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Optimal and orthogonal Latin hypercube designs for computer experiments

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SUMMARY

Latin hypercube designs are often used in computer experiments as they ensure that few design points are redundant when there is effect sparsity. In this paper, designs suitable for factor screening are presented and they are shown to be efficient in terms of runs required per factor as well as having optimal and orthogonal properties. Designs orthogonal under full second-order models are also constructed.

Some key words: Discrete cosine transform; Fourier-polynomial; Optimality criteria; Resolution; Sensitivity analysis; Simulation model; Williams transformation.

1. INTRODUCTION

Computer simulation experiments are used in a wide range of applications to learn about the effect of input variables x on a response of interest y. The simulation programs are usually deterministic, so the response of each simulation is observed without error and is unchanged if a design point is replicated. This presents different challenges to traditional design of experiments problems where replication is often recommended in the presence of experimental errors.

The design of computer experiments has received much recent interest and this is likely to grow as more and more simulation models are used to carry out research; see Sacks, Welch et al. (1989), Sacks, Schiller & Welch (1989), Welch et al. (1992), Morris et al. (1993) and Bates et al. (1996). The designs proposed for computer experiments have almost exclusively been Latin hypercube designs; see McKay et al. (1979). The main attraction of these designs is that they have good one-dimensional projective properties which ensure that there is little redundancy of design points when some of the factors have a relatively negligible effect, called effect sparsity.

An $n \times m$ discrete Latin hypercube is a design for m factors in n runs, where each factor occurs exactly once at each of n equally spaced levels $x = 1, 2, \ldots, n$. Thus, the columns of the $n \times m$ design matrix X are required to be permutations of $(1, 2, \ldots, n)$. An example of an 11×5 Latin hypercube design has design matrix

$$X = \begin{pmatrix} 4 & 2 & 1 & 3 & 5 & 7 & 9 & 11 & 10 & 8 & 6 \\ 2 & 3 & 7 & 11 & 8 & 4 & 1 & 5 & 9 & 10 & 6 \\ 1 & 7 & 10 & 4 & 3 & 9 & 8 & 2 & 5 & 11 & 6 \\ 3 & 11 & 4 & 5 & 10 & 2 & 7 & 8 & 1 & 9 & 6 \\ 5 & 8 & 3 & 10 & 1 & 11 & 2 & 9 & 4 & 7 & 6 \end{pmatrix}'. \tag{1}$$

This design will be considered later in §§ 3 and 5.

Various methods have been proposed for constructing Latin hypercube designs. Initially, randomised Latin hypercube designs were considered and they were shown by McKay et al. (1979), Stein (1987) and Owen (1992) to perform much better than completely randomised designs. More recently, algorithms have been used to construct systematic Latin hypercube designs under various optimality criteria. Sacks, Welch et al. (1989), Sacks, Schiller & Welch (1989) and Park (1994) use the integrated mean squared error criterion under a spatial model. Currin et al. (1991) and Bates et al. (1996) consider an entropy-based design criterion. Johnson et al. (1990) and Morris & Mitchell (1995) develop a maximin distance criterion which maximises the minimum distance between design points. Iman & Conover (1982) and Owen (1994) find designs by minimising a linear correlation criterion for pairwise factors. This is modified into a polynomial canonical correlation criterion by Tang (1998).

Morris (1991) and Kleijnen (1997) make it clear that many simulation models involve several hundred factors or even more. Consequently, factor screening is vital in computer experiments for reducing the dimension of the factor space before carrying out more detailed experimentation. Methods for constructing factor screening designs have previously been considered by Welch et al. (1992) and Morris (1991). An alternative approach is to use system partitioning, as described in Bates et al. (1996).

In this paper, three types of Latin hypercube design are constructed. By analogy with two-level factorial experiments and because of their orthogonality properties, the types of design are called near-resolution III, resolution IV and resolution V Latin hypercube designs. The resolution IV and near-resolution III designs are very competitive in terms of the number of runs required per factor and consequently are highly suitable for factor screening. The resolution V designs require more runs per factor but are orthogonal under a full second-order model.

