal arrays based on difference matrices. An $r \times c$ difference matrix is an array with entries from a finite abelian group $\mathcal{A}$ with g elements such that every element of $\mathcal{A}$ appears equally often in the vector difference between any two columns of the array (Hedayat et al., 1999). We denote such an array by D(r, c, g). Throughout $\mathcal{A}$ corresponds to the additive group associated with a Galois field. For a prime power s, a D(s, s, s) can be obtained by constructing the $s \times s$ multiplication table of GF(s), where the rows and columns are labelled by all distinct elements of GF(s) (Hedayat et al., 1999). Hereinafter, in describing such a table, we call a row or column labelled with an element $f(x) \in \text{GF}(s)$ as row or column $f(x)$. Here we assume $u_2 \mid u_1$, and use the projection ϕ and relevant notation from § 3.

Now define a special type of difference matrix. Let A be a D(r_1, c, s_1) based on GF(s_1). Suppose the r_1 rows of this array can be partitioned into v subarrays with r_2 rows, denoted by A_i, and each $\phi(A_i)$ is a D(r_2, c, s_2), where $r_1 > r_2$. Then A, or more precisely $(A_1, \ldots, A_v)$, is called a sliced difference matrix.

Let A_0 be the multiplication table of $F = \text{GF}(s_1)$. By taking the columns of A_0 labelled by the elements of G, obtain a matrix A. Next partition A into groups. For $j = 1, \ldots, q$ with $q = s_1/s_2$, obtain a matrix A_j by taking the rows of A labelled with the elements of $\Gamma(:, j)$.

LEMMA 3. *For A and the A_js,*

(i) *the matrix A is a* D(s_1, s_2, s_1);
(ii) *the submatrices A_j form a partition of A and $\phi(A_j)$ is a* D(s_2, s_2, s_2).

Only (ii) needs a proof. It follows readily from Lemma 1 and the fact $\phi\{\Gamma(:, j)\} = G (j = 1, \ldots, q)$.

Next we develop A into a sliced orthogonal array. Let $C_i = A + \alpha_i$ for $\alpha_i \in F$ $(i = 0, \ldots, s_1 - 1)$. Obtain an array B by juxtaposing C_is: $B = (C_0' \; C_1' \; \ldots \; C_{s_1-1}')'$. Then partition B as follows. For $j, k = 1, \ldots, q$, let $C_{jk}^{(i)} = A_j + \Gamma(i, k)$ $(i = 1, \ldots, s_2)$. Next obtain an array B_{jk} as $[\{C_{jk}^{(1)}\}' \ldots \{C_{jk}^{(s_2)}\}']'$.

Table 1. *The matrix A in Example 7*

	0	1	x^2+x	x^2+x+1
0	0	0	0	0
1	0	1	x^2+x	x^2+x+1
x	0	x	x^3+x^2	x^3+x^2+x
$x+1$	0	$x+1$	x^3+x	x^3+1
x^2	0	x^2	x^3+x+1	x^3+x^2+x+1
x^2+1	0	x^2+1	x^3+x^2+1	x^3
x^2+x	0	x^2+x	x^2+x+1	1
x^2+x+1	0	x^2+x+1	1	x^2+x
x^3	0	x^3	x^2+1	x^3+x^2+1
x^3+1	0	x^3+1	$x+1$	x^3+x
x^3+x	0	x^3+x	x^3+1	$x+1$
x^3+x+1	0	x^3+x+1	x^3+x^2+x+1	x^2
x^3+x^2	0	x^3+x^2	x^3+x^2+x	x
x^3+x^2+1	0	x^3+x^2+1	x^3	x^2+1
x^3+x^2+x	0	x^3+x^2+x	x	x^3+x^2
x^3+x^2+x+1	0	x^3+x^2+x+1	x^2	$x^3+x+1.$

THEOREM 4. *For B and the B_{jk}s,*

(i) *the matrix B is an* $\mathrm{OA}(s_1^2, s_2, s_1, 2)$;

(ii) *the submatrices B_{jk} form a partition of B and $\phi(B_{jk})$ is an* $\mathrm{OA}(s_2^2, s_2, s_2, 2)$;

(iii) *the matrix $\phi(B_{jk})$ is completely resolvable, i.e. equivalent to the juxtaposition of s_2 arrays such that each factor occurs in each of these arrays once at each level.*

Only (ii) and (iii) need a proof. They can be readily verified by using Lemmas 1 and 3 and the fact $\Gamma(:, k) = G (k = 1, \ldots, q)$.

