Handout #13: **Fractional factorial designs and orthogonal arrays**

When the number of factors is large, it may be feasible to observe only a fraction of all the treatment combinations. Under such a fractional factorial design, not all factorial effects can be estimated. In this handout, we introduce an important combinatorial structure called orthogonal arrays, and describe how they can be used to run factorial experiments. We discuss the estimability of factorial effects under an orthogonal array, and show that when some effects are assumed to be negligible, other effects become estimable and their estimates are uncorrelated. Several examples are given to illustrate different types of orthogonal arrays, in particular, the distinction between regular and nonregular designs. We briefly discuss Hadamard matrices, an important class of nonregular designs, and also present a useful design construction technique called foldover. In this and the next few handouts, we assume that the experimental units are unstructured and the experiment is to be conduced with complete randomization. Multi-stratum fractional factorial designs will be discussed in a later handout.

13.1. Model for completely randomized factorial experiments

When the experimental units are unstructured, a factorial design can be specified by the number of observations to be taken on each treatment combination. For a design d, let $n_d(x_1, \cdots, x_n)$ be the number of observations on treatment combination $(x_1, \cdots, x_n)^T$ and let $\boldsymbol{n}_d$ be the $(s_1 \cdots s_n) \times 1$ vector whose entries are the $n_d(x_1, \cdots, x_n)$'s arranged in lexicographic order. Then d is determined by $\boldsymbol{n}_d$. We have $\boldsymbol{n}_d^T \mathbf{1} = N$, where N is the run size. When $n_d(x_1, \cdots, x_n) = 0$ or 1, $\boldsymbol{n}_d$ can also be viewed as the indicator function of the selected treatment combinations.

Let $y_1, \cdots, y_N$ be the N observed responses. Without loss of generality, we may assume that $y_1, \cdots, y_N$ are uncorrelated with constant variance, and if y_i is an observation on the treatment combination $(x_1, \cdots, x_n)^T$, then

$$\mathrm{E}(y_i) = \mu + \alpha(x_1, \cdots, x_n),$$

where $\alpha(x_1, \cdots, x_n)$ is the effect of treatment combination $(x_1, \cdots, x_n)$. We have seen in Handout #9 how to parametrize $\alpha(x_1, \cdots, x_n)$ in terms of various factorial effects. In general, let $\boldsymbol{p}_0 = \mathbf{1}_{s_1 \cdots s_n}$ and let $\boldsymbol{p}_1^T \boldsymbol{\alpha}, \cdots, \boldsymbol{p}_{s_1 \cdots s_n - 1}^T \boldsymbol{\alpha}$ be $s_1 \cdots s_n - 1$ mutually orthogonal treatment contrasts representing the factorial effects, with $\boldsymbol{p}_i^T \boldsymbol{\alpha}$ being a k-factor interaction contrast if the entries of $\boldsymbol{p}_i$ only depend on the levels of k factors. Then $\boldsymbol{\alpha}$ can be expressed as $\boldsymbol{P\beta}$, where $\boldsymbol{P} = [\mathbf{1} \vdots \boldsymbol{p}_1 \vdots \cdots \vdots \boldsymbol{p}_{s_1 \cdots s_n - 1}]$ and $\boldsymbol{\beta} = (\beta_0, \beta_1, \cdots, \beta_{s_1 \cdots s_n - 1})^T$, with $\beta_i = \frac{1}{\|\boldsymbol{p}_i\|^2} \boldsymbol{p}_i^T \boldsymbol{\alpha}$. We shall absorb μ into β_0 and still denote $\mu + \beta_0$ as β_0. Then a full model with all factorial effects present can be expressed as

$$\mathrm{E}(\boldsymbol{y}) = \mu\mathbf{1} + \boldsymbol{X}_T\boldsymbol{\alpha} = \boldsymbol{X}_T\boldsymbol{P}\boldsymbol{\beta}, \tag{13.1.1}$$

where $\boldsymbol{y}$ is the $N \times 1$ vector of observed responses. Often some of the factorial effects are assumed to be negligible; then the associated terms are dropped from (13.1.1). This leads to a linear model

$$\mathrm{E}(\boldsymbol{y}) = \boldsymbol{X}_T\boldsymbol{Q}\widetilde{\boldsymbol{\beta}}, \tag{13.1.2}$$

where $\boldsymbol{Q}$ is obtained from $\boldsymbol{P}$ by deleting the columns of $\boldsymbol{P}$ that correspond to negligible factorial effects, and $\widetilde{\boldsymbol{\beta}}$ is the subvector of $\boldsymbol{\beta}$ consisting of the nonnegligible effects.