2. MODELS

Latin hypercube designs will be constructed under three different models, namely a full second-order model, a first-order model and a second-order main effects model. The full second-order model usually considered is the second-order polynomial model

$$y = \mu + \sum_{i=1}^{m} \alpha_i x_i + \sum_{i=1}^{m} \gamma_i x_i^2 + \sum_{i=1}^{m} \sum_{j=i+1}^{m} \beta_{ij} x_i x_j + \varepsilon, \tag{2}$$

where $\varepsilon \sim N(0, \sigma^2)$. Note that, although observations in computer experiments are usually observed without error, the error term ε is required in order to model higher-order systematic effects. The polynomial model (2) appears to be more difficult to use in the context of Latin hypercube designs than the closely related second-order model

$$\begin{aligned} y = \mu - \sqrt{2} \sum_{i=1}^{m} \alpha_i \cos\left\{\frac{\pi(x_i - 0{\cdot}5)}{n}\right\} + \sqrt{2} \sum_{i=1}^{m} \gamma_i \cos\left\{\frac{2\pi(x_i - 0{\cdot}5)}{n}\right\} \\ + 2 \sum_{i=1}^{m} \sum_{j=i+1}^{m} \beta_{ij} \cos\left\{\frac{\pi(x_i - 0{\cdot}5)}{n}\right\} \cos\left\{\frac{\pi(x_j - 0{\cdot}5)}{n}\right\} + \varepsilon. \end{aligned} \tag{3}$$

For reasons given below, this model will be referred to as a second-order Fourier-polynomial model. Note that the first-order terms in (3) with parameters α_i complete only half a cycle from $x = 0$ to $x = n$. Consequently, the terms are different from the trigonometric functions usually included in Fourier models such as in Riccomagno et al. (1997).

Model (3) also provides a link with spatial processes, which have often been considered in the context of computer experiments. The link is that the Fourier terms in (3) correspond to the eigenvectors with the lowest frequencies in the discrete cosine transform; see for example Buckley (1994) and Butler (1998). Note that the discrete cosine transform is based on reflective boundary assumptions which lead to far more realistic boundary properties than do the periodic boundary assumptions under the discrete Fourier transform. The lowest frequencies in the discrete cosine transform have the highest variances or spectral densities under positively correlated spatial models. Consequently, (3) is able to model the larger-scale spatial trends and so may be interpreted as an approximation to spatial models. This approximation may be a good one when there are very few runs per factor as in this case there will be little information about small-scale spatial trends.

The Fourier-polynomial model (3) is so called as it is also closely related to polynomial models. To see this, define $p_1(x) = x - n/2$ as the polynomial linear function of x orthogonal to a constant on $[0, n]$ and $p_2(x) = (x - n/2)^2 - n^2/12 = x^2 - nx + n^2/6$ as the polynomial quadratic function of x orthogonal on $[0, n]$ to both a constant and $p_1(x)$. Then the relationship between (3) and polynomial models is highlighted by the inner products

$$\int_0^n -p_1(x)\cos\left(\frac{\pi x}{n}\right)dx = 0{\cdot}993\left\{\int_0^n p_1(x)^2\,dx\right\}^{\frac{1}{2}}\left\{\int_0^n \cos^2\left(\frac{\pi x}{n}\right)dx\right\}^{\frac{1}{2}},$$

$$\int_0^n p_2(x)\cos\left(\frac{2\pi x}{n}\right)dx = 0{\cdot}961\left\{\int_0^n p_2(x)^2\,dx\right\}^{\frac{1}{2}}\left\{\int_0^n \cos^2\left(\frac{2\pi x}{n}\right)dx\right\}^{\frac{1}{2}}.$$

The above equations show that the inner products of the linear and quadratic polynomials with the corresponding Fourier terms are close to one under normalisation. In addition, the inner product of the interactions equals $(0{\cdot}993)^2 = 0{\cdot}986$ under normalisation and so is also close to one. This indicates that the second-order Fourier-polynomial model (3) is a good approximation to the polynomial model (2). The close relationship between linear and Fourier-linear terms is further illustrated in § 3 on a specific design.

