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Industrial Experimentation for Screening

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1. Introduction

Industrial managers are becoming increasingly aware of the benefits of running statistically designed experiments. Statistical experimental designs, first developed by Sir R. A. Fisher in the 1920's, largely originated from agricultural problems. Designing experiments for industrial problems and for agricultural problems are similar in their basic concerns. There are, however, many differences. The differences listed in Table 1 are based upon the overall characteristics of all problems. Exceptions can be found in some particular cases, of course.

- Industrial problems tend to contain a much larger number of factors under investigation and usually involve a much smaller number of runs in total.
- Industrial results are more reproducible; that is, industrial problems contain a much smaller replicated variation (pure error) than that of agricultural problems.
- Industrial experimenters are obliged to run their experimental points in sequence and naturally plan their follow-up experiments guided by previous results. In contrast, agricultural problems harvest all results at one time. Doubts and complications can be resolved in industry by immediate follow-up experiments. Confirmatory experimentation is readily available for industrial problems and has become a routine procedure to assess validity of assumptions.
- The concept of blocking arose naturally in agriculture, but often is not obvious for industrial problems. Usually, industrial practitioners need certain specialized training to recognize and handle blocking variables.
- Missing values seem to occur more often in agriculture (mainly due to natural losses) than industry. Usually, such problems can be avoided for industrial problems by well-designed experiments.

The design method considered in this chapter suggests some screening methods for industrial problems involving a large number of potential relevant factors. It may not be an appropriate method for some agricultural problems.

Consider the simple fact that when there is an effect, there is a cause. Quality engineers are constantly faced with distinguishing between factors which have substantial effects (causal or "active" factors) and those which do not have a substantial effects

Table 1
Differences between agricultural and industrial experiments

Subject	Agriculture	Industry
Number of factors	Small	Large
Number of runs	Large	Small
Reproducibility	Less likely	More likely
Time taken	Long	Short
Blocking	Nature	Not obvious
Missing values	Often	Seldom

(inert of "null" factors). The null factors are then adjusted appropriately to lower the cost; while the active factors are adjusted appropriately to yield better quality. To distinguish between them, a large number of factors can often be listed as possible sources of potential effects. Preliminary investigations (e.g., using subject-matter knowledge) may quickly remove some of these "candidate factors". It is not unusual, however, to find that more than twenty sources of effects exist, and among those factors only a small portion are actually active. The goal here is to apply the Pareto principle of separating the vital few effects from the trivial many. A problem frequently encountered in this area is how to reduce the total number of experiments in such a screening structure. This is particularly important in situations where the cost of an individual run is expensive (e.g., regarding money or time). With powerful statistical software readily available for data analysis, there is no doubt that data collection is the most important part of such problems.

We initially consider an experimental situation in which a response y depends upon k factors $x_1, \ldots, x_k$ with a first order relationship of the form

$$y = \beta_0 + \beta_1 x_1 + \cdots + \beta_k x_k + \varepsilon = \boldsymbol{X}\beta + \varepsilon,$$

where y is an $n \times 1$ vector of observations, the design matrix $\boldsymbol{X}$ is $n \times (k+1)$ whose jth row is of the form $(1, x_{1j}, x_{2j}, \ldots, x_{kj})$, $j = 1, 2, \ldots, n$, β is the $(k+1) \times 1$ vector of coefficients to be estimated, and ε is the noise vector. In a two-level factorial design, each x_i can be coded as ± 1 (or simply $\pm$). The design is then determined by the $n \times k$ matrix of elements ± 1. The ith column gives the sequence of factor levels for factor x_i; each row constitutes a *run*. When $k = n - 1$, the design is called a *saturated* design and the design matrix $\boldsymbol{X}$ is an $n \times n$ square matrix. Note that $n = k+1$ is the minimal number of points (rows) required to estimate all coefficients of interest (the β_i's). Typically, many possible factors are suggested for investigation, but it is often anticipated that only a "small" subset of these will be "active". Assume there are n experimental runs and k factors under study, of which p are active. Let $\boldsymbol{A} = \{j_1, j_2, \ldots, j_p\}$ and $\boldsymbol{N} = \{j_{p+1}, \ldots, j_k\}$ denote indexes of active and inert factors, respectively, so that $\boldsymbol{A} \cup \boldsymbol{N} = \{1, \ldots, k\} = \boldsymbol{S}$. In the multiple hypothesis-testing framework, we have null and alternative pairs H_j: $\beta_j = 0$ and H_j^c: $\beta_j \neq 0$ with H_j true for $j \in \boldsymbol{N}$ and H_j^c true for $j \in \boldsymbol{A}$.

In this chapter, we discuss screening designs that are useful for finding the β_j for $j \in \boldsymbol{A}$. The chapter is organized as follows. Section 2 introduces some popular designs for screening purposes. These are minimal-point or near minimal point designs. This includes the 2^{k-p}_{III} series designs, Plackett and Burman designs, alphabetic optimality designs, T-optimal design, regular simplex, p-efficient designs, and uniform designs. Section 3 discusses the usefulness of supersaturated designs. A supersaturated design is essentially a fractional factorial design in which the number of factors exceeds the number of runs. Section 4 provides some additional designs which are useful for computer experiments. The common equal variance assumption $\mathrm{Var}(\varepsilon) = \sigma^2$ is made in Sections 2–4. Section 5 discusses the impact of dispersion effects (when the equal variance assumption does not hold) when analyzing fractional factorial designs.

2. Screening designs

Screening designs are typically used in the initial stages of an experimental investigation. Because of their relative simplicity, the 2^{k-p} fractional factorial designs are popular in practice. A fractional two-level design is one that employs only a fractional of the complete 2^k runs. Many such designs use a 2^{-p} fraction of the whole 2^k runs and have been designated 2^{k-p} fractional factorials. Strictly speaking, however, any selection of the 2^k runs forms a fractional design, but not necessarily a 2^{k-p} fraction. Two-level factorial and fractional factorial designs have been used for many years, certainly since Yates (1935). A large compilation of 2^{k-p} designs was made by the National Bureau of Standard (1957), for example.

An important characteristic of a 2^{k-p} design is its *resolution*, a concept recognized by Bose (1947) and Rao (1947) and defined by Box and Hunter (1961) as follows: "A design of resolution R is one in which no p factor effect is confounded with any other effect containing less than $R - p$ factors." Therefore, a resolution III design permits the estimation of all main effects when (two- or higher-order) interaction effects are negligible. Because of its simplicity and orthogonality, the two-level fractional factorial design of resolution III, denoted by 2^{k-p}_{III}, is probably the most popular screening design. In general, it can study n factors in $n - 1$ runs, where n is power of two. This may be feasible for many industrial experiments. These designs are available in many design textbooks and statistical software packages.

In this section, we will introduce some other advanced screening designs. This includes Plackett and Burman (PB) designs, p-efficient designs, regular simplex designs, optimal designs, T-optimal designs, and uniform designs. The 2^{k-p}_{III} design is only available when the run size n is a power of two. The Plackett and Burman design which can be viewed as a special class of Hadamard matrices, however, is available for any n that is a multiple of four. Compared to the regular 2^{k-p}_{III} design, the Plackett and Burman design has a much more complicated alias structure. The regular simplex design and the T-optimal design are both orthogonal designs, but give up the two-level property. On the other hand, the p-efficient design keeps the two-level property, but does not have perfect orthogonality. The optimal design requires prior knowledge of

the underlying model, and the uniform design is constructed based on the uniformity of the design points in the design space.

2.1. Plackett and Burman design

Plackett and Burman (1946) provided a series of two-level fractional factorial designs for examining $n-1$ factors in n runs, where n is a multiple of four and $n \leqslant 100$. They omitted the case $n = 92$ which was later provided by Baumert, Golomb and Hall (1962). When only main effects exist, these designs estimate all of them. Moreover, they are available for all run sizes that are a multiple of four (versus a power of two as in a 2^{k-p} design). PB designs are thus extremely useful in screening situations.

Construction of Plackett and Burman designs
A 12-run Plackett and Burman design can be obtained as follows:

1. Write down the set of signs $++-+++---+-$, provided by Plackett and Burman (1946).
2. Permute the signs in 11 rows total, by taking the sign from the right hand side and moving it to the left-hand side.
3. Add a 12th row of all minus signs.

$$\boldsymbol{PB}_{12} = \begin{bmatrix} + & + & - & + & + & + & - & - & - & + & - \\ + & - & + & + & + & - & - & - & + & - & + \\ - & + & + & + & - & - & - & + & - & + & + \\ + & + & + & - & - & - & + & - & + & + & - \\ + & + & - & - & - & + & - & + & + & - & + \\ + & - & - & - & + & - & + & + & - & + & + \\ - & - & - & + & - & + & + & - & + & + & + \\ - & - & + & - & + & + & - & + & + & + & - \\ - & + & - & + & + & - & + & + & + & - & - \\ + & - & + & + & - & + & + & + & - & - & - \\ - & + & + & - & + & + & + & - & - & - & + \\ - & - & - & - & - & - & - & - & - & - & - \end{bmatrix}.$$

For $n \leqslant 24$, all of the Plackett and Burman designs can be obtained by such a cyclic permutation. The signs for the first rows are:

$n = 8$: $+++-+--$
$n = 12$: $++-+++---+-$
$n = 16$: $++++-+-++--+---$
$n = 20$: $++--++++-+-+----++-$
$n = 24$: $+++++-+-++--++--+-+----$.

For n a power of two (e.g., $n = 8$ and 16), we obtain a standard 2^{k-p} design. Note that Plackett and Burman designs can be viewed as a special class of Orthogonal Array. A complete list of OAs is given in Hedayat, Sloane and Stufken (1999) and can be found at the website `http://www.research.att.com/~njas/oadir/`.

Table 2
Projection of a 12-run PB design into q dimensions

q	Design	Description
2	2.1	$2^2 \times 3$ (2^2 design with 3 replicates)
3	3.1	$2^3 + \frac{1}{2}2^3$ (2^3 design plus 2^{3-1} design)
4	4.1	Add one more runs to form a 2^{4-1}_{IV} design
		Add five more runs to form a 2^4 design
5	5.1	Add two more runs to form a 2^{5-2}_{III} design
		Add six more runs to form a 2^{5-1}_{V} design
	5.2	Add two more runs to form a 2^{5-2}_{III} design
		Add eight more runs to form a 2^{5-1}_{IV} design
		Add ten more runs to form a 2^{5-1}_{V} design

Projection properties
When an n-run screening design is employed, it is expected that only a subset of factors be important. This permits the use of fractionated designs with complicated alias structures. The alias structure of PB designs can be found in Lin and Draper (1993). After the initial analysis, the whole design is then projected into a lower-dimensional space which contains only the q apparently important factors. The projection properties of PB design are worth mentioning.

To see what the projection of the 12-run design is in any q of the 11 factor dimensions, we select q columns and examine the design that results by ignoring the other $11-q$ columns. Table 2 summarizes the situation of $n = 12$ runs and $q \leqslant 5$. An important aspect of this table is that, for $q \leqslant 4$, only one projected design type is obtained apart from variations caused by changes of signs in the columns. For details and projection in larger PB designs, see Lin and Draper (1992, 1995).

2.2. Optimal design

The problem of selecting a suitable design is a formidable one (see Box and Draper, 1975). Many design criteria have been proposed for choosing the design matrix $\boldsymbol{X}$, or for comparing design matrices. Essentially, most of them deal with the eigenvalues of the matrix $\boldsymbol{X'X}$, $\lambda_1, \lambda_2, \ldots, \lambda_k$. The major alphabetical optimality criteria are:

- *D-optimality*: maximize $\|\boldsymbol{X'X}\| = \lambda_1 \times \lambda_2 \times \cdots \times \lambda_k$.
- *A-optimality*: minimize $\text{trace}(\boldsymbol{X'X})^{-1} = \sum_{i=1}^{k} \lambda_i^{-1}$.
- *E-optimality*: maximize the smallest eigenvalue of the $\boldsymbol{X'X}$ matrix.
- *G-optimality*: minimize the maximum prediction variance over the operation region.
- *V-optimality*: minimize the average prediction variance over the operation region.

More (generalized) design optimalities can be found in Kiefer (1959), or more recently Pukelsheim (1993). In essence, given the underlying model and the optimality criterion, any modern optimization technique can be used to generate an optimal design for the

practitioner. However, the resulting design may not have desirable design properties, such as orthogonality, few levels in each factor, symmetry, etc., as in a 2^{k-p}_{III} design.

The problem of finding a D-optimal design has been very thoroughly explored mathematically; two early articles are by Hotelling (1944) and by Mood (1946). For two-level saturated D-optimal designs, the problem becomes finding an $n \times n$ matrix with all its elements being either 1 or -1 such that its determinant is maximized. Such a "det-max" matrix problem has received a great deal of attention in the literature. Many of the resulting designs are available in software. If the underlying first-order design is believed to be true and if the optimality criterion is appropriate, these optimal designs can be very helpful.

The practical value of saturated D-optimal designs, apart from Plackett and Burman (1946) designs, is worthy of further investigation. First, these designs do not contain an equal number of high-level and low-level values. This can be quite disturbing to experimenters. The nonequal occurrence property implies that the factor is being partially confounded with the constant term (the column with all +'s), which is usually significantly different from zero. Second, unlike orthogonal designs, these designs lack similarity relationships among all the columns. For example, the correlations between every pair of columns are not necessarily the same. This raises questions about which factors to assign to which columns and whether it matters. This leads to the study of p-efficient and T-optimal cyclic designs, as will be discussed below.

2.3. *p-efficient design*

For screening situations, Lin (1993a, 1993b) argued that the focus should be on the potential projective models, rather than the full model. This section discusses some practical concerns in choosing a design and presents some first-order saturated designs having two desirable properties: (near-) equal occurrence and (near-) orthogonality. These saturated designs are shown to be reasonably efficient for estimating the parameters of projective submodels, and thus are called p-efficient designs.