Theorem 4(iii) implies that B_{jk} can be further divided into s_2 subgroups, each becoming a Latin hypercube design with s_2 levels (McKay et al., 1979) after the levels of B_{jk} are collapsed according to ϕ. This property will be further explored in § 7.

Example 7. Let $p = 2, u_1 = 4$ and $u_2 = 2$ with $s_1 = 16$ and $s_2 = 4$. Use $p_1(x) = x^4 + x + 1$ for $F = \mathrm{GF}(16)$ with $\alpha = x$. Let G be the subfield $\{0, 1, x^2 + x, x^2 + x + 1\}$ of F with $\beta = x^2 + x$. The mapping from the elements of F to those of G by ϕ was given in Example 2. Table 1 presents the matrix A, which is a D(16, 4, 16). The dashed lines in the table separate $A_1, \ldots, A_4$ and each $\phi(A_i)$ is a D(4, 4, 4). For example,

$$\phi(A_1) = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & \beta & \beta^2 \\ 0 & \beta & \beta^2 & 1 \\ 0 & \beta^2 & 1 & \beta \end{pmatrix}.$$

The matrix B is an OA(256, 4, 16, 2) and $\phi(B_{jk})$ is an OA(16, 4, 4, 2) with complete resolvability. For example, the transpose of $\phi(B_{11})$ is

$$\begin{pmatrix} 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & \beta & \beta & \beta & \beta & \beta^2 & \beta^2 & \beta^2 & \beta^2 \\ 0 & 1 & \beta & \beta^2 & 1 & 0 & \beta^2 & \beta & \beta & \beta^2 & 0 & 1 & \beta^2 & \beta & 1 & 0 \\ 0 & \beta & \beta^2 & 1 & 1 & \beta^2 & \beta & 0 & \beta & 0 & 1 & \beta^2 & \beta^2 & 1 & 0 & \beta \\ 0 & \beta^2 & 1 & \beta & 1 & \beta & 0 & \beta^2 & \beta & 1 & \beta^2 & 0 & \beta^2 & 0 & \beta & 1 \end{pmatrix},$$

which can be further partitioned into four submatrices, in each of which every element of G appears exactly once in each column.

7. GENERATION OF SLICED SPACE-FILLING DESIGNS

In this section we present a procedure for using the constructed sliced orthogonal arrays in the previous sections to generate sliced space-filling designs. It consists of two steps. First, for the quantitative factors a Latin hypercube design is generated based on a sliced orthogonal array and then it is partitioned into different groups, where the points in each group achieve good space-filling properties in low dimensions. Second, these groups are associated with different level combinations of the qualitative factors. Since the second step is rather straightforward, our discussion focuses on the first step. Because the sliced orthogonal arrays in §§ 4–6 have different structures, we discuss them separately. Throughout we assume that each of the quantitative factors takes values in the interval [0, 1]. When we say that a design is space filling or achieves uniformity in low dimensions, we mean that, when projected onto low dimensions, the design points are evenly scattered in the design region.

First, suppose B is a sliced orthogonal array from Theorem 3, where B is an OA$(n_1, m_2, s_1, 2)$, $B_1, \ldots, B_v$ are a partition of B and $\varphi(B_i)$ is an OA$(n_2, m_2, s_2, 2)$. In constructing a Latin hypercube design based on B, the s_1 levels of B, currently represented by the elements of a Galois field, have to be relabelled as $1, \ldots, s_1$. The projection φ divides the s_1 levels into s_2 groups, each of size $q = s_1/s_2$ and the levels $f_1(x)$ and $f_2(x)$ belong to the same group if $\phi\{f_1(x)\} = \phi\{f_2(x)\}$. To ensure that the points corresponding to each B_i have good space-filling properties, following Qian et al. (2009), we label the s_1 levels of B in such a way that the group of levels that are mapped to the same level should form a consecutive subset of $\{1, \ldots, s_1\}$. The s_2 groups can be arbitrarily labelled as groups $1, \ldots, s_2$, and the q levels within the ith group can be arbitrarily labelled as $(i-1)q+1, \ldots, (i-1)q+q$ for $i = 1, \ldots, s_2$. After labelling the levels of B as $1, \ldots, s_1$ as discussed above, we now use B to obtain an orthogonal array-based Latin hypercube design D (Tang, 1993). Let D_i be the subset of D corresponding to B_i. Then D achieves uniformity on $s_1 \times s_1$ grids in two dimensions, in addition to achieving maximum uniformity in one dimension; and $\mathrm{D}_1, \ldots, \mathrm{D}_v$ are a partition of D and D_i achieves uniformity on $s_2 \times s_2$ grids in two dimensions.