The full second-order Fourier-polynomial model (3) may also be expressed in the linear-model form as

$$Y = Z\theta + \varepsilon, \quad \varepsilon \sim N(0, \sigma^2 I_n), \tag{4}$$

where Y is the n-vector of observations and

$$\theta = (\mu, \alpha_1, \ldots, \alpha_m, \gamma_1, \ldots, \gamma_m, \beta_{11}, \beta_{12}, \ldots, \beta_{m-1,m})$$

is the vector of model parameters. Furthermore, $Z = (1_n, Z_L, Z_Q, Z_I)$ is the corresponding design matrix with

$$(Z_L)_{ti} = -\surd 2\cos\left\{\frac{\pi(X_{ti} - 0{\cdot}5)}{n}\right\}, \quad (Z_Q)_{ti} = \surd 2\cos\left\{\frac{2\pi(X_{ti} - 0{\cdot}5)}{n}\right\},$$

$$(Z_I)_{t,(i,j)} = 2\cos\left\{\frac{\pi(X_{ti} - 0{\cdot}5)}{n}\right\}\cos\left\{\frac{\pi(X_{tj} - 0{\cdot}5)}{n}\right\},$$

for $t = 1, 2, \ldots, n$, $1 \leqslant i, j \leqslant m$ and $(i, j) = j + m(i-1) - i(i+1)/2$ for $i < j$. Note that Z_L is the design matrix of the Fourier-linear effects, Z_Q is the design matrix of the Fourier-quadratic effects and Z_I is the design matrix of the interactions between the Fourier-linear effects. Note that for a Latin hypercube design Z_L and Z_Q satisfy the constraints

$1_n' Z_L = 0_m'$ and $1_n' Z_Q = 0_m'$. Hence all Fourier-linear effects and Fourier-quadratic effects are orthogonal to the overall mean effect.

A first-order Fourier-polynomial model is similarly defined by (4) with $\theta = (\mu, \alpha_1, \ldots, \alpha_m)$ and $Z = (1_n, Z_L)$. This model is closely related to a first-order polynomial model because of the high inner product between the Fourier-linear terms and the orthogonal linear functions $p_1(x_i)$. The third and final type of model considered in this paper is the second-order main effects model (4) with $\theta = (\mu, \alpha_1, \ldots, \alpha_m, \gamma_1, \ldots, \gamma_m)$ and $Z = (1_n, Z_L, Z_Q)$. This model is likely to be particularly appropriate when the assumption of effect sparsity is valid as there will then be relatively few active interactions compared with the main effects.

3. Construction of designs

Latin hypercube designs will be constructed using what will be called the Williams transformation (Williams, 1949), which is a one-one transformation between n one-dimensional locations $x = 1, 2, \ldots, n$ and n codes $w = 0, 1, \ldots, n-1$ used to construct designs. In the case when $n = 11$, the one-one transformation is given by

$$\begin{array}{cccccccccccc} x & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 & 11 \\ w & 0 & 10 & 1 & 9 & 2 & 8 & 3 & 7 & 4 & 6 & 5 \end{array}.$$

More generally, the Williams transformation determines the locations x from the codes w using the formulae

$$x(w) = \begin{cases} 2w + 1 & (w < n/2), \\ 2(n - w) & (w \geqslant n/2). \end{cases}$$

Williams (1949) used the transformation to construct Latin square designs that are balanced for nearest neighbours. These designs are useful in a variety of applications including field trials, cross-over trials and multilevel factorial experiments. Bailey (1984) provides other transformations that can be used to construct neighbour-balanced designs. Bailey (1982) and Edmondson (1993) provide designs orthogonal to polynomial trends which can be based on the Williams transformation.

The Williams transformation will be used to construct two types of design, denoted by $D_n(g_1, g_2, \ldots, g_m)$ and $E_n(g_1, g_2, \ldots, g_r)$. The designs $D_n(g_1, g_2, \ldots, g_m)$ have $m \leqslant n_0$, where $n_0 = (n-1)/2$, and the designs $E_n(g_1, g_2, \ldots, g_r)$ have $m = n_0 + r$ for some $1 \leqslant r \leqslant n_0$.

The $n \times m$ design matrix X of the design $D_n(g_1, g_2, \ldots, g_m)$ has elements $X_{ti} = x(w_{ti})$ for $t = 1, 2, \ldots, n$ and $i = 1, 2, \ldots, m$, where $w_{ti} \in \{0, 1, \ldots, n-1\}$ and

$$w_{ti} \equiv \begin{cases} t g_i + (n-1)/4 \bmod n, & \text{for } n \equiv 1 \bmod 4, \\ t g_i + (3n-1)/4 \bmod n, & \text{for } n \equiv 3 \bmod 4. \end{cases}$$

To ensure that the factors x_i are not completely confounded, the generators g_i are required to be distinct elements in the set $\{1, 2, \ldots, n_0\}$. The constants in the above equations of $(n-1)/4$ for $n \equiv 1 \bmod 4$ and $(3n-1)/4$ for $n \equiv 3 \bmod 4$ ensure that the designs include the centre point of the design space.