The contrasts $\beta_1, \cdots, \beta_{s_1\cdots s_n-1}$ can be constructed by using finite geometry or by the method as described in Theorem 9.6.3. In this Handout, we will use the latter method. Then $\boldsymbol{P}$ is as in (9.6.18). We follow the notation in (9.6.17) to write each β_i as $\beta^{\boldsymbol{z}}$, where $\boldsymbol{z} \in S_1 \times \cdots \times S_n$. Let $\boldsymbol{q}^{\boldsymbol{z}}$ be the column of $\boldsymbol{X}_T\boldsymbol{Q}$ corresponding to a nonnegligible $\beta^{\boldsymbol{z}}$. If the nonzero entries of $\boldsymbol{z}$ are $z_{i_1}, \cdots, z_{i_k}$, then the entry of $\boldsymbol{q}^{\boldsymbol{z}}$ corresponding to an observation on the treatment combination $(x_1, \cdots, x_n)^T$ is equal to $\prod_{j=1}^{k} p^{i_j}_{x_{ij}, z_{ij}}$ as defined in (9.6.12).

We define the *Hadamard product* of two vectors $\boldsymbol{x} = (x_1, \cdots, x_n)^T$ and $\boldsymbol{y} = (y_1, \cdots, y_n)^T$ to be $\boldsymbol{x} \odot \boldsymbol{y} = (x_1y_1, \cdots, x_ny_n)^T$. Let $\boldsymbol{q}^{\boldsymbol{u}}$ and $\boldsymbol{q}^{\boldsymbol{v}}$ be two different columns of $\boldsymbol{X}_T\boldsymbol{Q}$, and $u_{i_1}, \cdots, u_{i_r}$ and $v_{j_1}, \cdots, v_{j_s}$ be the nonzero entries of $\boldsymbol{u}$ and $\boldsymbol{v}$, respectively. Then $\boldsymbol{q}^{\boldsymbol{u}}$ and $\boldsymbol{q}^{\boldsymbol{v}}$ can be expressed as

$$\boldsymbol{q}^{\boldsymbol{u}} = \boldsymbol{q}^{u_{i_1}\boldsymbol{e}_{i1}} \odot \cdots \odot \boldsymbol{q}^{u_{i_r}\boldsymbol{e}_{ir}},$$

$$\boldsymbol{q}^{\boldsymbol{v}} = \boldsymbol{q}^{v_{j_1}\boldsymbol{e}_{j1}} \odot \cdots \odot \boldsymbol{q}^{v_{j_s}\boldsymbol{e}_{j_s}},$$

where the ith entry of $\boldsymbol{e}_i$ is equal to 1, and all its other entries are zero; i.e., each column corresponding to an interaction contrast is the Hadamard product of the relevant main-effect columns. If each treatment combination is observed exactly once (that is, we have one replicate of the *complete* factorial), none of the factorial effects is negligible, and the entries of $\boldsymbol{y}$ and $\boldsymbol{\beta}$ are arranged in lexicographic order, then $\boldsymbol{X}_T$ is the identity matrix and $\boldsymbol{Q} = \boldsymbol{P} = \boldsymbol{P}_{s_1} \otimes \boldsymbol{P}_{s_2} \otimes \cdots \otimes \boldsymbol{P}_{s_n}$. In this case, the information matrix $(\boldsymbol{X}_T\boldsymbol{Q})^T\boldsymbol{X}_T\boldsymbol{Q} = \boldsymbol{Q}^T\boldsymbol{X}_T^T\boldsymbol{X}_T\boldsymbol{Q} = \boldsymbol{Q}^T\boldsymbol{Q} = \boldsymbol{P}^T\boldsymbol{P}$ is a diagonal matrix. As a consequence, the least squares estimates of the factorial effects are uncorrelated and can be calculated easily: $\widehat{\beta^{\boldsymbol{z}}} = \frac{1}{\|\boldsymbol{p}^{\boldsymbol{z}}\|^2}(\boldsymbol{p}^{\boldsymbol{z}})^T\boldsymbol{y}$.