Much theoretical work has been done in this area to select designs that meet certain optimization criteria. Note that a typical preliminary investigation contains a large number of potentially relevant factors, but often only a few are believed to have *actual* effects. Once these actual effects are identified, the initial design is then projected into a much smaller dimension. In such a screening situation, considering the optimality properties based upon the full model may be irrelevant.

An optimal (D-optimal, for example) design for the full model is not necessarily optimal for the submodel that contains only the active factors. Since we do not know in advance which factors will be important, it is reasonable to have designs that are *balanced* in all factors. This naturally leads to the desirability of the (near-) equal occurrence and (near-) orthogonality properties as explained below.

(1) (*Near-*) *equal occurrence*. For each factor, both high- and low-level values are usually of equal interest, and each experimental result, y_i, should have equal influence. This leads to the equal occurrence property – an equal number of high-level and low-level points for each factor in a design. When n is odd, however, the equal occurrence property is unattainable. We thus seek a design to be as near to equal occurrence as possible by specifying that the numbers of +'s and −'s should differ by no more than one.

Without loss of generality, for odd n, we assume that there are $(n+1)/2$ +'s and $(n-1)/2$ −'s. Denote the largest correlation with the constant term among all factors by c as a measure of equal occurrence. A large value for c is undesirable. The designs given here have $c = 0$ for even n and $c = 1/n$ for odd n.

(2) (*Near-*) *orthogonality*. Orthogonality was considered as an important design principle by R. A. Fisher and F. Yates back in the 1920's. The degree of nonorthogonality between factors x_i and x_j can be measured by $s_{ij} = \sum_{u=1}^{n} x_{iu}x_{ju}$ ($s_{ij} = 0$ implies orthogonality). Even if circumstances are such that exact orthogonality is unattainable, it is still preferable to make the design as nearly orthogonal as possible. Denote the largest $|s_{ij}|$ among all pairs of factors for a given design by s ($s \geqslant 0$). We thus desire a design to have a minimum value for s. Under the equal occurrence assumption, it is shown that $s_{ij} \equiv n \pmod 4$, namely that the smallest $s = |s_{ij}|$ possible are 0, 1, 2, and 1 for $n \equiv 0, 1, 2,$ and 3 (mod 4) respectively. If two designs have the same value of s, we prefer the one in which the frequency of such s is smaller. Thus, we minimize the the average of s^2, denoted by ave(s^2). For a specific design, ave(s^2) is computed by $\sum s_i^2 f_i / \binom{n-1}{2}$, where f_i is the frequency of s_i of all $\binom{n-1}{2}$ pairs of columns. This criterion was first proposed by Booth and Cox (1962) in the context of supersaturated designs (see Section 3). We see that when $n \equiv 0 \pmod 4$, the Plackett and Burman designs are optimal in the sense of meeting both of these requirements.

Now, consider a design's projective property, i.e., consider the submodel that contains only the $q \leqslant k = (n-1)$ active factors. The projective design in any p of the k factor dimensions will always preserve the original (near-) equal occurrence property and (near-) orthogonality, no matter which q factors are designated as the survivor columns. Moreover, these designs have high d-efficiency in terms of the reduced model, when p is small, e.g., $q \leqslant 5$. Because of this property, we call them *p-efficient* designs.

Consider the case $n = 7$ to investigate six factors, as an example. Table 3 gives the D-optimal and the p-efficient designs. Suppose two factors are found to be important (the first two columns, say). The D-optimal design for the full model (see Williamson, 1946) could then project into $(+-+-+++)'$ and $(++--- -)'$ whose

Table 3
The d-optimal and the p-efficient designs for $n = 7$

No.	d-optimal design						p-efficient design					
	x_1	x_2	x_3	x_4	x_5	x_6	x_1	x_2	x_3	x_4	x_5	x_6
1	1	1	1	1	1	1	1	1	−1	−1	−1	−1
2	−1	1	1	−1	−1	1	−1	−1	1	1	−1	−1
3	1	1	−1	−1	−1	−1	−1	−1	−1	−1	1	1
4	−1	−1	−1	1	1	−1	−1	1	−1	1	−1	1
5	1	−1	1	−1	1	−1	−1	1	1	−1	1	−1
6	1	−1	1	1	−1	−1	1	−1	−1	1	1	−1
7	1	−1	−1	−1	−1	1	1	−1	1	−1	−1	1

$\boldsymbol{X}'_{\text{sub}}\boldsymbol{X}_{\text{sub}} = \begin{bmatrix} 7 & 3 & 1 \\ 3 & 7 & 1 \\ 1 & 1 & 7 \end{bmatrix}$ is no longer D-optimal for the submodel. On the other hand, the p-efficient design results in $\boldsymbol{X}'_{\text{sub}}\boldsymbol{X}_{\text{sub}} = 8\boldsymbol{I} - \boldsymbol{J}$ which is optimal in many senses (including D-optimality), no matter which two columns are selected. Furthermore, the first design column for the D-optimal design consists of two $-$'s and five $+$'s. Thus, the experimenters may be confused as to which level to be assigned as $+$. For larger n, the problem is even more severe.

The fact that saturated designs are often used in screening situations where it is expected that there only will be a few important factors leads to the practical value of these designs. The p-efficient designs discussed here are attractive because their (near-) equal occurrence property and (near-) orthogonality are preserved when projecting into $q \leqslant k$ dimensions. Further, for estimating from a submodel, it is shown that these designs are more efficient than D-optimal designs. Even for the full model, the D-optimal designs are not substantially more efficient than the p-efficient designs.

D-optimality has an appealing property of invariance under a nonsingular linear transformation, a property clearly possessed by the p-efficient design. This is not true for most of the other optimalities (including A-, E-, G-, L-, and R-optimality; see Kiefer, 1959, p. 294). We note that blindly following a single optimality criterion is dangerous, although the p-efficient designs should perform well in general because of their better balance property. The p-efficient designs for $n < 30$ are given in Lin (1993b).

2.4. *Regular simplex design*

Orthogonality is probably one of the most important properties for designed experiments. For extreme economy of experimentation, a class of orthogonal design was proposed by Box (1952), called *regular simplex design*. It was shown in Box (1952) that the $n = k + 1$ design points must be distributed over a k-dimensional sphere, centered at the origin, radius $(n-1)^{1/2}$, in the x-space, in such a way that the angle subtended at the origin by any pair of points is the same and has cosine $(-1/(n-1))$. Thus the design consists of the vertices of a regular k-dimensional simplex. One particular type of orientation is given in Table 4.

Table 4
Regular simplex design for k factors

u	x_{1u}	x_{2u}	$\cdots$	x_{ku}
1	-1	-1	$\cdots$	-1
2	1	-1	$\cdots$	-1
3	0	2	$\cdots$	-1
4	0	0	$\cdots$	-1
.	.	.	$\cdots$	.
.	.	.	$\cdots$	.
n	0	0	$\cdots$	k

For example, the design for $k = 3$ is

$$\begin{pmatrix} -1 & -1 & -1 \\ 1 & -1 & -1 \\ 0 & 2 & -1 \\ 0 & 0 & 3 \end{pmatrix}.$$

After standardizing (so that the length of each design column is one), the design becomes

$$\begin{pmatrix} -\sqrt{2} & -\sqrt{2/3} & -1/\sqrt{3} \\ \sqrt{2} & -\sqrt{2/3} & -1/\sqrt{3} \\ 0 & 2\sqrt{2/3} & -1/\sqrt{3} \\ 0 & 0 & \sqrt{3} \end{pmatrix}.$$

2.5. *T-optimal design*

Although orthogonality may be one of the most important features in selecting a design, it is not always possible under certain constraints. For example, in the case of a two-level design, the Plackett and Burman type orthogonal design is only available when n is a multiple of four. On the other hand, some first-order orthogonal designs, such as regular simplex designs (Box, 1952), are presented in an asymmetric manner, which may create practical problems. For example, allocating factors to design columns or determining the experimental regions which suitably fit the coded variables are not trivial matters. Lin and Chang (2001) thus consider the first-order orthogonal design with cyclic structure. The cyclic structure has been adapted to generate symmetry among all design columns. Here, "symmetry" refers to identical experimental range and the common structure of all design columns.

Consider the first-order polynomial model in k variables as in Section 1: $Y = \boldsymbol{X}\beta + \varepsilon = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_k x_k + \varepsilon$, where Y is the response variable and x_i's are the independent variables. A cyclic design in k variables with its first row being $[x_1, x_2, \ldots, x_k]$ can be constructed by cyclically permuting the values in the first row to create $k-1$ more rows and then adding a row of all -1's as the final row. Thus, the design matrix X for a cyclic design in k variables can be written in the general form as

$$\boldsymbol{X} = \begin{bmatrix} x_1 & x_2 & x_3 & \cdots & x_k \\ x_2 & x_3 & x_4 & \cdots & x_1 \\ x_3 & x_4 & x_5 & \cdots & x_2 \\ . & . & . & \cdots & . \\ . & . & . & \cdots & . \\ x_k & x_1 & x_2 & \cdots & x_{k-1} \\ -1 & -1 & -1 & \cdots & -1 \end{bmatrix}.$$

A first-order design is orthogonal if the inner product of any two columns of the X matrix equals zero.

Table 5
T-optimal designs for $k \leqslant 10$

k	$(x_1, x_2, \ldots, x_k)$	Tightness	d-efficiency
1	(1.00)	2.0000	1.0000
2	(1.37, −0.37)	2.3666	0.7990
3	(−1.00, 1.00, 1.00)	2.000	1.000
4	(0.81, −1.43, 0.81, 0.81)	2.2361	0.8365
5	(−0.79, 0.20, −1.00, 1.29, 1.29)	2.2923	0.7966
6	(−1.06, 0.61, −1.06, −0.08, 1.30.1.30)	2.3595	0.7532
7	(1.00, −1.00, −1.00, 1.00, 1.00, 1.00, −1.00)	2.000	1.000
8	(−1.01, 0.40, −1.01, 0.44, −0.58, −0.43, 1.60, 1.60)	2.605	0.6251
9	(−1.12, −0.07, −1.12, −0.07, 1.24, −1.12, 0.77, 1.24, 1.24)	2.3621	0.7412

Lin and Chang (2001) showed a cyclic orthogonal design exists for any positive integer k and it is not unique. Furthermore it is shown that the determinant of $X'X$ is a constant $(k+1)^{k+1}$. For a fair comparison on design efficiency, the design columns need to be rescaled into $[-1, 1]$ range. It turns out that the D-optimal cyclic orthogonal design essentially involves minimizing the tightness of experimental range, namely the difference of $x_{(k+1)} - x_{(1)}$. Cyclic orthogonal designs with minimal tightness are called T-optimal designs. The resulting designs for $k \leqslant 10$ is given in Table 5. Here, the tightness is defined as $\max(x_i) - \min(x_i) = x_{(k+1)} - x_{(1)}$, and the d-efficiency is defined as

$$\text{d-efficiency} = \frac{\|\boldsymbol{X}'\boldsymbol{X}\|^{1/n}}{n}.$$

Clearly, D-optimal designs will yield the highest d-efficiency values, this being the reason for their name. Under our setting, the d-efficiency is equal to 1 only for Plackett and Burman designs; usually it is less than 1.

Take $k = 6$ as an example. From the table we have the first column

$$(-1.06, 0.61, -1.06, -0.08, 1.30, 1.30)'.$$

The resulting design is thus

$$\begin{pmatrix} -1.06 & 0.61 & -1.06 & -0.08 & 1.30 & 1.30 \\ 0.61 & -1.06 & -0.08 & 1.30 & 1.30 & -1.06 \\ -1.06 & -0.08 & 1.30 & 1.30 & -1.06 & 0.61 \\ -0.08 & 1.30 & 1.30 & -1.06 & 0.61 & -1.06 \\ 1.30 & 1.30 & -1.06 & 0.61 & -1.06 & -0.08 \\ 1.30 & -1.06 & 0.61 & -1.06 & -0.08 & 1.30 \\ -1 & -1 & -1 & -1 & -1 & -1 \end{pmatrix}.$$

Table 6
The $U_{12}(12^3 \times 3)$ uniform design

No.	**1**	**2**	**3**	**4**
1	1	10	4	2
2	2	5	11	1
3	3	1	7	3
4	4	6	1	2
5	5	11	10	3
6	6	9	8	1
7	7	4	5	3
8	8	2	3	1
9	9	7	12	2
10	10	12	6	1
11	11	8	2	3
12	12	3	9	2

Table 7
A summarized comparions on selected screening designs

Section	Design	Run	Level	Remarks
2.0	2^{k-p}_{III}	2^t	2	Orthogonal & symmetry
2.1	P&B	4t	2	Orthogonal & symmetry
2.2	Optimal	any	many	Nonorthogonal & asymmetry
2.3	p-eff	$k+1$	2	Nonorthogonal & symmetry
2.4	Simplex	$k+1$	many	Orthogonal & asymmetry
2.5	T-opt	$k+1$	many	Orthogonal & symmetry
2.6	Uniform	any	any	Symmetry

2.6. *Uniform design*

When the relationship between the response and factors is nonlinear or when the experimental domain is large, two-level designs are known to be insufficient. A powerful class of screening designs for more than two-level factors is *Uniform Design*. The uniform experimental design is one of (high level) fractional factorial design which seeks its design points to be uniformly scattered on the experimental domain. The detailed discussion on the uniformity criterion, the construction methods, the resulting designs, as well as the applications to the real life problems can be found in Fang and Lin (Chapter 4). Table 6 gives an example of the $U_{12}(12^3 \times 3)$ design which can be used to investigate three factors at 12 levels and one factor at 3 levels. Most uniform design tables are available at the website `http://www.math.hkbu.edu.hk/UniformDesign`.

2.7. *Summary of screening designs*

All the screening designs discussed above are summarized below for a brief comparison. The experimenter shall choose an appropriate design, based upon his own needs. The term "any" indicates that the experimenter can choose any value, while the term "many" indicates that the number of levels are determined by the design, typically more than two levels.