The above designs could, in theory, be constructed for any odd number of runs n and any $m \leqslant n_0$ factors. However, it will be assumed here that n is prime as this guarantees, amongst other things, that the resulting design is a Latin hypercube. Note that the above method of applying cyclic generators to the Williams code w should not be confused with the more established method of applying the generators to the locations x; see for example Fang & Wang (1994).

For $n=11$ and $m=5$, the Williams codes of the design $D_{11}(1,2,3,4,5)$ are given by the matrix

$$W=\begin{pmatrix} 9 & 10 & 0 & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 \\ 10 & 1 & 3 & 5 & 7 & 9 & 0 & 2 & 4 & 6 & 8 \\ 0 & 3 & 6 & 9 & 1 & 4 & 7 & 10 & 2 & 5 & 8 \\ 1 & 5 & 9 & 2 & 6 & 10 & 3 & 7 & 0 & 4 & 8 \\ 2 & 7 & 1 & 6 & 0 & 5 & 10 & 4 & 9 & 3 & 8 \end{pmatrix}'.$$

On applying the Williams transformation to the elements of W, we find that $D_{11}(1,2,3,4,5)$ is the same as the design X in (1).

The other type of design $E_n(g_1, g_2, \ldots, g_r)$ has $n \times m$ design matrix $X=(X_0, X_1)$, where X_0 is the $n \times n_0$ design matrix of the design $D_n(1,2,\ldots,n_0)$, and X_1 is an $n \times r$ design matrix with elements

$$(X_1)_{ti} = x(w_{ii}),$$

where

$$w_{ti} \equiv tg_i \bmod n, \quad w_{ti} \in \{0, 1, \ldots, n-1\},$$

for $t=1,2,\ldots,n$ and $i=1,2,\ldots,r$. It is again assumed that n is prime and that the generators $g_1, g_2, \ldots, g_r$ of X_1 are distinct elements in $\{1,2,\ldots,n_0\}$.

Note that the design $E_n(1,2,\ldots,n_0)$ is a saturated design for $n-1$ factors and n runs under the first-order model. The saturated design $E_7(1,2,3)$, for $n=7$ and $m=6$, has design matrix

$$X=\begin{pmatrix} 2 & 1 & 3 & 3 & 5 & 7 \\ 1 & 5 & 6 & 5 & 6 & 2 \\ 3 & 6 & 1 & 7 & 2 & 5 \\ 5 & 2 & 7 & 6 & 3 & 4 \\ 7 & 3 & 2 & 4 & 7 & 3 \\ 6 & 7 & 5 & 2 & 4 & 6 \\ 4 & 4 & 4 & 1 & 1 & 1 \end{pmatrix}.$$

For this design, the correlations R_X between the columns of X and the correlations R_{Z_L} between the columns of Z_L are

$$R_X=\begin{pmatrix} 1 & 0{\cdot}07 & -0{\cdot}07 & -0{\cdot}21 & 0{\cdot}07 & 0 \\ 0{\cdot}07 & 1 & -0{\cdot}07 & 0 & -0{\cdot}21 & -0{\cdot}07 \\ -0{\cdot}07 & -0{\cdot}07 & 1 & -0{\cdot}07 & 0 & -0{\cdot}21 \\ -0{\cdot}21 & 0 & -0{\cdot}07 & 1 & 0{\cdot}07 & 0{\cdot}11 \\ 0{\cdot}07 & -0{\cdot}21 & 0 & 0{\cdot}07 & 1 & 0{\cdot}11 \\ 0 & -0{\cdot}07 & -0{\cdot}21 & 0{\cdot}11 & 0{\cdot}11 & 1 \end{pmatrix},$$

$$R_{Z_L} = \begin{pmatrix} 1 & 0 & 0 & -0{\cdot}22 & 0 & 0 \\ 0 & 1 & 0 & 0 & -0{\cdot}22 & 0 \\ 0 & 0 & 1 & 0 & 0 & -0{\cdot}22 \\ -0{\cdot}22 & 0 & 0 & 1 & 0 & 0 \\ 0 & -0{\cdot}22 & 0 & 0 & 1 & 0 \\ 0 & 0 & -0{\cdot}22 & 0 & 0 & 1 \end{pmatrix}.$$

Note the similarity in the column correlations for X and Z_L. This illustrates the close relationship between linear effects and Fourier-linear effects. The correlations are small in both cases as the design $E_7(1, 2, 3)$ will be shown in § 4 to have near-orthogonal and near-optimal properties.