Now suppose B is a sliced orthogonal array from Theorem 4 with $(B_{11}, \ldots, B_{qq})$ as its partition. Using this B to generate a sliced space-filling design can be done similarly as above, where D denotes the orthogonal array-based Latin hypercube design and D_{jk} denotes the subset of D corresponding to B_{jk}. Due to the complete resolvability of B_{jk}, D_{jk} can be further divided into s_2 groups D_{jkl}. Then D achieves uniformity on $s_1 \times s_1$ grids in two dimensions, in addition to achieving maximum uniformity in one dimension; D_{jk} achieves uniformity on $s_2 \times s_2$ grids in two dimensions and D_{jkl} achieves uniformity in one dimension with respect to s_2 equally spaced intervals.

Next, consider using a sliced orthogonal array B from Theorem 1. The procedure with an array from Theorem 2 is similar. Unlike the previous situations, this array can have strength three or higher. For easier presentation, assume B is an OA$(n_1, m_2, s_1, 3)$ based on F and B_is denote a partition of B, where $\phi(B_i)$ is an OA$(n_2, m_2, s_2, 3)$ based on G. For $j = 0, \ldots, s_2 - 1$, obtain a submatrix B_{ij} of B_i by taking the rows whose entries in the first column take values in $\phi^{-1}(\beta_j)$. Obtain a matrix C_{ij} by deleting the first column of B_{ij}. Finally, delete the first column of B_i to generate a matrix C_i and delete the first column of B to generate a matrix C. Here, $\phi(C_i)$ is an OA$(n_2, m_2 - 1, s_2, 3)$ and $\phi(C_{ij})$ is an OA$(n_3, m_2 - 1, s_2, 2)$, where $n_3 = n_2/s_2$ and $m_2 - 1 \geqslant 3$. We then label the levels of C with $1, \ldots, s_1$ as done above and use C to construct an orthogonal

Table 2. *The matrix B in Example 8*

Run #	x_1	x_2	x_3	x_4	x_5	Run #	x_1	x_2	x_3	x_4	x_5
1	1	1	1	1	1	33	1	8	8	8	8
2	3	1	3	5	7	34	3	8	6	4	2
3	5	1	5	8	4	35	5	8	4	1	5
4	7	1	7	4	6	36	7	8	2	5	3
5	8	1	8	7	2	37	8	8	1	2	7
6	6	1	6	3	8	38	6	8	3	6	1
7	4	1	4	2	3	39	4	8	5	7	6
8	2	1	2	6	5	40	2	8	7	3	4
9	1	3	3	3	3	41	1	6	6	6	6
10	3	3	1	7	5	42	3	6	8	2	4
11	5	3	7	6	2	43	5	6	2	3	7
12	7	3	5	2	8	44	7	6	4	7	1
13	8	3	6	5	4	45	8	6	3	4	5
14	6	3	8	1	6	46	6	6	1	8	3
15	4	3	2	4	1	47	4	6	7	5	8
16	2	3	4	8	7	48	2	6	5	1	2
17	1	5	5	5	5	49	1	4	4	4	4
18	3	5	7	1	3	50	3	4	2	8	6
19	5	5	1	4	8	51	5	4	8	5	1
20	7	5	3	8	2	52	7	4	6	1	7
21	8	5	4	3	6	53	8	4	5	6	3
22	6	5	2	7	4	54	6	4	7	2	5
23	4	5	8	6	7	55	4	4	1	3	2
24	2	5	6	2	1	56	2	4	3	7	8
25	1	7	7	7	7	57	1	2	2	2	2
26	3	7	5	3	1	58	3	2	4	6	8
27	5	7	3	2	6	59	5	2	6	7	3
28	7	7	1	6	4	60	7	2	8	3	5
29	8	7	2	1	8	61	8	2	7	8	1
30	6	7	4	5	2	62	6	2	5	4	7
31	4	7	6	8	5	63	4	2	3	1	4
32	2	7	8	4	3	64	2	2	1	5	6