A complete factorial experiment requires $s_1 \cdots s_n$ runs. Cost and other practical considerations often call for observing only a fraction of the treatment combinations.

Indeed if only a subset of the factorial effects are expected to be important, then observing a fraction of the treatment combinations would be sufficient Under such a *fractional factorial design*, not all the factorial effects are estimable. There are two interesting issues. Given a model where some of the factorial effects are assumed negligible, under what designs can the nonnegligible effects be estimated? Given a fractional factorial design, what models can it entertain? In the former question, one may also ask, under what designs are the estimators of the nonnegligible effects uncorrelated? In the next section, we introduce orthogonal arrays and provide some answers to this question.

13.2 Orthogonal arrays

Orthogonal arrays were first introduced by Rao (1946, 1947) for the case where all the factors have the same number of levels. Such arrays will be referred to as *symmetric* orthogonal arrays. Rao (1973) extended the definition to also cover a*symmetrical* (*mixed-level*) orthogonal arrays. A useful reference is the book "Orthogonal Arrays: Theory and Applications" by Hedayat, Sloane and Stufken, Springer, 1999.

Definition 13.2.1. An orthogonal array OA$(N, s_1 \times \cdots \times s_n, t)$ is an $N \times n$ matrix with s_i distinct symbols in the ith column, $1 \leq i \leq n,$ such that in each $N \times t$ submatrix, all combinations of the symbols appear equally often as row vectors. The positive integer t is called the *strength* of the orthogonal array. If $s_1 = \cdots = s_n = s$, then it is called a *symmetric* orthogonal array and is denoted as OA(N, s^n, t).

From the definition it follows immediately that if an OA(N, s^n, t) exists, then N must be a multiple of s^t.

An OA$(N, s_1 \times \cdots \times s_n, t)$ can be used to define a factorial design of size N for n factors with $s_1, \cdots, s_n$ levels: each column corresponds to one factor and each row represents a treatment combination. The following result explains the role of the strength and the utility of orthogonal arrays.

Theorem 13.2.2. An orthogonal array of strength $t = 2k$ ($k \geq 1$) can be used to estimate all the main-effect contrasts and all interaction contrasts involving up to k factors, assuming that all the interactions involving more than k factors are negligible. An orthogonal array of strength $t = 2k - 1$ ($k \geq 2$) can be used to estimate all the main-effect contrasts and all interaction contrasts involving up to $k - 1$ factors, assuming that all the interactions involving more than k factors are negligible. In both cases, all the estimators are uncorrelated.

Proof. Suppose all the interactions involving more than k factors are negligible. Let $\boldsymbol{X}_T\boldsymbol{Q}$ be the model matrix as in (13.1.2). Then each column of $\boldsymbol{X}_T\boldsymbol{Q}$ is a $\boldsymbol{q}^{\boldsymbol{z}}$, where $\boldsymbol{z}$ contains at most k nonzero entries.

Case 1. $t = 2k$: We claim that the information matrix $(\boldsymbol{X}_T\boldsymbol{Q})^T(\boldsymbol{X}_T\boldsymbol{Q})$ is a diagonal matrix; then $(\boldsymbol{X}_T\boldsymbol{Q})^T(\boldsymbol{X}_T\boldsymbol{Q})$ is invertible and all the unknown parameters in the model are estimable with uncorrelated estimators.