4. RESULTS

The Latin hypercube designs constructed in § 3 are now shown to have various optimal and orthogonal properties. By analogy with two-level factorial designs, the orthogonal properties of Latin hypercubes will be expressed in terms of the resolution of the design.

A Latin hypercube design will be said to have resolution III if the Fourier-linear effects are mutually orthogonal. This requires $Z_L' Z_L = nI_m$ as the diagonal elements are fixed for Latin hypercube designs. Similarly, a Latin hypercube design will be said to have resolution IV if the Fourier-linear effects are mutually orthogonal and orthogonal to all second-order effects, and if the overall mean effect is orthogonal to all second-order interactions. Note, as mentioned above, that the overall mean effect is automatically orthogonal to all Fourier-linear and Fourier-quadratic effects for a Latin hypercube design. Thus, a resolution IV Latin hypercube design requires that $Z_L' Z_L = nI_m$ and that all the elements of $Z_L' Z_Q$, $Z_L' Z_I$ and $1_n' Z_I$ equal zero. Finally, a Latin hypercube design will be said to have resolution V if all the effects in a full second-order model are orthogonal. This requires $Z'Z$ to be a diagonal matrix for $Z = (1_n, Z_L, Z_Q, Z_I)$. The proofs of all the results below are given in the Appendix.

LEMMA 1. *For the design* $D_n(1, 2, \ldots, n_0)$,

$$(Z_L)_{ti} = (-1)^d \sqrt{2} \sin\left(\frac{2\pi t i}{n}\right), \quad (Z_Q)_{ti} = -\sqrt{2} \cos\left(\frac{4\pi t i}{n}\right),$$

$$(Z_I)_{t,(i,j)} = \cos\left\{\frac{2\pi t(j-i)}{n}\right\} - \cos\left\{\frac{2\pi t(i+j)}{n}\right\} \quad (i<j),$$

$t = 1, 2, \ldots, n$ *and* $1 \leqslant i, j \leqslant n_0$, *where* $d = 0$ *for* $n \equiv 1 \bmod 4$, *and* $d = 1$ *for* $n \equiv 3 \bmod 4$.

THEOREM 1. *For n prime,* $D_n(1, 2, \ldots, n_0)$ *is a resolution* IV *Latin hypercube design, and is orthogonal and saturated under the second-order main effects model.*

COROLLARY 1. *Within the class of Latin hypercube designs for* $m \leqslant n_0$ *and n prime,* $D_n(g_1, g_2, \ldots, g_m)$ *is*

(i) *I-optimal and D-optimal under the first-order model,*
(ii) *I-optimal and D-optimal under the second-order main effects model,*
(iii) D_s*-optimal for the subset of first-order parameters under the full second-order model.*

As a result of the close link between polynomial and Fourier-polynomial effects, the designs $D_n(g_1, g_2, \ldots, g_m)$ also perform extremely well under the linear correlation criterion of Iman & Conover (1982) and the quadratic canonical correlation criterion of Tang (1998).

THEOREM 2. *For the design* $E_n(1, 2, \ldots, n_0)$,

$$(Z_L)_{ti} = (-1)^d \sqrt{2} \sin\left(\frac{2\pi ti}{n}\right), \quad (Z_L)_{t,n_0+i} = -\sqrt{2} \cos\left(\frac{2\pi ti}{n} + \frac{\pi}{2n}\right),$$

for $t = 1, 2, \ldots, n$ *and* $1 \leqslant i \leqslant n_0$, *where* $d = 0$ *for* $n \equiv 1 \bmod 4$, *and* $d = 1$ *for* $n \equiv 3 \bmod 4$. *Consequently,* $n^{-1} Z_L' Z_L = I_{n-1} + P$, *where* P *is an* $(n-1) \times (n-1)$ *matrix with nonzero elements*

$$P_{i,n_0+i} = P_{n_0+i,i} = (-1)^d \sin \pi/(2n) \quad (1 \leqslant i \leqslant n_0).$$

Note that the design $E_n(1, 2, \ldots, n_0)$ would be optimal under various criteria and orthogonal under the first-order model if all the elements of P were zero. As this is close to being achieved, particularly when n is large, the design is both near-optimal and near-orthogonal. Hence, $E_n(1, 2, \ldots, n_0)$ will be referred to as a near-resolution III Latin hypercube design.