3. Supersaturated designs

In order to obtain an unbiased estimate of the main effect of each factor, the number of experiments must exceed (or at least be equal to) the number of factors plus one (for estimating the grand average). When these two are equal, the design is called saturated and represents the minimum effort required to estimate all main effects. The standard advice given to users in such a screening process is to use the saturated design, which is "optimal" based upon certain theoretical optimality criteria. However, the nonsignificant effects are not of interest. Estimating all main effects may be wasteful if the goal is simply to detect those few active factors. If the number of active factors is indeed small, the use of a slightly biased estimate will still allow one to accomplish the identification of the active factors but significantly reduce the amount of experimental work. Developing such screening designs has long been a well-recognized problem, certainly since Satterthwaite (1959).

When all factors can be reasonably arranged into several groups, the so-called group screening designs can be used (see, for example, Watson, 1961). Only those factors in groups that are found to have large effects are studied further. The basic assumptions (such as the directions of possible effects are known, etc.), in fact, depend heavily upon the grouping scheme. Some recent developments in group screening can be found in Lewis and Dean (2001) and Dean and Lewis (2002). While such methods may be appropriate in certain situations (e.g., blood tests), we are interested in systematic supersaturated designs factorial designs (mostly two-level) that can examine k factors in $N < k+1$ experiments in which no grouping scheme needs to be made. Recent work in this area includes, for example, Lin (1991, 1993a, 1993b, 1994, 1995), Wu (1993), Deng and Lin (1994), Nguyen (1996), Deng, Lin and Wang (1996a, 1996b), Tang and Wu (1997), Yamada and Lin (1997, 1999), Chen and Lin (1998), Cheng (1997) and Fang, Lin and Ma (2000). Some results on supersaturated design with more than two levels (as well as mixed levels) will be addressed in Section 3.5.

3.1. *Supersaturated designs using Hadamard matrices*

Recently, Lin (1993a) proposed a class of special supersaturated designs which can be easily constructed via half-fractions of the Hadamard matrices. These designs can examine $k = N - 2$ factors with $n = N/2$ runs, where N is the order of the Hadamard matrix used. The Plackett and Burman (1946) designs, which can be viewed as a special class of Hadamard matrices, are used to illustrate the basic construction method.

Table 8 shows the original 12-run Plackett and Burman design. If we take column **11** as the branching column, then the runs (rows) can be split into two groups: Group I with the sign of $+1$ in column **11** (rows 2, 3, 5, 6, 7, and 11), and Group II with the sign of -1 in column **11** (rows 1, 4, 8, 9, 10, and 12). Deleting column **11** from Group I causes columns **1–10** to form a supersaturated design to examine $N - 2 = 10$ factors in $N/2 = 6$ runs (Runs 1–6, as indicated in Table 9). It can be shown that if Group II is used, the resulting supersaturated design is an equivalent one. In general, a Plackett and Burman (1946) design matrix can be split into two half-fractions according to a specific branching column whose signs equal $+1$ or -1. Specifically, take only

Table 8
A supersaturated design derived from the Hadamard matrix of order 12

R	#	1	2	3	4	5	6	7	8	9	10	11
	1	+	+	−	+	+	+	−	−	−	+	−
1	2	+	−	+	+	+	−	−	−	+	−	+
2	3	−	+	+	+	−	−	−	+	−	+	+
	4	+	+	+	−	−	−	+	−	+	+	−
3	5	+	+	−	−	−	+	−	+	+	−	+
4	6	+	−	−	−	+	−	+	+	−	+	+
5	7	−	−	−	+	−	+	+	−	+	+	+
	8	−	−	+	−	+	+	−	+	+	+	−
	9	−	+	−	+	+	−	+	+	+	−	−
	10	+	−	+	+	−	+	+	+	−	−	−
6	11	−	+	+	−	+	+	+	−	−	−	+
	12	−	−	−	−	−	−	−	−	−	−	−

Table 9
The resulting supersaturated design for $(n, k) = (6, 10)$

No.	x_1	x_2	x_3	x_4	x_5	x_6	x_7	x_8	x_9	x_{10}
1	+	−	+	+	+	−	−	−	+	−
2	−	+	+	+	−	−	−	+	−	+
3	+	+	−	−	−	+	−	+	+	−
4	+	−	−	−	+	−	+	+	−	+
5	−	−	−	+	−	+	+	−	+	+
6	−	+	+	−	+	+	+	−	−	−

the rows which have $+1$ in the branching column. Then, the $N - 2$ columns other than the branching column will form a supersaturated design for $N - 2$ factors in $N/2$ runs. Judged by various design criteria, including $E(s^2)$ proposed by Booth and Cox (1962), these designs have been shown to be superior to other existing supersaturated designs.

The construction methods here are simple. However, knowing in advance that Hadamard matrices entertain many "good" mathematical properties, the optimality properties of these supersaturated designs deserve further investigation. For example, the half-fraction Hadamard matrix of order $n = N/2 = 4t$ is closely related to a *balanced incomplete block design* with $(v, b, r, k) = (2t - 1, 4t - 2, 2t - 2, t - 1)$ and $\lambda = t - 1$. Consequently, the $E(s^2)$ value (see next section) for a supersaturated design from a half-fraction Hadamard matrix is $n^2(n-3)/[(2n-3)(n-1)]$ which can be shown to be the minimum within the class of designs with same size. Potentially promising theoretical results seem possible for the construction of a half-fraction Hadamard matrix. Theoretical implications deserve detailed scrutiny and will be discussed below. For more details regarding this issue, please consult with Cheng (1997) and Nguyen (1996).

Note that the interaction columns of Hadamard matrices are only partially confounded with other main effect columns. Wu (1993) makes use of such a property and proposes a supersaturated design that consists of all main-effect and two-factor interaction columns from any given Hadamard matrix of order N. The resulting design has N runs and can accommodate up to $N(N-1)/2$ factors. When there are $k < N(N-1)/2$ factors to be studied, choosing columns becomes an important issue to be addressed.

3.2. Capacity considerations

As mentioned, when a supersaturated design is used, the abandonment of perfect orthogonality is inevitable. The designs given in Lin (1993a) based on half-fractions of Hadamard matrices have a very nice mathematical structure but can only be used to examine $N-2$ factors in $N/2$ runs, where N is the order of the Hadamard matrix used. Moreover, these designs do not control the value of the maximal pairwise correlation r, and in fact, large values of r occur in some cases.

Consider a two-level k-factor design in n observations with maximal pairwise correlation r. Given any two of the quantities (n, k, r), Lin (1995) presents the possible values that can be achieved for the third quantity. Moreover, designs given in Lin (1995) may be adequate to allow examination of many prespecified two-factor interactions.

Table 10 shows the maximum number of factors, $k_{\max}$, that can be accommodated when both n (even) and r are specified for $3 \leqslant n \leqslant 25$ and $0 \leqslant r \leqslant 1/3$. We see that for $r \leqslant 1/3$, many factors can be accommodated. For fixed n, as the value of r increases, $k_{\max}$ also increases. That is, the larger the nonorthogonality, the more factors can be accommodated. In fact, $k_{\max}$ increases rapidly in this setting. Certainly the more factors accommodated, the more complicated are the biased estimation relationships that occur, leading to more difficulty in data analysis. On the other hand, for fixed r, the value of $k_{\max}$ increases rapidly as n increases. For $r \leqslant 1/3$, one can accommodate at most 111 factors in 18 runs or 66 factors in 12 runs; for $r \leqslant 1/4$, one can accommodate 42 factors in 16 runs; for $r \leqslant 1/5$, one can accommodate 34 factors in 20 runs. Provided that these maximal correlations are acceptable, this can be an efficient design strategy.

Table 10
Maximal number of factors found, $k_{\max}$, as a function of n and nr, for even $n \leqslant 24$ and $r \leqslant 1/3$

Number of runs	Maximum ($\lvert c_i' c_j \rvert$)				
(n)	0	2	4	6	8
4	3				
6	–	10			
8	7	–			
10	–	12			
12	11	–	66		
14	–	13	–	113	
16	15	–	42	–	
18	–	17	–	111	
20	19	–	34		
22	–	20	–	92	–
24	23	–	33	–	276

3.3. Data analysis methods

Several methods have been proposed in the literature to analyze the k effects, given only the n ($<k$) observations, mainly from the random balance design contents (see, for example, Satterthwaite, 1959). These methods can also be applied here. Quick methods such as these provide an appealing, straightforward comparison among factors, but it is questionable how much available information can be extracted using them. Combining several of these methods provides a more satisfying result. In addition, three data analysis methods for data resulting from a supersaturated design are discussed in Lin (1995): (1) normal plotting, (2) stepwise selection, and (3) ridge regression.

When studying so many columns in only a few runs, the probability of a false-positive reading (Type I error) is a major risk. An alternative to the forward selection procedure to control these false-positive rates has been investigated. Recall that we have null and alternative pairs H_j: $\beta_j = 0$ and H_j^c: $\beta_j \neq 0$ with H_j true for $j \in N$ and H_j^c true for $j \in A$ (see Section 1). Forward selection proceeds by identifying the maximum F-statistics at successive stages. Let $F_j^{(s)}$ denote the F-statistic for testing H_j at stage s. Consequently, define

$$j_t = \underset{j \in S - \{j_1, \ldots, j_{t-1}\}}{\arg\max} F_j^{(t)},$$

where $F_j^{(s)} = \mathrm{SSR}(j \mid j_1, \ldots, j_{s-1})/\mathrm{MSE}(j, j_1, \ldots, j_{s-1})$. Letting $\max F_j^{(s)} = F^{(s)}$, the forward selection procedure is defined by selecting variables $j_1, \ldots, j_f$, where $F^{(f)} \leqslant \alpha$ and $F^{(f+1)} > \alpha$. If $F^{(1)} > \alpha$, then no variables are selected.

The Type I (false positive) error rate may be controlled using the adjusted p-value method of Westfall and Young (1993). Algorithmically, at stage j, if $p^{(j)} > \alpha$, then stop; otherwise, enter X_j and continue. This procedure controls the Type I error rate exactly at level α under the complete null hypothesis since $P(\text{Rejects at least one } H_i \mid \text{all } H_i \text{ true}) = P(F^{(1)} \leqslant f_\alpha^{(1)}) = \alpha$. In addition, if the first s variables are *forced* and the test is used to evaluate the significance of the next entering variable (of the remaining $k-s$), the procedure is again exact under the complete null hypothesis of no effects among the $k-s$ remaining variables. The exactness disappears with simulated p-values, but the errors can be made very small, particularly with control variates. The analysis of data from supersaturated designs along this direction can be found in Westfall, Young and Lin (1993).

Beattie, Fong and Lin (2002) detail a two-stage Bayesian model selection strategy combining recent methodologies: the Stochastic Search Variable Selection (SSVS) method of George and McCulloch (1993, 1997) and the Intrinsic Bayes Factor (IBF) method of Berger and Pericchi (1996). This strategy is able to keep all possible models under consideration, provides a direct comparison between any two competing models, and provides a level of robustness akin to Bayesian analyses incorporating noninformative priors. The two-stage procedure is able to keep all possible models under consideration while providing a level of robustness akin to Bayesian analyses incorporating noninformative priors. Note that Bayesian methods are able to supplement observational information using prior information on the parameters. This allows straightforward computation of posterior probabilities, a more intuitive concept than the p-value.

Recent development of the Gibbs sampling algorithm (Gelfand and Smith, 1990) and other Markov chain Monte-Carlo techniques (see, for example, Gilks et al., 1996), in tandem with computational advances, have brought many Bayesian ideas mainstream. However, the use of these methods in analyzing supersaturated designs may require a departure from noninformative priors to guarantee the existence of a proper posterior distribution, thus leaving room for controversy on the objectivity of the results.

Li and Lin (2002) proposed a variable selection procedure for identifying active factors in supersaturated design, via nonconvex penalized least square approach. With a proper choice of the regularization parameter, it is shown that the resulting estimator is root n consistent and possesses an oracle property. This is believed to be the most reliable data analysis method for supersaturated design. For details, see Li and Lin (2002, 2003).

3.4. Theoretical construction methods

Deng, Lin and Wang (1994) proposed a supersaturated design of the form $\boldsymbol{X}_c = [\boldsymbol{H}, \boldsymbol{RHC}]$, where $\boldsymbol{H}$ is a normalized Hadamard matrix, $\boldsymbol{R}$ is an orthogonal matrix, and $\boldsymbol{C}$ is an $n \times (n-c)$ matrix representing the operation of column selection. Besides the fact that some new designs with nice properties can be obtained this way, the $\boldsymbol{X}_c$ matrix covers many existing supersaturated designs. This includes the supersaturated designs proposed by Lin (1993a), Wu (1993) and Tang and Wu (1997). It can be shown that

$$\boldsymbol{X}_c'\boldsymbol{X}_c = \begin{pmatrix} n\boldsymbol{I}_n & \boldsymbol{H}'\boldsymbol{RHC} \\ \boldsymbol{C}'\boldsymbol{H}'\boldsymbol{R}'\boldsymbol{H} & n\boldsymbol{I}_{n-c} \end{pmatrix} = \begin{pmatrix} n\boldsymbol{I}_n & \boldsymbol{WC} \\ \boldsymbol{C}'\boldsymbol{W}' & n\boldsymbol{I}_{n-c} \end{pmatrix},$$

where $\boldsymbol{W} = \boldsymbol{H}'\boldsymbol{RH} = (w_{ij}) = (\boldsymbol{h}_i'\boldsymbol{R}\boldsymbol{h}_j)$ and $\boldsymbol{h}_j$ is the jth column of $\boldsymbol{H}$. It can be further shown that:

THEOREM 1. *Let $\boldsymbol{H}$ be a Hadamard matrix of order n and $\boldsymbol{B} = (b_1, \ldots, b_r)$ be a $n \times r$ matrix with all entries ± 1 and $\boldsymbol{V} = \boldsymbol{H}'\boldsymbol{B} = (v_{ij}) = \boldsymbol{h}_i'b_j$. Then*

(1) *for any fixed $1 \leqslant j \leqslant r$, $n^2 = \sum_{i=1}^n v_{ij}^2$.*
(2) *In particular, let $\boldsymbol{B} = \boldsymbol{RH}$ and $\boldsymbol{W} = \boldsymbol{H}'\boldsymbol{RH} = (w_{ij})$. We have*

- *$\frac{1}{n}\boldsymbol{W}$ is an $n \times n$ orthogonal matrix,*
- *$n^2 = \sum_{i=1}^n w_{ij}^2 = \sum_{j=1}^n w_{ij}^2$,*
- *w_{ij} is always a multiple of 4, and*
- *if $\boldsymbol{H}'$ is column balanced, then $\pm n = \sum_{i=1}^n w_{ij} = \sum_{j=1}^n w_{ij}$.*

COROLARRY. *For any $\boldsymbol{R}$ and $\boldsymbol{C}$ such that (1) $\boldsymbol{R}'\boldsymbol{R} = \boldsymbol{I}$ and (2) $\operatorname{rank}(\boldsymbol{C}) = n - c$, then the X_c matrix has the same $E(s^2)$ values.*

This implies that the popular $E(s^2)$ criterion used in supersaturated designs is invariant for any choice of $\boldsymbol{R}$ and $\boldsymbol{C}$. Therefore, it is not effective for comparing supersaturated designs. In fact, following the argument in Tang and Wu (1997), the designs given here will always have the minimum $E(s^2)$ values within the supersaturated design of this type. One important feature of the goodness of a supersaturated screening design is its projection property (as discussed in Section 3.5 and in Lin, 1993b). We thus consider the r-rank property as defined below.