array-based Latin hypercube design D. Denote by D_i the subset of D corresponding to C_i and D_{ij} the subset of D corresponding to C_{ij}. Then D achieves uniformity on $s_1 \times s_1 \times s_1$ grids in three dimensions, in addition to achieving maximum uniformity in one dimension; D_i achieves uniformity on $s_2 \times s_2 \times s_2$ grids in three dimensions and D_{ij} achieves uniformity on $s_2 \times s_2$ grids in two dimensions.

Example 8. Consider Example 6, which has five quantitative factors x_1 to x_5 and two qualitative factors z_1 and z_2 at two levels $-$ and $+$. We label $\{0, x^2+x+1\}$ as levels 1 and 2, $\{1, x^2+x\}$ as levels 3 and 4, $\{x, x^2+1\}$ as levels 5 and 6 and $\{x+1, x^2\}$ as levels 7 and 8. Table 2 presents the array B after using such labelling, where B_{11}, B_{21}, B_{12}, B_{22} correspond to runs 1–4, 9–12, 17–20, 25–28; runs 33–36, 41–44, 49–52, 57–60; 5–8, 13–16, 21–24, 29–32; and runs 37–40, 45–48, 53–56, 61–64, respectively. We then use B to construct an orthogonal array-based Latin hypercube D for x_1 to x_5. Now partition D into D_{ij} with points corresponding to B_{ij}, $i, j = 1, 2$. Finally, D_{11}, D_{12}, D_{21}, D_{22} are associated with the level combinations $(z_1, z_2) = (-, -)$, $(z_1, z_2) = (-, +)$, $(z_1, z_2) = (+, -)$ and $(z_2, z_2) = (+, +)$, respectively. Figure 1 presents the bivariate projections of D and D_{11}, where both designs achieve uniformity on 4×4 grids in two dimensions, and D also achieves maximum uniformity in one dimension.

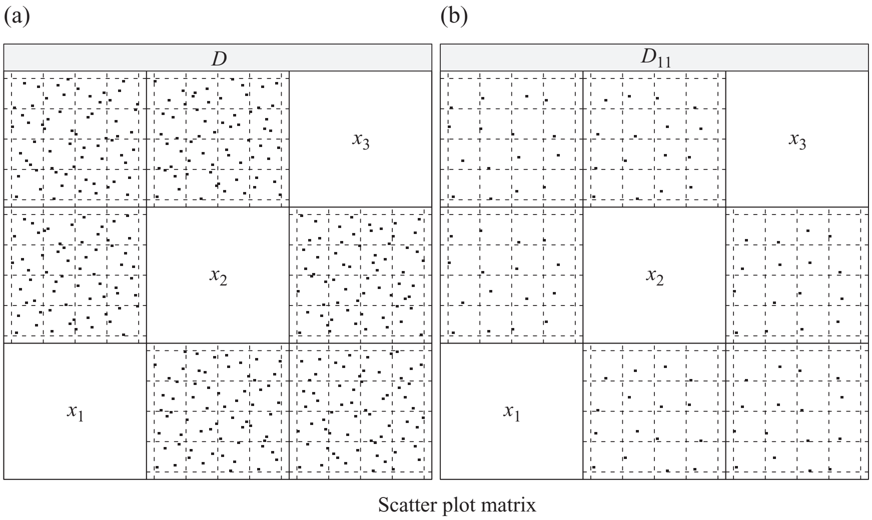

Fig. 1. (a) Bivariate projections among x_1, x_2, x_3 of D in Example 8; (b) bivariate projections among x_1, x_2, x_3 of D_{11} in Example 8.

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