THEOREM 3. *For n prime,* $D_n(g_1, g_2, \ldots, g_m)$ *is a resolution* V *Latin hypercube design if all the elements*

$$\min(2g_i, n - 2g_i) \quad (1 \leqslant i \leqslant m),$$

$$|g_j - g_i|, \quad \min(g_i + g_j, n - g_i - g_j) \quad (1 \leqslant i < j \leqslant m)$$

are distinct.

The conditions in Theorem 3 bear a resemblance to those in Theorem 2 of Riccomagno et al. (1997). However, a different model is being considered, as mentioned in § 2.

Note that the above resolution V Latin hypercube designs are not necessarily optimal under the second-order model (3) as there could be other designs which provide more information about the interactions. However, these other designs would require more design points near the corners of the grid and this is likely to result in poorer projective properties.

The conditions in Theorem 3 can only hold if $n \geqslant 2m^2 + 1$, otherwise there will be confounding between the second-order effects. The lower bound of $n = 2m^2 + 1$ is attainable for $m = 2$ and $m = 3$ factors but not it appears for $m > 3$. For $m = 2$, the design $D_9(1, 2)$ is an orthogonal Latin hypercube design requiring the minimum number of 9 runs. For $m = 3$, $D_{19}(2, 3, 5)$ and $D_{19}(1, 7, 8)$ are examples of orthogonal Latin hypercube designs attaining the lower bound of $n = 19$ runs. Note that the two-factor projections of $D_{19}(1, 7, 8)$ for factors 1 and 7 and factors 1 and 8 may be observed in Fig. 1.

For $m = 4$, the lowest number of runs for an orthogonal Latin hypercube designs is 37, which exceeds the lower bound of 33. A suitable orthogonal design in this case is $D_{37}(3, 5, 6, 10)$. For $m = 5$, the orthogonal Latin hypercube design $D_{59}(6, 8, 11, 12, 19)$ requires the minimum number of runs for orthogonality under the second-order model. Suitable designs for $m \geqslant 6$ are not provided as they are relatively inefficient in terms of the number of runs required per factor.

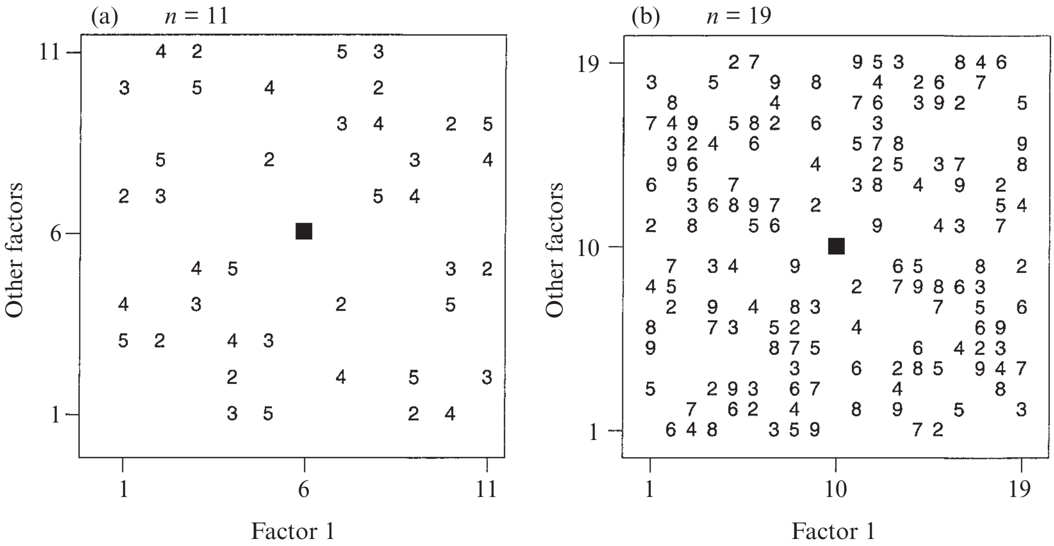

Fig. 1. Two-factor projections of the Latin hypercube design $D_n(1, 2, \ldots, n_0)$ for 11 and 19 runs. Points i represent the projection of factor 1 and factor i ($i = 2, 3, \ldots, n_0$).