DEFINITION. Let $\boldsymbol{X}$ be a equal occurrence design matrix. The resolution rank (or r-rank, for short) of $\boldsymbol{X}$ is defined as $f = d - 1$, where d is the minimum number of subset columns that are linearly dependent.

The following results are provided by Deng, Lin and Wang (1994).

(1) If no column in any supersaturated design $\boldsymbol{X}$ is fully aliased, then the r-rank of $\boldsymbol{X}$ is at least 3.
(2) $n\boldsymbol{R}\boldsymbol{h}_j = \sum_{i=1}^n w_{ij}\boldsymbol{h}_i$.
(3) Let $\boldsymbol{W} = \boldsymbol{H}'\boldsymbol{D}(\boldsymbol{h}_l)\boldsymbol{H}$, where $\boldsymbol{D}(\boldsymbol{h}_l)$ is the diagonal matrix associated with $\boldsymbol{h}_l$, namely, the lth column vector of $\boldsymbol{H}$, and $n = 4t$, then

- If t is odd, then there can be exactly three 0's in each row, or each column, of $\boldsymbol{W}$. The rest of w_{ij} can only be of the form $\pm 8k + 4$, for some nonnegative integer k.
- If t is even, then every entry w_{ij} in $\boldsymbol{W}$ can be of the form $\pm 8k$, for some nonnegative integer k.

These results are only the first step. Extension of these results to a more general class of supersaturated designs in the form $\boldsymbol{S}_K = (\boldsymbol{R}_1\boldsymbol{H}\boldsymbol{C}_1, \ldots, \boldsymbol{R}_K\boldsymbol{H}\boldsymbol{C}_K)$ are promising.

Recently, a series of "optimal" supersaturated designs via combinatorial design theory has been obtained by Fang, Ge, Liu and Qin (2001). A website for all supersaturated design obtained will be established in the near future.

3.5. Optimality criteria

When a supersaturated design is employed, as previously mentioned, the abandonment of orthogonality is inevitable. It is well known that lack of orthogonality results in lower efficiency; therefore we seek a design that is as "near orthogonal" as possible. One way to measure the degree of nonorthogonality between two columns, c_i and c_j, is to consider their cross-product, $s_{ij} = c_i'c_j$. A larger $|s_{ij}|$ implies less orthogonality. As discussed in Section 2.5, denote the largest $|s_{ij}|$ among all pairs of columns for a given design by s, and we desire a minimum value for s ($s = 0$ implies orthogonality). The quantity s can be viewed as the degree of orthogonality that the experimenter is willing to give up with small s indicating a better design. This is intimately connected with the expectation of s^2, $E(s^2)$, defined in Section 2.2. Intuitively, $E(s^2)$ gives the increment in variance of estimation arising from non-orthogonality. It is, however, a measurement for pairwise relationships only. More general criteria have been obtained in Wu (1993) and Deng, Wang and Lin (1994, 1996b). Deng and Lin (1994) outline eight criteria useful for supersaturated designs: $s = \max c_i'c_j$; $E(s^2)$; ρ (Lin, 1995); D_f, A_f, E_f (Wu, 1993); B-criterion (Deng, Lin and Wang, 1996a, 1996b); and r-rank (Deng, Lin and Wang, 1999). Further theoretical justification is currently under study. Optimal designs in light of these approaches deserve further investigations. In addition, the notion of multi-factor (non-)orthogonality is closely related to multicollinearity in linear model theory.

For 3-level supersaturated designs, Yamada and Lin (1999) defined a measure of dependency between two design columns $\boldsymbol{x}_i$ and $\boldsymbol{x}_j$ by

$$\chi^2(\boldsymbol{x}_i, \boldsymbol{x}_j) = \sum_{u,v=1}^{3} \frac{(n_{uv}^{(ij)} - n/9)^2}{n/9}, \tag{1}$$

where $n_{uv}^{(ij)}$ is the number of (u, v)-pairs in $(\boldsymbol{x}_i, \boldsymbol{x}_j)$. Then they defined a criterion for the whole design $\boldsymbol{X}$ by

$$\text{ave}\,\chi^2 = \sum_{1 \leqslant i < j \leqslant k} \chi^2(\boldsymbol{x}_i, \boldsymbol{x}_j) \Big/ \binom{k}{2}$$

and also showed a lower bound of

$$\text{ave}\,\chi^2 \geqslant \frac{2n(2k - n + 1)}{(n-1)(k-1)}. \tag{2}$$

Recently, Fang, Lin and Liu (2000) proposed a new criterion for supersaturated design, suitable for any mixed level design. For any two design columns $\boldsymbol{x}_i$ and $\boldsymbol{x}_j$, define

$$f_{NOD}^{ij} = \sum_{u=1}^{q_i} \sum_{v=1}^{q_j} \left(n_{uv}^{(ij)} - \frac{n}{q_i q_j} \right)^2, \tag{3}$$

where $n_{uv}^{(ij)}$ is the number of (u, v)-pairs in $(\boldsymbol{x}_i, \boldsymbol{x}_j)$, and $n/(q_i q_j)$ stands for the average frequency of level-combinations in each pair of columns $\boldsymbol{x}_i$ and $\boldsymbol{x}_j$. A new criterion $E(f_{NOD})$ is defined as the following,

$$E(f_{NOD}) = \sum_{1 \leqslant i < j \leqslant m} f_{NOD}^{ij} \Big/ \binom{m}{2}. \tag{4}$$

It is obvious that $E(f_{NOD}) = 0$ for an orthogonal array. Let $\lambda_{kl} = \sum_{j=1}^{m} 1_{\{x_{kj} = x_{lj}\}}$, where 1_A is the indicator function of A, i.e., λ_{kl} is the number of coincidences between the two columns $\boldsymbol{x}_k$ and $\boldsymbol{x}_l$. It is obvious that $\lambda_{kk} = m$. The following theorem defines the $E(f_{NOD})$ criterion and gives its lower bound (in terms of λ_{kl}'s). The formal definition of U-type design $\mathcal{U}(n, q_1, \ldots, q_m)$ can be found in Chapter 4.

THEOREM 2. *For any design matrix $\boldsymbol{X} \in \mathcal{U}(n, q_1, \ldots, q_m)$, we have*

$$E(f_{NOD}) = \frac{\sum_{k,l=1, k \neq l}^{n} \lambda_{kl}^2}{m(m-1)} + C(n, q_1, \ldots, q_m) \tag{5}$$

$$\geqslant \frac{n(\sum_{j=1}^{m} n/q_j - m)^2}{m(m-1)(n-1)} + C(n, q_1, \ldots, q_m), \tag{6}$$

where

$$C(n, q_1, \ldots, q_m) = \frac{nm}{m-1} - \frac{1}{m(m-1)} \left(\sum_{i=1}^{m} \frac{n^2}{q_i} + \sum_{i,j=1, j \neq i}^{m} \frac{n^2}{q_i q_j} \right)$$

depends on $\boldsymbol{X}$ only through $n, q_1, \ldots, q_m$, and the lower bound of $E(f_{NOD})$ can be achieved if and only if $\lambda = (\sum_{j=1}^{m} n/q_j - m)/(n-1)$ is a positive integer and all the λ_{kl}'s for $k \neq l$ are equal to λ.

For any two factors $\boldsymbol{x}_i$ and $\boldsymbol{x}_j$ of the design $\boldsymbol{X}$, the equal occurrence of -1 and 1 implies that $f_{NOD}^{ij} = s_{ij}^2/4$, where $f_{NOD}^{ij} = \sum_{u,v=-1,1} (n_{uv}^{(ij)} - n/4)^2$. This, in turn, implies that f_{NOD}^{ij} is essentially the same measure as s_{ij}^2 for two-level designs. Furthermore, $\chi^2(\boldsymbol{x}_i, \boldsymbol{x}_j) = f_{NOD}^{ij} q_i q_j / n$, for three-level columns. The next theorem follows immediately.

THEOREM 3. *For any design matrix $\boldsymbol{X} \in \mathcal{U}(n; q_1, \ldots, q_m)$, the three design criteria $E(f_{NOD})$, $E(s^2)$ and* ave χ^2 *satisfy the following relations*:

$$E(f_{NOD}) = \frac{n}{9}\,\text{ave}\,\chi^2, \quad \textit{when } q_i = 3, i = 1, \ldots, m, \quad \textit{and} \tag{7}$$

$$E(f_{NOD}) = \frac{1}{4} E(s^2), \quad \textit{when } q_i = 2, i = 1, \ldots, m, \textit{ with two levels } -1 \textit{ and } 1. \tag{8}$$

Furthermore, the lower bound of $E(f_{NOD})$ includes those lower bounds of $E(s^2)$ and of ave χ^2 *as special cases.*

This theorem sets up the equivalence between the three criteria for supersaturated designs, $E(s^2)$, ave χ^2 and $E(f_{NOD})$. It also provides a justification for using $E(f_{NOD})$ as a design criterion for supersaturated designs. Unlike the $E(s^2)$ and ave χ^2 criteria, the $E(f_{NOD})$ criterion can be used for mixed level designs.

3.6. *Computer algorithmic construction methods*

More and more researchers are benefiting from using computer power to construct designs for specific needs. Unlike some cases from the optimal design perspective (such as D-optimal design), computer construction of supersaturated designs is not currently well-developed. Lin (1991) introduced the first computer algorithm to construct supersaturated designs. Lin (1995) examines the maximal number of factors that can be accommodated in such a design when r and n are given.

Al Church at GenCorp Company utilized the projection properties in Draper and Lin (1992) to develop a software package named "DOE0" to generate designs for mixed-level discrete variables. Such a program has been used by several sites in GenCorp. A program named "DOESS" is one of the results and is currently in a test stage.

Dr. Nam-Ky Nguyen (CSIRO, Australia) also independently works on this subject. He uses an exchange procedure to construct supersaturated designs and near-orthogonal arrays. A commercial product called "Gendex" is available for public sale, as a result. Algorithmic approaches to constructing supersaturated designs seem to be a hot topic in the recent year. For example, Li and Wu (1997) develop a so-called columnwise-pairwise exchange algorithm. Such an algorithm seems to perform well for constructing supersaturated designs by various criteria.

3.7. Some recent advances on supersaturated design

Marginally oversaturated designs

A special class of supersaturated design, called marginally over saturated design (MOSD), in which the number of variables under investigation (k) is only slightly larger than the number of experimental runs (n), is presented in Deng, Lin and Wang (1996a, 1996b). The construction method builds on two major theorems which provide an efficient way to evaluate the resolution rank criterion. They provided such designs for $n = 8$, 12, 16, and 20. Recall that the resolution rank (r) is defined as $r = \max\{c$: for any $(\boldsymbol{x}_{i1}, \ldots, \boldsymbol{x}_{ic})$ of $\boldsymbol{X}, \boldsymbol{x}_{i1}, \ldots, \boldsymbol{x}_{ic}$ are linearly independent$\}$.

THEOREM 4. *Let $\boldsymbol{X} = [\boldsymbol{H}, \boldsymbol{v}]$, $\boldsymbol{w} = \boldsymbol{H}'\boldsymbol{v}$, where $\boldsymbol{H}$ is a Hadamard matrix of order n. Let R_1 be the number of nonzero entries in $\boldsymbol{w}$. Then*

$$r = R_1,$$

where r is the resolution rank of $\boldsymbol{X}$.

THEOREM 5. *Let $\boldsymbol{X} = [\boldsymbol{H}, \boldsymbol{v}_1, \boldsymbol{v}_2]$ and $\boldsymbol{w}_1 = \boldsymbol{H}'\boldsymbol{v}_1$, $\boldsymbol{w}_2 = \boldsymbol{H}'\boldsymbol{v}_2$, where $\boldsymbol{H}$ is a Hadamard matrix of dimension n. Let*

$$R_1 = \min\bigl[S(\boldsymbol{w}_1), \boldsymbol{S}(\boldsymbol{w}_1)\bigr]$$

and

$$R_2 = \min\bigl[S(\boldsymbol{b}_1\boldsymbol{w}_1 + \boldsymbol{b}_2\boldsymbol{w}_2)\bigr] + \boldsymbol{1},$$

where $S(\boldsymbol{u})$ represents the number of nonzero elements in the vector $\boldsymbol{u}$ and b_1, b_2 can take on all possible values. Then

$$r = \min[R_1, R_2],$$

where r is the resolution rank of $\boldsymbol{X}$.

For example, with $n = 12$, the MSOD is given as follows, where $(1, \boldsymbol{x}_1, \ldots, \boldsymbol{x}_1\boldsymbol{1})$ form a 12-run Hadamard matrix and $\boldsymbol{v}_1$ and $\boldsymbol{v}_2$ are the optimal added columns from Theorems above.