Let $\boldsymbol{q}^{\boldsymbol{u}}$ and $\boldsymbol{q}^{\boldsymbol{v}}$ be two different columns of $\boldsymbol{X}_T\boldsymbol{Q}$, and $u_{i_1}, \cdots, u_{i_r}$ and $v_{j_1}, \cdots, v_{j_s}$ be the nonzero entries of $\boldsymbol{u}$ and $\boldsymbol{v}$, respectively. Then $(\boldsymbol{q}^{\boldsymbol{u}})^T\boldsymbol{q}^{\boldsymbol{v}}$ is equal to the sum of the entries of $\boldsymbol{q}^{\boldsymbol{u}} \odot \boldsymbol{q}^{\boldsymbol{v}} = (\boldsymbol{q}^{u_{i_1}\boldsymbol{e}_{i1}} \odot \cdots \odot \boldsymbol{q}^{u_{i_r}\boldsymbol{e}_{ir}}) \odot (\boldsymbol{q}^{v_{j_1}\boldsymbol{e}_{j1}} \odot \cdots \odot \boldsymbol{q}^{v_{j_s}\boldsymbol{e}_{j_s}})$. Since $r,\, s \le k$, $r+s$ is no more than the strength of the orthogonal array. Therefore each row of the $N \times (r+s)$ matrix $[\boldsymbol{q}^{u_{i_1}\boldsymbol{e}_{i1}} \vdots \cdots \vdots\, \boldsymbol{q}^{u_{i_r}\boldsymbol{e}_{ir}} \vdots\, \boldsymbol{q}^{v_{j_1}\boldsymbol{e}_{j1}} \vdots \cdots \vdots\, \boldsymbol{q}^{v_{j_s}\boldsymbol{e}_{j_s}}]$ is replicated $s_1s_2\cdots s_n/N$ times in the $(s_1s_2\cdots s_n) \times (r+s)$ matrix $[\boldsymbol{p}^{u_{i_1}\boldsymbol{e}_{i1}} \vdots \cdots \vdots\, \boldsymbol{p}^{u_{i_r}\boldsymbol{e}_{ir}} \vdots\, \boldsymbol{p}^{v_{j_1}\boldsymbol{e}_{j1}} \vdots \cdots \vdots\, \boldsymbol{p}^{v_{j_s}\boldsymbol{e}_{j_s}}]$. It follows that $(\boldsymbol{q}^{\boldsymbol{u}})^T\boldsymbol{q}^{\boldsymbol{v}} = \frac{N}{s_1s_2\cdots s_n}(\boldsymbol{p}^{\boldsymbol{u}})^T\boldsymbol{p}^{\boldsymbol{v}} = 0$.

Case 2. $t = 2k-1$: Partition $\boldsymbol{X}_T\boldsymbol{Q}$ as $[\boldsymbol{U}_1 \vdots \boldsymbol{U}_2]$, where $\boldsymbol{U}_1$ consists of all the $\boldsymbol{q}^{\boldsymbol{z}}$'s where $\boldsymbol{z}$ contains at most $k-1$ nonzero entries, and $\boldsymbol{U}_2$ consists of all the $\boldsymbol{q}^{\boldsymbol{u}}$'s where $\boldsymbol{u}$ contains k nonzero entries. Then the information matrix for the effects involving up to $k-1$ factors is equal to $\boldsymbol{U}_1^T\boldsymbol{U}_1 - \boldsymbol{U}_1^T\boldsymbol{U}_2(\boldsymbol{U}_2^T\boldsymbol{U}_2)^-\boldsymbol{U}_2^T\boldsymbol{U}_1$. Similar to the proof of case 1, $\boldsymbol{U}_1^T\boldsymbol{U}_1$ is a diagonal matrix, and $\boldsymbol{U}_1^T\boldsymbol{U}_2 = \boldsymbol{0}$. Thus $\boldsymbol{U}_1^T\boldsymbol{U}_1 - \boldsymbol{U}_1^T\boldsymbol{U}_2(\boldsymbol{U}_2^T\boldsymbol{U}_2)^-\boldsymbol{U}_2^T\boldsymbol{U}_1 = \boldsymbol{U}_1^T\boldsymbol{U}_1$ is a diagonal matrix. $\square$

In either case, the least squares estimators of the factorial effects of interest are uncorrelated and can be calculated easily: $\widehat{\beta^{\boldsymbol{z}}} = \frac{1}{\|\boldsymbol{q}^{\boldsymbol{z}}\|^2}(\boldsymbol{q}^{\boldsymbol{z}})^T\boldsymbol{y}$.