5. Discussion

The resolution IV and near-resolution III designs resulting from Theorems 1 and 2 respectively are appropriate for factor screening as they require very few experimental runs per factor. In particular, the resolution IV designs $D_n(1, 2, \ldots, n_0)$ are half-saturated under a first-order model and are saturated under a second-order main effects model. Moreover, the near-resolution III designs $E_n(1, 2, \ldots, n_0)$ are saturated under a first-order model. These designs are thus a Latin hypercube equivalent of Plackett–Burman designs (Plackett & Burman, 1946).

In addition to their optimal and orthogonal properties, the suitability of the resolution IV designs is further confirmed by their projective properties. Figure 1 provides the two-factor projections involving factor 1 for the Latin hypercube designs $D_n(1, 2, \ldots, n_0)$ for $n = 11$ and $n = 19$. In every case, the projection includes the centrepoint $((n+1)/2, (n+1)/2)$. Note that the projections of $D_{11}(1, 2, 3, 4, 5)$ may be confirmed from the design matrix (1).

Although Fig. 1 provides the projections only involving factor 1, it follows from the cyclical nature of the designs that each factor has exactly the same projections for some permutation of the factors and with some of the factors reflected about the middle level $(n+1)/2$. The important features in Fig. 1 are the relative positions of the points under the same projection, i.e. the points with the same number. Note that, for each projection, approximately a quarter of the points are in each quadrant.

The worst projections between pairs of factors x_i and x_j in terms of the distribution of design points occur when $g_j \equiv \pm 3g_i \bmod n$ or $g_i \equiv \pm 3g_j \bmod n$. Note that it can be shown that none of these projections occurs for the resolution V designs as a result of the conditions in Theorem 3. For values of $m < n_0$ but where m is too large for a resolution V design, it would be reasonable to select the generators $g_1, g_2, \ldots, g_m$ to avoid as many of these projections as possible. This is a topic for further research.

The resolution V designs in this paper are suitable for more detailed experimentation of the response surface once the factors having the most substantial effect on the response have been identified. These are called the active factors. The active factors may be identified during factor screening using a combination of graphical methods, estimation under first-order models and forward subset selection methods (Welch et al., 1992).

In some computer experiments, the number of factors m may be larger than the number of available runs n (Morris, 1991; Kleijnen, 1997). In such cases, the designs constructed in this paper could not be used. Instead, factor screening could be performed using supersaturated designs. Supersaturated designs have mainly been studied in the context of two-level factorial experiments; see Butler et al. (2001) and the references therein. However, research is currently being carried out on developing supersaturated Latin hypercube designs.

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Appendix

Proofs

Proof of Lemma 1. First note that under the Williams transformation

$$x(w) - 0{\cdot}5 = \begin{cases} 2w + 0{\cdot}5 & (w < n/2), \\ 2n - (2w + 0{\cdot}5) & (w \geqslant n/2). \end{cases}$$

Consequently,

$$(Z_L)_{ti} = -\surd 2 \cos\left\{\frac{\pi(X_{ti} - 0{\cdot}5)}{n}\right\} = -\surd 2 \cos\left\{\frac{\pi(2w_{ti} + 0{\cdot}5)}{n}\right\} = (-1)^d \surd 2 \sin\left(\frac{2\pi t i}{n}\right),$$

where $d = 0$ for $n \equiv 1 \bmod 4$, and $d = 1$ for $n \equiv 3 \bmod 4$. Also

$$(Z_Q)_{ti} = \surd 2 \cos\left\{\frac{2\pi(X_{ti} - 0{\cdot}5)}{n}\right\} = \surd 2 \cos\left\{\frac{2\pi(2w_{ti} + 0{\cdot}5)}{n}\right\} = -\surd 2 \cos\left(\frac{4\pi t i}{n}\right),$$

$$\begin{aligned}(Z_I)_{t,(i,j)} &= 2 \cos\left\{\frac{\pi(X_{ti} - 0{\cdot}5)}{n}\right\} \cos\left\{\frac{\pi(X_{tj} - 0{\cdot}5)}{n}\right\} \\ &= 2 \sin\left(\frac{2\pi t i}{n}\right) \sin\left(\frac{2\pi t j}{n}\right) = \cos\left\{\frac{2\pi t(j-i)}{n}\right\} - \cos\left\{\frac{2\pi t(i+j)}{n}\right\}.\end{aligned}$$