$\boldsymbol{1}$	$\boldsymbol{x}_1$	$\boldsymbol{x}_2$	$\boldsymbol{x}_3$	$\boldsymbol{x}_4$	$\boldsymbol{x}_5$	$\boldsymbol{x}_6$	$\boldsymbol{x}_7$	$\boldsymbol{x}_8$	$\boldsymbol{x}_9$	$\boldsymbol{x}_{10}$	$\boldsymbol{x}_{11}$	$\boldsymbol{v}_1$	$\boldsymbol{v}_2$
+	+	+	−	+	+	+	−	−	−	+	−	+	−
+	+	−	+	+	+	−	−	−	+	−	+	+	+
+	−	+	+	+	−	−	−	+	−	+	+	+	+
+	+	+	+	−	−	−	+	−	+	+	−	+	+
+	+	+	−	−	−	+	−	+	+	−	+	+	+
+	+	−	−	−	+	−	+	+	−	+	+	−	+
+	−	−	−	+	−	+	+	−	+	+	+	+	−
+	−	−	+	−	+	+	−	+	+	+	−	−	+
+	−	+	−	+	+	−	+	+	+	−	−	−	−
+	+	−	+	+	−	+	+	+	−	−	−	−	−
+	−	+	+	−	+	+	+	−	−	−	+	−	−
+	−	−	−	−	−	−	−	−	−	−	−	−	−

Three-level supersaturated designs

Given a two-level orthogonal array $\boldsymbol{C}$ of size (n, m), Yamada and Lin (1999) provided a series of three-level supersaturated designs of the form $(N, K) = (3n, 4m)$ as follows.

$$\boldsymbol{D} = \begin{bmatrix} \phi^{12}(\boldsymbol{C}) & \phi^{12}(\boldsymbol{C}) & \phi^{13}(\boldsymbol{C}) & \phi^{23}(\boldsymbol{C}) \\ \phi^{23}(\boldsymbol{C}) & \phi^{13}(\boldsymbol{C}) & \phi^{23}(\boldsymbol{C}) & \phi^{12}(\boldsymbol{C}) \\ \phi^{31}(\boldsymbol{C}) & \phi^{23}(\boldsymbol{C}) & \phi^{12}(\boldsymbol{C}) & \phi^{13}(\boldsymbol{C}) \end{bmatrix}, \tag{9}$$

where $\phi^{ab}(\,)$ is an operator which transforms the elements from -1 to a and from 1 to b on the matrix/vector in $(\,)$. Such a design can study $K = 4m$ factors in $N = 3n$ runs. It is clearly a three-level supersaturated design. It is also shown in Yamada and Lin (1999) that such designs have a relatively small value of ave χ^2 as previously defined.

Multi-level supersaturated designs

Fang, Lin and Ma (2000) obtained a new class of multi-level supersaturated design by collapsing a U-type uniform design to an orthogonal array. This can be illustrated by the following example. Suppose that we extend the orthogonal design $\boldsymbol{L} = \boldsymbol{L}_9(\boldsymbol{3}^4)$ and a generating U-type design $\boldsymbol{U} = \boldsymbol{U}(\boldsymbol{9}, \boldsymbol{9}^2)$ to a S-design $S_9(3^8)$ by the collapsing method.

$$\boldsymbol{U} \oplus \boldsymbol{L} = \begin{bmatrix} 1 & 1 \\ 2 & 7 \\ 3 & 3 \\ 4 & 9 \\ 5 & 5 \\ 6 & 6 \\ 7 & 2 \\ 8 & 8 \\ 9 & 4 \end{bmatrix} \oplus \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 1 \\ 0 & 2 & 2 & 2 \\ 1 & 0 & 1 & 2 \\ 1 & 1 & 2 & 0 \\ 1 & 2 & 0 & 1 \\ 2 & 0 & 2 & 1 \\ 2 & 1 & 0 & 2 \\ 2 & 2 & 1 & 0 \end{bmatrix} = \boldsymbol{X} = \left[\begin{array}{cccc|cccc} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 1 & 2 & 0 & 2 & 1 \\ 0 & 2 & 2 & 2 & 0 & 2 & 2 & 2 \\ 1 & 0 & 1 & 2 & 2 & 2 & 1 & 0 \\ 1 & 1 & 2 & 0 & 1 & 1 & 2 & 0 \\ 1 & 2 & 0 & 1 & 1 & 2 & 0 & 1 \\ 2 & 0 & 2 & 1 & 0 & 1 & 1 & 1 \\ 2 & 1 & 0 & 2 & 2 & 1 & 0 & 2 \\ 2 & 2 & 1 & 0 & 1 & 0 & 1 & 2 \end{array}\right],$$

where the operation $\oplus$ is defined such that the ith block of $\boldsymbol{X}$ if essentially the matrix $\boldsymbol{L}$ by taking the row order of column i in matrix $\boldsymbol{U}$. Namely, the first block (the first four columns) of $\boldsymbol{X}$ is the original $\boldsymbol{L}$ and the second block (the last four columns) are formed by rearranging row vectors of $\boldsymbol{L}$ according to the order defined by the second column of $\boldsymbol{U}$. The crucial step of this collapsing method is how to choose the best U-type design $U(n, n^r)$ in the sense of minimizing any specific criterion (see Fang, Lin and Ma, 2000).

3.8. Summary of supersaturated designs

Using supersaturated designs involves more risk than using designs with more runs. However, their use is far superior to other experimentation approaches such as subjective selection of factors or changing factors one-at-a-time. The latter can be shown to have unresolvable confounding patterns, though such confounding patterns are important for data analysis and follow-up experiments.

Supersaturated designs are very useful in early stages of the experimental investigation of complicated systems and processes involving many factors. They are not used for a terminal experiment. Knowledge of the confounding patterns makes possible the interpretation of the results and provides the understanding of how to plan the follow-up experiments.

The success of a supersaturated design depends heavily on the "effect sparsity" assumption. Consequently, the projection properties play an important role in designing a supersaturated experiment. Combining several data analysis methods to analyze the data resulting from a supersaturated design is always recommended. Besides the stepwise selection procedure, PLS (partial least squares), adjusted p-value nonconvex penalized least square and Bayesian approaches are promising procedures used to identify active factors.

Another particularly suitable use for these designs is in testing "robustness," where the objective is not to identify important factors, but to vary all possible factors so that the response will remain within the specifications.

4. Computer experiments

4.1. Introduction

Computer models are often used to describe complicated physical phenomena encountered in science and engineering. These phenomena are often governed by a set of equations, including linear, nonlinear, ordinary, and partial differential equations. The equations are often too difficult to be solved simultaneously by any person, but can be by a computer modeling program. These programs, due to the number and complexity of the equations, may have long running times, making their use difficult for comprehensive scientific investigation.

The SOLA-PTS algorithm described in Daly and Torrey (1984), for example, has been developed at the Los Alamos National Laboratory for modeling the rapid cooling of a nuclear reactor wall as a result of cold water injected into the reactor's downcomer for containment during a nuclear accident. The authors' three-pronged goal is to study

the response of the reactor, to study the turbulent mixture of the cold water and the warm fluid already in the downcomer, and to predict the onset and growth of cracks in the reactor wall as a result of the rapid cooling. This algorithm simultaneously solves eight partial differential equations with eight inputs and takes approximately 90 minutes on a Cray supercomputer to run. It solves a large number of differential equations, is very computationally expensive in running time, and has a "black box" quality – one does not know in advance which factors have large effects and one would like to examine the response over a wide range of input combinations. This algorithm is typical of computer models needing designed experiments.

One goal in this setting is to build an approximating program which, although not as precise as the computer model, would run fast enough to study the phenomenon in detail. Construction of an adequate approximating function (or program) to the computer model requires the selection of design points (a designed experiment) at which to approximate. Because the computer models are mostly deterministic, these computer experiments require special designs. In physical experiments, if certain factors have no effect on the response and are taken out of the approximation function (linear model), then the replicated design points in the reduced design space can be used to estimate the random error present in the system. However, with computer experiments, there is no random error – only lack of fit. Standard factorial designs are inadequate here; in the absence of certain main effects, replication cannot be used to estimate this error, but instead produces redundancy. That is, they are hindered by their nonunique projections to lower dimensions. This section presents a new and simple strategy for designs for computer experiments, developed from the rotation of the standard factorial design to yield a Latin hypercube.

4.2. Design criteria and related work

Selection of an appropriate designed experiment depends to an extent on the experimental region, the model to be fit, and the method of analysis. The approach described here assumes the following: the experimental region is cuboidal (each factor is bound between values of interest), the true model is unknown to the experimenter and that he will approximate it by a polynomial of some degree *a priori* unknown to him, and the method of analysis will be ordinary least squares regression. Alternative methods are available (see Haaland et al., 1994).

In order to assess design criteria for computer experiments, it is valuable to study the progression of proposed designs. Koehler and Owen (1996) provide an overview of past and current approaches (see also Draper and Lin, 1996). The two main geometric designs are the standard (full or fractional) factorial designs and the Latin hypercube designs, but also include other traditional designs for physical experiments, such as central composite designs. Easterling (1989) points out that standard factorial designs have many attractive properties for physical experiments: balance (factor levels used an equal number of times), symmetry (permutation of design matrix columns yields same design), orthogonality (separability of main effects), collapsibility (projects to lower subspace as factorial design, sometimes redundantly), equally-spaced projections to each dimension, and straightforward measurability of main effects.

McKay, Beckman and Conover (1979) introduced the use of the Latin hypercube (LH) in computer experiments. A n-point LH design matrix is constructed by randomly permuting the integers $\{1, 2, \ldots, n\}$ for each factor and rescaling to the experimental region, so that the points project uniquely and equally-spaced to each dimension. The unique projections of LHs allow for great flexibility in model fitting. Box and Draper (1959) showed that when the true model is a polynomial of unknown degree, the best design places its points evenly spaced over the design region. Thus, equally-spaced projections are also of value. For these reasons, the LH has become the standard for computer experiments. However, random LHs are susceptible to high correlations between factors, even complete confounding, and to omitting regions of the design space.

Computer-generated designs include those of Sacks, Schiller and Welch (1989) and Sacks, Welch, Mitchell and Wynn (1989) that try to minimize the integrated mean square error (IMSE) of prediction when prediction errors are taken as a realization of a spatial stochastic process. Johnson, Moore and Ylvisaker (1990) proposed similar designs to minimize the correlations between observations when responses are taken as a realization of a spatial stochastic process. The latter authors' called a design D^* a maximin distance design if

$$\min_{x_1,x_2\in D^*} d(x_1, x_2) = \max_{D} \min_{x_1,x_2\in D} d(x_1, x_2), \tag{10}$$

where d is a distance measure and $\min_{x_1,x_2\in D} d(x_1, x_2)$ is the minimum interpoint distance (MID) of design D; that is, its points are moved as far apart from one another as possible.

Attempts have been made to bridge the gap between geometric designs and computer-generated designs. Tang (1993) and Owen (1992) introduced orthogonal-array based LHs to guarantee coverage of all regions for every subset of r factors. Morris and Mitchell (1992) and Tang (1994) proposed LHs that attain the largest MID among all LHs, called maximin Latin hypercubes. Owen (1994) attempted to control the correlations between design matrix columns of random LHs. These methods are a step forward in merging the good properties of Latin hypercubes with the optimization of computer-generated designs. However, being themselves computer-generated designs leaves susceptibilities to the aforementioned problems.

With this in mind, we seek a new design for computer experiments with these properties: the unique and equally-spaced projections to each dimension and flexibility in model selection provided by Latin hypercube design and the orthogonality and ease of construction provided by standard factorial designs. In addition, these new designs should perform reasonably well in terms of other criteria mentioned, such as MID correlation and coverage of the design space.

4.3. *Rotated factorial designs in two dimensions*

The strategy taken here is to modify the standard factorial design by rotation so as to yield a Latin hypercube. To see how this is done, first consider the standard 3^2 factorial design, represented by the 3×3 square of points in Figure 1, and how it can

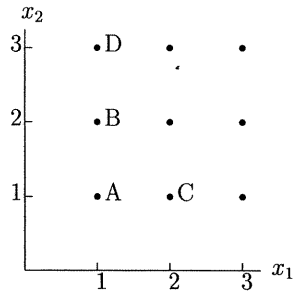

Fig. 1. Standard 3^2 factorial design before rotation.

be rotated to yield equally-spaced projections. The key to finding all such rotations is in the relationship between points A–D. We focus on nontrivial angles between 0 and 45 degrees clockwise due to the symmetry of the rotation problem.

The matrix equation to rotate a set of points clockwise by an angle w about the origin is

$$\begin{bmatrix} x_1 & x_2 \end{bmatrix} \times \begin{bmatrix} \cos(w) & -\sin(w) \\ \sin(w) & \cos(w) \end{bmatrix}$$

so that if (x_1, x_2) are the coordinates of a design point in the standard factorial design, then the rotation moves the point to $(x_1\cos(w) + x_2\sin(w), -x_1\sin(w) + x_2\cos(w))$. Notice first that as the points are rotated clockwise about the origin that A will have the smallest x_1-coordinate for any angle between $0°$ and $45°$. (A $45°$ rotation will place A directly on the x_1-axis and A is the closest point to the origin.) Also notice that the x_1-projections of points with the same initial x_1-coordinate (like A, B, and D) will be equally spaced, by $\sin(w)$, regardless of the rotation angle. Likewise, the x_1-projections of points with the same initial x_2-coordinate (like A and C) will be equally spaced, by $\cos(w)$, regardless of the rotation angle. It suffices to find all angles that make the x_1-projections of points A–D equally spaced. For the x_1-coordinates of A–D, see the table below.

Point	x_1-coordinate
A	$\cos(w) + \sin(w)$
B	$\cos(w) + 2\sin(w)$
C	$2\cos(w) + \sin(w)$
D	$\cos(w) + 3\sin(w)$

Between $0°$ and $45°$, $\sin(w) \leqslant \cos(w)$, so the point with the next smallest x_1-coordinate will always be B (although C will tie B when $w = 45°$) and the distance between the smallest two x_1-projections will always be $\sin(w)$. To achieve equally-spaced x_1-projections, the distance between all x_1-projections must equal $\sin(w)$. We've already seen that this is true when $w = 45°$ (equivalently, $\tan^{-1}(1)$) and both C and B have the second smallest x_1-coordinate.

Another possibility is that C will have the third smallest x_1-coordinate, and that the "x_1-distance" between B and C will be $\sin(w)$. However, the "x_1-distance" between B and D is always $\sin(w)$. In this case, C and D will have the same x_1-coordinate, hence

$$\cos(w) = 2\sin(w) \Longrightarrow w = \tan^{-1}(1/2).$$

Continuing in this manner, consider the case where C has the fourth smallest x_1-coordinate – after A, B, and D – and the "x_1-distance" between D and C is $\sin(w)$. Then

$$\cos(w) - 2\sin(w) = \sin(w) \Longrightarrow w = \tan^{-1}(1/3).$$

Point C cannot have the fifth smallest x_1-coordinate, so these three rotations are the only ones (again, among nontrivial angles between 0° and 45°) that yield equally-spaced x_1-projections from the 3^2 design. It is easily verified that these also yield equally-spaced x_2-projections.

Figure 2 displays the standard 3^2 factorial design, shown in open circles, and the designs that result from these rotations, shown in solid circles. Boxes are drawn around the rotated designs to identify the design regions. In practice, one would then scale this design (by subtraction and division) to the experimental region of interest. Along each axis, we have provided dot plots of the projections from which it is plain to see the equally-spaced property.

Among the rotated standard p^2 factorial designs with equally-spaced projections, only those obtained from rotation angles of $\tan^{-1}(1/p)$ contain no redundant projections. Therefore, we define a *p^2-point rotated full factorial design* to be a rotated standard p^2 factorial design with unique, equally-spaced projections to each dimension (which is a Latin hypercube). Among the rotated standard p^2 factorial designs with equally-spaced projections, only those obtained from rotation angles of $\tan^{-1}(1/p)$ contain no redundant projections. Following the argument above, a general result for factorial designs can be stated (see Beattie, 1999 for the proofs).

THEOREM 6. *For nontrivial rotations between 0° and 45°, a rotated standard p^2 factorial design will produce equally-spaced projections to each dimension if and only if the rotation angle is* $\tan^{-1}(1/k)$, *where* $k \in \{1, \ldots, p\}$.

THEOREM 7. *Any two-dimensional rotated factorial design has uncorrelated regression effects estimates.*

4.4. A sample construction example

To illustrate the basic idea of rotated design, we provide an example of rotating a 4^2 full factorial design. We have developed software to construct the rotated factorial designs presented in this paper. Users of S-Plus or C who are interested in obtaining this, please send email to sbeattie@stat.psu.edu.

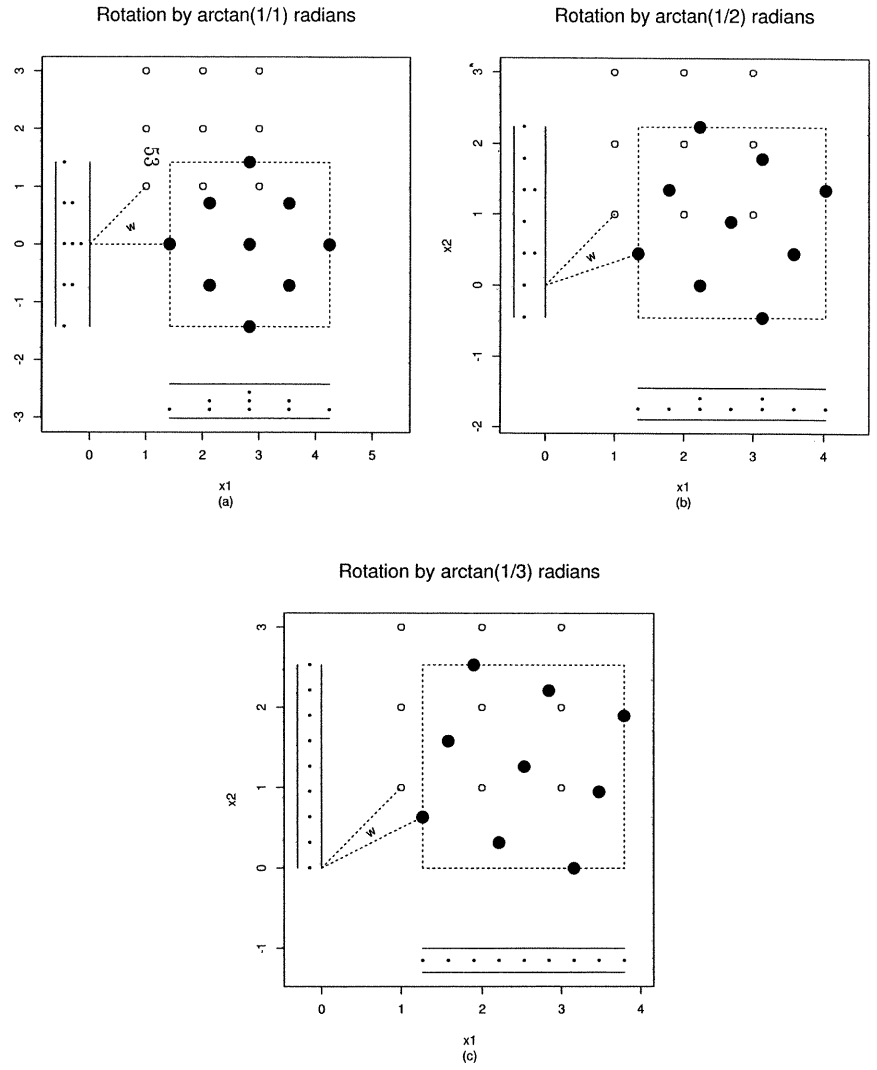

Fig. 2. Three rotations of A standard 3^2 factorial design: (a) $w = \tan^{-1}(1)$; (b) $w = \tan^{-1}(1/2)$; (c) $w = \tan^{-1}(1/3)$.

(1) *A $4^2 = 16$-run rotated factorial design.*
Start with a 4^2 standard factorial design.

$$\begin{bmatrix} 1 & 1 & 1 & 1 & 2 & 2 & 2 & 2 & 3 & 3 & 3 & 3 & 4 & 4 & 4 & 4 \\ 1 & 2 & 3 & 4 & 1 & 2 & 3 & 4 & 1 & 2 & 3 & 4 & 1 & 2 & 3 & 4 \end{bmatrix}'.$$

Rotate by $\tan^{-1}(1/4)$. This yields a 16-point rotated factorial design.

$$\begin{bmatrix}
1\cos(\tan^{-1}(1/4))+1\sin(\tan^{-1}(1/4)) & -1\sin(\tan^{-1}(1/4))+1\cos(\tan^{-1}(1/4)) \\
1\cos(\tan^{-1}(1/4))+2\sin(\tan^{-1}(1/4)) & -1\sin(\tan^{-1}(1/4))+2\cos(\tan^{-1}(1/4)) \\
1\cos(\tan^{-1}(1/4))+3\sin(\tan^{-1}(1/4)) & -1\sin(\tan^{-1}(1/4))+3\cos(\tan^{-1}(1/4)) \\
1\cos(\tan^{-1}(1/4))+4\sin(\tan^{-1}(1/4)) & -1\sin(\tan^{-1}(1/4))+4\cos(\tan^{-1}(1/4)) \\
2\cos(\tan^{-1}(1/4))+1\sin(\tan^{-1}(1/4)) & -2\sin(\tan^{-1}(1/4))+1\cos(\tan^{-1}(1/4)) \\
2\cos(\tan^{-1}(1/4))+2\sin(\tan^{-1}(1/4)) & -2\sin(\tan^{-1}(1/4))+2\cos(\tan^{-1}(1/4)) \\
2\cos(\tan^{-1}(1/4))+3\sin(\tan^{-1}(1/4)) & -2\sin(\tan^{-1}(1/4))+3\cos(\tan^{-1}(1/4)) \\
2\cos(\tan^{-1}(1/4))+4\sin(\tan^{-1}(1/4)) & -2\sin(\tan^{-1}(1/4))+4\cos(\tan^{-1}(1/4)) \\
3\cos(\tan^{-1}(1/4))+1\sin(\tan^{-1}(1/4)) & -3\sin(\tan^{-1}(1/4))+1\cos(\tan^{-1}(1/4)) \\
3\cos(\tan^{-1}(1/4))+2\sin(\tan^{-1}(1/4)) & -3\sin(\tan^{-1}(1/4))+2\cos(\tan^{-1}(1/4)) \\
3\cos(\tan^{-1}(1/4))+3\sin(\tan^{-1}(1/4)) & -3\sin(\tan^{-1}(1/4))+3\cos(\tan^{-1}(1/4)) \\
3\cos(\tan^{-1}(1/4))+4\sin(\tan^{-1}(1/4)) & -3\sin(\tan^{-1}(1/4))+4\cos(\tan^{-1}(1/4)) \\
4\cos(\tan^{-1}(1/4))+1\sin(\tan^{-1}(1/4)) & -4\sin(\tan^{-1}(1/4))+1\cos(\tan^{-1}(1/4)) \\
4\cos(\tan^{-1}(1/4))+2\sin(\tan^{-1}(1/4)) & -4\sin(\tan^{-1}(1/4))+2\cos(\tan^{-1}(1/4)) \\
4\cos(\tan^{-1}(1/4))+3\sin(\tan^{-1}(1/4)) & -4\sin(\tan^{-1}(1/4))+3\cos(\tan^{-1}(1/4)) \\
4\cos(\tan^{-1}(1/4))+4\sin(\tan^{-1}(1/4)) & -4\sin(\tan^{-1}(1/4))+4\cos(\tan^{-1}(1/4))
\end{bmatrix} = \begin{bmatrix}
1.21 & 0.73 \\ 1.46 & 1.70 \\ 1.70 & 2.67 \\ 1.94 & 3.64 \\ 2.18 & 0.49 \\ 2.43 & 1.46 \\ 2.67 & 2.43 \\ 2.91 & 3.40 \\ 3.15 & 0.24 \\ 3.40 & 1.21 \\ 3.64 & 2.18 \\ 3.88 & 3.15 \\ 4.12 & 0.00 \\ 4.37 & 0.97 \\ 4.61 & 1.94 \\ 4.85 & 2.91
\end{bmatrix}.$$

This can be rescaled to be a 16-point Latin hypercube by multiplying by 15/3.64 then subtracting 3.99 from the first column and adding 1.00 to the second column.

$$\begin{bmatrix}
1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 & 11 & 12 & 13 & 14 & 15 & 16 \\
4 & 8 & 12 & 16 & 3 & 7 & 11 & 15 & 2 & 6 & 10 & 14 & 1 & 5 & 9 & 13
\end{bmatrix}'.$$

(2) *A 12-run Type U design.*
Rotated full factorial designs have, by design, unique, equally-spaced projections to each dimension. When points are removed, the resulting design will no longer have the equally-spaced projection property, although it will have unique projections. We will refer to designs created by applying a deletion process to a rotated full factorial design as *Type U rotated factorial designs*, where U emphasizes these *unique* projections. To construct a 12-point Type U design, remove the 4 most extreme design points (from the prescaled matrix): the 1st, 4th, 13th, and 16th.

(3) *A 12-run Type E design.*
After the deletion process, these new designs can be given equally-spaced projections by adjusting the angle of rotation, although this may have the simultaneous effect of creating some redundant projections. We will refer to designs created by modifying the rotation angle of a Type U design to yield the greatest number of unique, equally-spaced projections as *Type E rotated factorial designs*, where E emphasizes the *equally-spaced* projections. To get a 12-point Type E rotated factorial design, adjust the rotation angle to $\tan^{-1}(2/3)$. Figuring out the correct rotation angle is easy. If the original design has p^2 points, then the angle is unadjusted if 0 points are removed and is adjusted to $\tan^{-1}(1/(p-1))$ if $\{2, 4, \ldots, 2p-2\}$ points are removed or to $\tan^{-1}(1/(p-2))$ if $\{2p, 2p+2, \ldots, 4p-8\}$ points are removed. However, there is one exception to this rule: if the new design has an even number of points which exceed a square by 3, then

the angle is adjusted to $\tan^{-1}(2/(p-1))$. (Note that 12 is such a number, making the rotation angle $\tan^{-1}(2/3)$.)

$$\begin{bmatrix}
1\cos(\tan^{-1}(2/3))+2\sin(\tan^{-1}(2/3)) & -1\sin(\tan^{-1}(2/3))+2\cos(\tan^{-1}(2/3)) \\
1\cos(\tan^{-1}(2/3))+3\sin(\tan^{-1}(2/3)) & -1\sin(\tan^{-1}(2/3))+3\cos(\tan^{-1}(2/3)) \\
2\cos(\tan^{-1}(2/3))+1\sin(\tan^{-1}(2/3)) & -2\sin(\tan^{-1}(2/3))+1\cos(\tan^{-1}(2/3)) \\
2\cos(\tan^{-1}(2/3))+2\sin(\tan^{-1}(2/3)) & -2\sin(\tan^{-1}(2/3))+2\cos(\tan^{-1}(2/3)) \\
2\cos(\tan^{-1}(2/3))+3\sin(\tan^{-1}(2/3)) & -2\sin(\tan^{-1}(2/3))+3\cos(\tan^{-1}(2/3)) \\
2\cos(\tan^{-1}(2/3))+4\sin(\tan^{-1}(2/3)) & -2\sin(\tan^{-1}(2/3))+4\cos(\tan^{-1}(2/3)) \\
3\cos(\tan^{-1}(2/3))+1\sin(\tan^{-1}(2/3)) & -3\sin(\tan^{-1}(2/3))+1\cos(\tan^{-1}(2/3)) \\
3\cos(\tan^{-1}(2/3))+2\sin(\tan^{-1}(2/3)) & -3\sin(\tan^{-1}(2/3))+2\cos(\tan^{-1}(2/3)) \\
3\cos(\tan^{-1}(2/3))+3\sin(\tan^{-1}(2/3)) & -3\sin(\tan^{-1}(2/3))+3\cos(\tan^{-1}(2/3)) \\
3\cos(\tan^{-1}(2/3))+4\sin(\tan^{-1}(2/3)) & -3\sin(\tan^{-1}(2/3))+4\cos(\tan^{-1}(2/3)) \\
4\cos(\tan^{-1}(2/3))+2\sin(\tan^{-1}(2/3)) & -4\sin(\tan^{-1}(2/3))+2\cos(\tan^{-1}(2/3)) \\
4\cos(\tan^{-1}(2/3))+3\sin(\tan^{-1}(2/3)) & -4\sin(\tan^{-1}(2/3))+3\cos(\tan^{-1}(2/3))
\end{bmatrix} = \begin{bmatrix}
1.94 & 1.11 \\ 2.50 & 1.94 \\ 2.22 & -0.28 \\ 2.77 & 0.55 \\ 3.33 & 1.39 \\ 3.88 & 2.22 \\ 3.05 & -0.83 \\ 3.61 & 0.00 \\ 4.16 & 0.83 \\ 4.71 & 1.66 \\ 4.44 & -0.55 \\ 4.99 & 0.28
\end{bmatrix}.$$