This completes the proof. □

Proof of Theorem 1. The elements of $Z_L'Z_L$, $Z_L'Z_Q$, $Z_L'Z_I$ and $1_n'Z_I$ depend on sums of the form

$$S_1 = \sum_{t=1}^{n} \sin\left(\frac{2\pi p t}{n}\right) \sin\left(\frac{2\pi q t}{n}\right), \quad S_2 = \sum_{t=1}^{n} \cos\left(\frac{2\pi p t}{n}\right) \cos\left(\frac{2\pi q t}{n}\right),$$

$$S_3 = \sum_{t=1}^{n} \sin\left(\frac{2\pi p t}{n}\right) \cos\left(\frac{2\pi q t}{n}\right),$$

where p and q are integers. Standard trigonometric results show the following: $S_3 = 0$ for any integers p, q; $S_1 = 0$ and $S_2 = n$ for $(p, q) \equiv (0, 0) \bmod n$; $S_1 = n/2$ and $S_2 = n/2$ for $p - q \equiv 0 \bmod n$, and $(p, q) \not\equiv (0, 0) \bmod n$; $S_1 = -n/2$ and $S_2 = n/2$ for $p + q \equiv 0 \bmod n$, and $(p, q) \not\equiv (0, 0) \bmod n$; $S_1 = 0$ and $S_2 = 0$ for any other values of (p, q).

It follows from these results that $Z_L'Z_L = nI_{n_0}$ and that all the elements of $Z_L'Z_Q$, $Z_L'Z_I$ and $1_n'Z_I$ equal zero. Therefore, $D_n(1, 2, \ldots, n_0)$ satisfies the conditions required of a resolution IV Latin hypercube design. Also, for n prime, it can be shown that $Z_Q'Z_Q = nI_{n_0}$ and hence $Z'Z = nI_{2n_0+1} = nI_n$, where $Z = (1_n, Z_L, Z_Q)$ is the design matrix under the second-order main effects model. Consequently, the design is both orthogonal and saturated under this model. □

Proof of Corollary 1. Now D-optimality selects designs which maximise the determinant $\det(Z'Z)$, whilst I-optimality minimises

$$\int_{[0,n]^m} U(x)\,dx = \mathrm{tr}\,\{W(Z'Z)^{-1}\},$$

where $U(x)$ is the variance function at $x \in [0, n]^m$, $z(x)$ is the vector of covariates at x, and $W = \int_x z(x)z(x)'\,dx$. Under each of the models considered in this paper $W = n^m I_{m+1}$. Hence, in these cases, I-optimality turns out to be equivalent to A-optimality.

For any Latin hypercube design, it has been noted that all the diagonal elements of $Z'Z$ equal n under the first-order and second-order main effects model. Therefore, any design for which $Z'Z = nI_n$ is D-optimal and A-optimal, and hence I-optimal. This proves points (1) and (2) in the Corollary. Point (3) is a consequence of the design being of resolution IV. □

Proof of Theorem 2. For the factors in X_1,

$$(Z_L)_{t,n_0+i} = -\surd 2 \cos\left\{\frac{\pi(X_{ti} - 0{\cdot}5)}{n}\right\} = -\surd 2 \cos\left\{\frac{\pi(2w_{ti} + 0{\cdot}5)}{n}\right\} = -\surd 2 \cos\left\{\frac{2\pi ti}{n} + \frac{\pi}{2n}\right\}.$$

Therefore, by the above standard trigonometric results, all the off-diagonal elements of $Z_L'Z_L$ equal zero except for

$$(Z_L'Z_L)_{i,n_0+i} = -2(-1)^d \sum_{t=1}^{n} \sin\left(\frac{2\pi ti}{n}\right) \cos\left(\frac{2\pi ti}{n} + \frac{\pi}{2n}\right) = n(-1)^d \sin\left(\frac{\pi}{2n}\right)$$

and similarly for $(Z_L'Z_L)_{n_0+i,i}$. The result then follows. □

Proof of Theorem 3. For the design to be of resolution V, all columns of the design matrix $Z = (1_n, Z_L, Z_Q, Z_I)$ are required to be orthogonal. If we use the formulae for the columns of the design matrix given by Lemma 1, the above standard trigonometric results can be used to show that the columns of Z are orthogonal if the conditions on the generators in the Theorem hold. □

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