Once constructed, these designs can be rescaled to the experimental region. For example, to convert the 12-point Type E design matrix to LH notation, multiply by 11/3.05 then subtract 6.00 from the first column and add 3.99 to the second column

$$\begin{bmatrix}
1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 & 11 & 12 \\
8 & 11 & 3 & 6 & 9 & 12 & 1 & 4 & 7 & 10 & 2 & 5
\end{bmatrix}'.$$

4.5. *High-dimensional rotation theory*

Consider a standard full factorial design consisting of d factors, each with p levels. The goal is to rotate this design to convert it into a LH design, so that the p^d points create unique and equally-spaced projections to each individual factor. For certain values of d (notably when d is a power of 2) such a rotation exists, but not for general d. The following proof proceeds in three parts: identification of the required form of the rotation matrix, construction of the power-of-2 rotation matrix, and failure of the transformation matrix to be a rotation matrix when d is not a power of two.

A p-level, d-factor standard full factorial design can be represented by a $p^d \times d$ matrix, D, with entries from $\{1, 2, \ldots, p\}$ and all p^d combinations represented.

$$D = \begin{bmatrix}
1 & 1 & & \cdots & & 1 & \cdots & p & p & & \cdots & & p \\
\vdots & & & & & & & \vdots & & & & & \vdots \\
1 & 1 & \cdots & 1 & \cdots & p & p & \cdots & p & \cdots & 1 & 1 & \cdots & 1 & \cdots & p & p & \cdots & p \\
1 & 2 & \cdots & p & \cdots & 1 & 2 & \cdots & p & \cdots & 1 & 2 & \cdots & p & \cdots & 1 & 2 & \cdots & p
\end{bmatrix}^{\mathrm{T}}. \tag{11}$$

A rotation of this matrix is accomplished by post-multiplication by a $d \times d$ matrix R with the property that $R^{\mathrm{T}}R = I_d$ where I_d is the $d \times d$ identity matrix. Let the multiplication matrix R have entries denoted as $r_{[i,j]}$, which is the entry from the ith row and jth column. Lemma 1 below will not be concerned with whether the multiplication matrix is indeed a rotation matrix, but with how such a matrix would yield unique and equally-spaced projections to each dimension.

LEMMA 1. *The entries of each column of the transformation matrix R must be unique from the set $\{p^t \mid t = 0, 1, \ldots, d-1\}$ in order to yield unique and equally-spaced projections.*

This lemma shows that every column of the transformation matrix must be a permutation of the set $\{1, p, \ldots, p^{d-1}\}$ (allowing sign changes to elements and multiplication of entire columns by a constant). However, every rotation matrix R satisfies $R^{\mathrm{T}}R = kI_d$, so that the sum of squares for all columns of R must be equal. Then, without lose of generality, every column of the transformation matrix must be a permutation of the set $\{1, p, \ldots, p^{d-1}\}$ (allowing only sign changes to elements).

It is obvious that the columns of the transformation matrix cannot be identical, for otherwise the columns of the transformed matrix would be identical. The following lemma shows that the ith entries for the d columns must be unique in magnitude in order for the transformation to be a rotation.

LEMMA 2. *For a rotation matrix R, the ith entries of the d columns are unique in magnitude for all i.*

Lemmas 1 and 2 proved that all the rows and columns of the transformation matrix must be permutations of the set $\{1, p, \ldots, p^{d-1}\}$ (up to sign changes). However, this is not sufficient to guarantee that R will be a rotation matrix. Another requirement implied by the rotation condition $R^{\mathrm{T}}R = kI_d$ is that the columns of R must be orthogonal. Any matrix satisfying the requirements of the lemmas and this last condition will rotate factorial designs into Latin hypercubes. The remainder of this section shows how to create these matrices for d that are powers of two and illustrates why other choices of d, in general, have no such rotation matrix.

Let d be a power of 2. Let $c = \log_2 d$. Let

$$V_1 = [v_1 \quad v_2] = \begin{bmatrix} +1 & -p \\ +p & +1 \end{bmatrix}. \tag{12}$$

Now, for $c > 1$, let V_c be defined inductively from V_{c-1} as follows:

$$V_c = \begin{bmatrix} V_{c-1} & -(p^{2^{c-1}} V_{c-1})^* \\ p^{2^{c-1}} V_{c-1} & (V_{c-1})^* \end{bmatrix}, \tag{13}$$

where the operator $(\cdot)^*$ works on any matrix with an even number of rows by multiplying the entries in the top half of the matrix by -1 and leaving those in the bottom half unchanged.

THEOREM 8. *The matrix V_c is a rotation of the d-factor ($d = 2^c$), p-level standard full factorial design which yields unique and equally-spaced projections to each dimension.*

Reviewing the two-dimensional result from Section 4.3, when $d = 2 = 2^1$, the rotate matrix with $w = \tan^{-1}(1/p)$ can be re-expressed as

$$\begin{aligned} V_1 &= \begin{bmatrix} \cos(\tan^{-1}(1/p)) & -\sin(\tan^{-1}(1/p)) \\ \sin(\tan^{-1}(1/p)) & \cos(\tan^{-1}(1/p)) \end{bmatrix} \\ &= \frac{1}{\sqrt{1+p^2}} \begin{bmatrix} +1 & -p \\ +p & +1 \end{bmatrix}, \end{aligned} \tag{14}$$

which is the correctly scaled rotation matrix V_1 given in Eq. (12).

Other scaled rotation matrices for cases of interest ($d = 4, 8$ corresponding to $c = 2, 3$) are

$$V_2 = \sqrt{\frac{p^2-1}{p^8-1}} \begin{bmatrix} +1 & -p & +p^2 & -p^3 \\ +p & +1 & -p^3 & -p^2 \\ +p^2 & -p^3 & -1 & +p \\ +p^3 & +p^2 & +p & +1 \end{bmatrix} \tag{15}$$

and

$$V_3 = \sqrt{\frac{p^2-1}{p^{16}-1}} \begin{bmatrix} +1 & -p & +p^2 & -p^3 & +p^4 & -p^5 & +p^6 & -p^7 \\ +p & +1 & -p^3 & -p^2 & +p^5 & +p^4 & -p^7 & -p^6 \\ +p^2 & -p^3 & -1 & +p & -p^6 & +p^7 & +p^4 & -p^5 \\ +p^3 & +p^2 & +p & +1 & -p^7 & -p^6 & -p^5 & -p^4 \\ +p^4 & -p^5 & +p^6 & -p^7 & -1 & +p & -p^2 & +p^3 \\ +p^5 & +p^4 & -p^7 & -p^6 & -p & -1 & +p^3 & +p^2 \\ +p^6 & -p^7 & -p^4 & +p^5 & +p^2 & -p^3 & -1 & +p \\ +p^7 & +p^6 & +p^5 & +p^4 & +p^3 & +p^2 & +p & +1 \end{bmatrix}, \tag{16}$$

respectively.

The choice of rotation matrices for higher dimensions ($d > 2$) is not unique. Other inductive definitions for V_c in Eq. (13) are possible, namely

$$\begin{bmatrix} V_{c-1} & -p^{2^{c-1}} V_{c-1} \\ p^{2^{c-1}} V_{c-1} & V_{c-1} \end{bmatrix}. \tag{17}$$

However, the point is still clear, such rotations do exist.

Owen (1994) showed why orthogonality of design matrix columns is important in the estimation of Monte-Carlo integrals and attempted to control the column correlations within Latin hypercubes. Theorem 9 will prove that all designs obtained by rotation of standard factorial designs, specifically rotated full factorial designs, will also be orthogonal. Let k be the sum of squares of the first column of X. As X is an orthogonal matrix, $X^{\mathrm{T}}X = kI_d$. So $(XR)^{\mathrm{T}}(XR) = R^{\mathrm{T}}X^{\mathrm{T}}XR = R^{\mathrm{T}}kI_dR = kR^{\mathrm{T}}R = kI_d$, a diagonal matrix. Therefore, the rotated design matrix XR is an orthogonal design.

THEOREM 9. *Let X be an orthogonal design matrix of n rows and d columns in which the sums of squares for columns are equal. Let R be a $d \times d$ rotation matrix. The design resulting from the matrix product XR is also an orthogonal design.*

Since computation of Monte-Carlo integrals is, in effect, a computer experiment, it is beneficial for designs for computer experiments to have uncorrelated regression estimates of main effects. The following theorem shows this to be true for all designs obtained by rotation of standard full factorial designs, specifically rotated factorial designs.

THEOREM 10. *Any p^d-point rotated factorial design has uncorrelated regression estimates of main effects.*

Recall that Johnson et al. (1990) introduced the use of minimum interpoint distance (MID) as an important design criterion (see Eq. (10)). It can be shown that the MID using Euclidean distance for a p^d-point rotated factorial design scaled to the unit hypercube, $[0, 1]^d$, is $\sqrt{1 + p^2 + \cdots + p^{d+1}}/(p-1) = \sqrt{(p^{2d}-1)/((p^2-1)(p-1)^2)}$. Additionally, it can be shown this is the maximal MID for $d = 2$. A formal proof for higher dimensions has not been obtained as yet.

Table 11 lists the MIDs for several of the four-dimensional RFDs requiring fewer than 100 points and for the respective Latin hypercube designs of Morris and Mitchell (1992, denoted by MmLH) and maxmin U designs of Tang (1994, denoted by MmU). MmLH designs (Latin hypercube designs of Morris and Mitchell, 1992) and MmU designs (maxmin U designs of Tang, 1994). Due to the computational requirements of obtaining designs from other methods, some were results not available (N/A). It is clear that the easily-constructed RFDs have similar (if not equal) MIDs to other computing extensive constructed designs.

Table 11
MID comparisons of four-dimensional MmLH, RFD, and MmU designs

No. of Pts	Maximin Latin H-cube	Rotated factorial design		Maximin U design
		Type U	Type E	
8	0.9258 †	0.8692	0.7071 (3)	0.7954 ◁
9	0.8101 †	0.5762	1.0000 (3)	0.6960 ◁
10	0.7857 †	*	*	*
11	0.7416 †	*	*	*
12	0.7216 †	*	*	*
16	0.6218 ◇	0.6146	0.6146 (16)	0.5292 ◁
24	0.5325 ◇	0.3963	0.3963 (24)	N/A
28	N/A	0.3951	0.4167 (7)	*
36	N/A	0.3725	0.3725 (36)	N/A
40	N/A	0.5192	0.5192 (40)	N/A
41	0.4507 ◇	0.5062	0.5062 (41)	*
54	N/A	0.3641	0.3641 (54)	N/A
67	N/A	0.3825	0.3825 (67)	*
68	N/A	0.3751	0.3751 (68)	*
81	N/A	0.3579	0.3579 (81)	N/A

*No design can be constructed as defined.
†Published in Morris and Mitchell (1992).
◇Obtained via Morris and Mitchell (1992), but algorithm by the author.
◁Obtained by author's algorithm.

5. Dispersion effects in screening designs

When studying both location and dispersion effects in unreplicated fractional factorial designs, a "standard" procedure is to identify location effects using ordinary least squares analysis, fit a model, then identify dispersion effects by analyzing the residuals. Traditionally, the primary use of these designs has been in detecting and modeling location effects (changes in the mean response). An assumption of constant variance is usually made. In this section, we show that if the model in the above procedure does not include all active location effects, then null dispersion effects may be mistakenly be identified as active. We also derive an exact relationship between location and dispersion effects.

5.1. An illustrative example

Montgomery (1990) analyzed data from an injection molding experiment where the response to be optimized was shrinkage. The factors studied were mold temperature (A), screw speed (B), holding time (C), gate size (D), cycle time (E), moisture content (F), and holding pressure (G). The design is a 2^{7-3}_{IV} fractional factorial. The generators of this design are E = ABC, F = BCD, and G = ACD. The data are shown in Table 12.

Table 12
Design matrix and response for injection molding experiment

		A	B	C	D							E		G	F		
$i \downarrow j \rightarrow$	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	y_M
1	1	−	−	−	−	+	+	+	+	+	+	−	−	−	−	+	6
2	1	+	−	−	−	−	−	−	+	+	+	+	+	+	−	−	10
3	1	−	+	−	−	−	+	+	−	−	+	+	+	−	+	−	32
4	1	+	+	−	−	+	−	−	−	−	+	−	−	+	+	+	60
5	1	−	−	+	−	+	−	+	−	+	−	+	−	+	+	−	4
6	1	+	−	+	−	−	+	−	−	+	−	−	+	−	+	+	15
7	1	−	+	+	−	−	−	+	+	−	−	−	+	+	−	+	26
8	1	+	+	+	−	+	+	−	+	−	−	+	−	−	−	−	60
9	1	−	−	−	+	+	+	−	+	−	−	−	+	+	+	−	8
10	1	+	−	−	+	−	−	+	+	−	−	+	−	−	+	+	12
11	1	−	+	−	+	−	+	−	−	+	−	+	−	+	−	+	34
12	1	+	+	−	+	+	−	+	−	+	−	−	+	−	−	−	60
13	1	−	−	+	+	+	−	−	−	−	+	+	+	−	−	+	16
14	1	+	−	+	+	−	+	+	−	−	+	−	−	+	−	−	5
15	1	−	+	+	+	−	−	−	+	+	+	−	−	−	+	−	37
16	1	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	52

The least squares regression coefficients were obtained from fitting a saturated model. Figure 3 is a half-normal probability plot of the estimated regression coefficients ($\hat{\beta}_j$s). Montgomery used a normal probability plot of the estimated effects and determined that columns 1, 2, and 5 (A, B, and AB) produce active location effects. He fit this location model, which we denote M1.

(M1) $\hat{y} = 27.3125 + 6.9375\text{A} + 17.8125\text{B} + 5.9375\text{AB}.$

The estimated residuals under M1 are $(-2.50, -0.50, -0.25, 2.00, -4.50, 4.50, -6.25, 2.00, -0.50, 1.50, 1.75, 2.00, 7.50, -5.50, 4.75, -6.00)$. As a measure of the dispersion effect magnitude for column j, Montgomery calculates the statistic $F_j^* = \ln s_{j+}^2/s_{j-}^2$ which is the natural logarithm of the ratio of the sample variances of the residuals at the $+1$ and -1 levels of column j. Note that Box and Meyer (1986b) point out this statistic is *approximately* normally distributed with mean 0 and variance 1. Montgomery compared these statistics to an appropriate normal quantile to determine significance. He also used a normal plot of these statistics. Using either the normal quantile or the probability plot, it is evident that column 3 (C) has a dispersion effect with

$$F_{3|\text{M1}}^* = \ln \frac{s_{3+|\text{M1}}^2}{s_{3-|\text{M1}}^2} = \ln \frac{32.44}{2.66} = 2.50.$$

Thus, Montgomery (1990) concludes that factors A (mold temperature) and B (screw speed) impact the mean shrinkage of the mold and that factor C (holding time) impacts the variation in shrinkage. By studying the interaction between mold temperature and screw speed, it is apparent that the low screw speed is better for reducing mean shrinkage and that the setting of mold temperature is not crucial at this speed. To reduce the variation in shrinkage, holding time should be set at its low level.

This logical procedure has been used by many and has become a standard practice. However, the identification of dispersion effects is quite sensitive to the location model that is fit. To illustrate, note that another reasonable interpretation of Figure 3 is that columns 7 and 13 have active location effects in addition to columns 1, 2, and 5. Due to the confounding associated with this design, column 13 represents not just the factor G effect alone, but also the ACD interaction and other effects. The AD interaction effect appears in column 7 and the interaction of columns 7 and 13 appears in column 3.

We denote this model with five location effects (columns 1, 2, 5, 7, and 13) as M2.

(M2) $\hat{y} = 27.3125 + 6.9375\text{A} + 17.8125\text{B} + 5.9375\text{AB} - 2.6875\text{AD} - 2.4375\text{ACD}.$

The residuals from model M2 are $(-2.250, -0.750, 0.000, 1.750, 0.625, -0.625, -1.125, -3.125, -0.750, 1.750, 1.500, 2.250, 2.375, -0.375, -0.375, -0.875)$. From

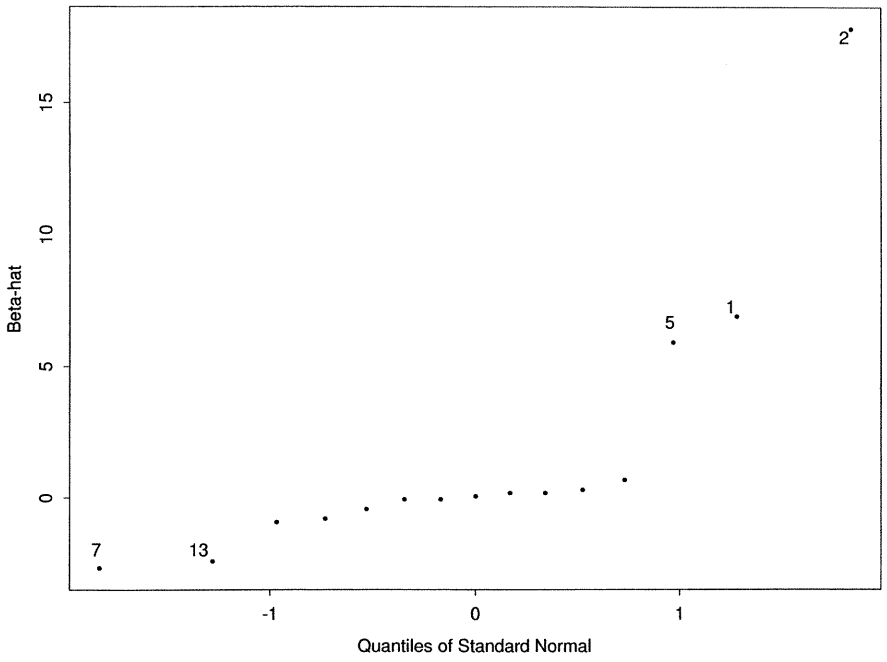

Fig. 3.

this model we have the F_j^* statistic for column 3,

$$F_{3|\text{M2}}^* = \ln \frac{s_{3+|\text{M2}}^2}{s_{3-|\text{M2}}^2} = \ln \frac{2.42}{2.58} = -0.06.$$

Here, it is apparent there is no dispersion effect associated with column 3 (factor C) as the sample variance of residuals is quite similar at the -1 and $+1$ levels of column 3.

So we have two feasible models for mold shrinkage, M1 and M2. M1 shows two factors important for determining the location (mean) of the response, and also includes another factor that is important for controlling the variation in the response. M2 includes four factors that affect the mean response and no dispersion factors. Which model is more appropriate? Is one model better than the other? Some additional information may be helpful.

The experiment actually included four center points (25, 29, 24, 27) in addition to the fractional factorial. From these center points, we have an estimate of the variance of the response, σ^2, of $\hat{\sigma}^2 = 4.92$. M1 produces $\hat{\sigma}_{\text{M1}}^2 = 20.73$ and M2 produces $\hat{\sigma}_{\text{M2}}^2 = 3.81$. The M2 estimate is in much better agreement with the center point estimate.

Therefore, a reasonable conclusion based on model M2 is that there are four important factors: mold temperature, screw speed, holding time and gate size (D). If

this experiment is truly a screening experiment, then fitting M1 would have eliminated a potentially important factor, gate size.

So we have two distinctly different possibilities:

- Failing to include a pair of location effects created a spurious dispersion effect, or
- Failing to account for a dispersion effect created two location effects.

These spurious dispersion effects are not uncommon. We will show that the exclusion of a pair of active location effects will create an apparent (spurious) dispersion effect in the interaction of these two columns. Box and Meyer (1986a, 1986b) and Bergman and Hynèn (1997) both noted a relationship between location and dispersion effects. We will derive the exact relationship. In the next section, we will provide a theoretical explanation showing that failure to include two location effects in a model before calculating residuals can produce a spurious dispersion effect.

5.2. *Spurious dispersion effects*

Assume some method is used to identify m active location effects in an unreplicated fractional factorial design. A model is fit and residuals are estimated, but assume there are two active location effects that are excluded from this model. Let the excluded active location effects be in columns $\boldsymbol{x}_j$ and $\boldsymbol{x}_{j'}$ and let $\boldsymbol{x}_d$ be the column associated with the interaction of $\boldsymbol{x}_j$ and $\boldsymbol{x}_{j'}$. Then $x_{ij}x_{ij'} = x_{id}$. Let $\hat{\beta}_j$ and $\hat{\beta}_{j'}$ be the usual least squares estimators of β_j and $\beta_{j'}$, the regression coefficients associated with $\boldsymbol{x}_j$ and $\boldsymbol{x}_{j'}$ respectively. We will show that failure to include β_j and $\beta_{j'}$ in the regression model will create a difference in the expected value of the sample variances at the $+1$ and -1 levels of $\boldsymbol{x}_d$.

Define the following sets of rows using the convention P for 'plus' and M for 'minus':

$$M = \{i\colon x_{id} = -1\}, \qquad P = \{i\colon x_{id} = +1\}.$$

A dispersion effect occurs when the variance of the response, independent of the location effects (or equivalently, the variance of the residuals from a known location model), is higher at one level of a column than the other. We can compare sample variances of the residuals at the plus and minus levels of a column to determine if it has a dispersion effect. Let

$$s_{d+}^2 = \frac{2}{n-2}\sum_{i\in P}(e_i - \bar{e}_p)^2 \quad \text{and} \quad s_{d-}^2 = \frac{2}{n-2}\sum_{i\in M}(e_i - \bar{e}_m)^2,$$

where

$$\bar{e}_m = \frac{2}{n}\sum_{i\in M} e_i \quad \text{and} \quad \bar{e}_p = \frac{2}{n}\sum_{i\in P} e_i.$$

It is shown in the Appendix that the expected sample variance of the residuals when $x_{id} = -1$ $(i \in M)$ is

$$E[s_{d-}^2] = E\left[\frac{2}{n-2}\sum_{i\in M}(e_i - \bar{e}_m)^2\right] = \frac{n-1-m}{n-1}\sigma^2 + \frac{n}{n-2}(\beta_j - \beta_{j'})^2 \tag{18}$$

and when $x_{id} = +1$ $(i \in P)$,

$$E[s_{d+}^2] = E\left[\frac{2}{n-2}\sum_{i\in P}(e_i - \bar{e}_p)^2\right] = \frac{n-1-m}{n-1}\sigma^2 + \frac{n}{n-2}(\beta_j + \beta_{j'})^2. \tag{19}$$

From (18) and (19) we have

$$E[s_{d+}^2] - E[s_{d-}^2] = \frac{4n}{n-2}\beta_j\beta_{j'}. \tag{20}$$

Consider the following three scenarios involving β_j and $\beta_{j'}$:

- If $\beta_j = \beta_{j'} = 0$, then these two location effects are not active and $E[s_{d-}^2] = E[s_{d+}^2] = \frac{n-1-m}{n-1}\sigma^2$ and $E[s_{d+}^2] - E[s_{d-}^2] = 0$. Thus, any difference is just random error so there will should be no spurious dispersion effect.
- If only one of the coefficients is nonzero, then (20) is still zero as mentioned in Bergman and Hynèn (1997), although both are biased upwards as estimates of σ^2.
- If β_j and $\beta_{j'} \neq 0$, the residuals will have different expected variance at the -1 and $+1$ levels of $\boldsymbol{x}_d$. Thus, excluding two location effects from a model and then studying residuals can create a spurious dispersion effect.

Returning to the injection molding example, if we assume columns 7 and 13 produce active location effects but were left out of the model, then we have

$$\widehat{E[s_{3+|\mathrm{M1}}^2]} - E[s_{3-|\mathrm{M1}}^2] = \frac{4n}{n-2}\hat{\beta}_7\hat{\beta}_{13} = \frac{(4)(16)}{14}(-2.6875)(-2.4375) = 29.95.$$

Recalling that $s_{3-|\mathrm{M1}}^2 = 2.66$ and $s_{3+|\mathrm{M1}}^2 = 32.44$, we have

$$s_{3+|\mathrm{M1}}^2 - s_{3-|\mathrm{M1}}^2 = 29.79.$$

So the observed difference in sample variances is almost the same as that caused by not including β_7 and β_{13} in the model. This indicates the dispersion effect detected by fitting model M1 is spurious.

5.3. Some theoretical results

McGrath and Lin (2001a) showed that (1) failing to include a pair of location effects creates a spurious dispersion effect in its interaction column; and (2) two dispersion effects create a dispersion effect in their interaction column. They also provide a way to simultaneously analyze the location and dispersion effects. Furthermore, the following results were given (see McGrath and Lin, 2001a).

- Let $\hat{\beta}_j$ and $\hat{\beta}_{j'}$ be the OLS estimates for columns $\boldsymbol{x}_j$ and $\boldsymbol{x}_{j'}$ respectively in a 2^{k-p} experiment. If the interaction of $\boldsymbol{x}_j$ and $\boldsymbol{x}_{j'}$ is in column $\boldsymbol{x}_d$, $\mathrm{Var}(\varepsilon_i | x_{id} = -1) = \sigma^2_{d-}$ and $\mathrm{Var}(\varepsilon_i | x_{id} = 1) = \sigma^2_{d+}$, then the correlation of $\hat{\beta}_j$ and $\hat{\beta}_{j'}$ is

$$\rho_{j,j'|d} = \frac{\sigma^2_{d+} - \sigma^2_{d-}}{\sigma^2_{d+} + \sigma^2_{d-}}. \tag{21}$$

- Let m be the number of active location effects in the model fit from a 2^{k-p} experiment. Let g = the number of alias pairs $(\boldsymbol{x}_j, \boldsymbol{x}_{j'})$ not in the model such that $x_{ij}x_{ij'} = x_{id}$ for $i = 1, \ldots, n$. Then s^2_{d+} and s^2_{d-} are independent if and only if $g = (n - 1 - m)/2$ and $\boldsymbol{x}_d$ is in the effect matrix for the fitted model.

6. Discussion

This chapter introduced some recently developed designs suitable for industrial experimentation. Apart from the introduction, it can be roughly split into four parts: Part 1 (Section 2) discussed some useful screening designs for physical experiments. Part 2 (Section 3) discussed the supersaturated design, a class of screening designs in which the number of factors is large and the cost of experiment is high (and thus a small number of runs is required). Specifically, the design is named because its number of runs is smaller than the number of factors. Part 3 (Section 4) provides a class of screening designs for computer experiments, and finally Part 4 (Section 5) discusses the impact of dispersion effects in analyzing the screening designs, using 2^{k-p} design as an example. Most designs discussed here provide somewhat unique features to the experimenters. Many are available through popular computer software packages. Whenever appropriate, the related websites or emails are listed.

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