For orthogonal arrays of odd strengths, one can prove a result somewhat stronger than that in Theorem 13.2.2. Under an OA of strength $2k-1$, we may not be able to estimate all interaction contrasts involving k factors. However, consider the model which contains all the main-effect contrasts, all interaction contrasts involving up to $k-1$ factors, and all the k-factor interaction contrasts involving a *given* factor. In this case, the information matrix $(\boldsymbol{X}_T\boldsymbol{Q})^T(\boldsymbol{X}_T\boldsymbol{Q})$ for all the nonnegligible effects is also diagonal. This is because, as in the proof of Theorem 13.2.2, each off-diagonal entry of $(\boldsymbol{X}_T\boldsymbol{Q})^T(\boldsymbol{X}_T\boldsymbol{Q})$ is the sum of all the entries of the Hadamard product of relevant main-effect columns of $\boldsymbol{X}_T\boldsymbol{Q}$. The total number of factors involved in each of these Hadamard products is no more than $2k-1$, since a common factor is involved in all the nonnegligible k-factor interactions. Then the same argument as in the proof of Theorem 13.2.2 shows that all the off-diagonal entries of $(\boldsymbol{X}_T\boldsymbol{Q})^T(\boldsymbol{X}_T\boldsymbol{Q})$ are zero since the strength of the array is $2k-1$. We state this result in the following theorem.

Theorem 13.2.3. An orthogonal array of strength $t = 2k-1$ ($k > 1$) can be used to estimate all the main-effect contrasts, all interaction contrasts involving up to $k-1$ factors, and all the k-factor interaction contrasts involving a given factor, assuming that all the other interaction contrasts are negligible.

By counting the numbers of degrees of freedom for the estimable orthogonal treatment contrasts, from Theorem 13.2.2 and Theorem 13.2.3, we obtain the following general lower bounds on the run sizes of orthogonal arrays due to Rao (1947).

Theorem 13.2.4. If there exists an OA(N, s^n, t), then

(i) for $t = 2k,\ N \geq \sum_{i=0}^{k} \binom{n}{i}(s-1)^i$;

(ii) for $t = 2k-1$, $N \geq \sum_{i=0}^{k-1} \binom{n}{i}(s-1)^i + \binom{n-1}{k-1}(s-1)^k$.

The following result follows easily from Theorem 13.2.4.

Corollary 13.2.5.

(i) If there exists an OA$(N, s^n, 2)$, then $n \leq (N-1)/(s-1)$. In particular, if there exists an OA$(N, 2^n, 2)$, then $n \leq N-1$.

(ii) If there exists an OA$(N, 2^n, 3)$, then $n \leq N/2$.

An orthogonal array achieving the bound in Corollary 13.2.5(i) can accommodate the maximum possible number of factors for a given run size, and is called a *saturated* orthogonal array of strength two.

13.3 Examples of orthogonal arrays

We list a few examples of orthogonal arrays. The first three are symmetric two-level arrays in which the two levels are denoted by 1 and -1. The fourth is asymmetrical with seven three-level factors and one two-level factor. The first two designs are examples of the so called *regular* fractional factorial designs, while the last two designs are nonregular. Regular designs are discussed in the next section and Handout #14.

Example 13.3.1. an OA$(8, 2^6, 2)$:

$$\begin{array}{rrrrrr} -1 & -1 & -1 & 1 & 1 & -1 \\ 1 & -1 & -1 & -1 & 1 & 1 \\ -1 & 1 & -1 & -1 & -1 & 1 \\ 1 & 1 & -1 & 1 & -1 & -1 \\ -1 & -1 & 1 & 1 & -1 & 1 \\ 1 & -1 & 1 & -1 & -1 & -1 \\ -1 & 1 & 1 & -1 & 1 & -1 \\ 1 & 1 & 1 & 1 & 1 & 1 \end{array} \tag{13.3.1}$$

Example 13.3.2 an $\mathrm{OA}(16, 2^8, 3)$:

$$
\begin{array}{rrrrrrrr}
1 & -1 & -1 & 1 & -1 & 1 & 1 & -1 \\
1 & 1 & -1 & -1 & -1 & -1 & 1 & 1 \\
1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 \\
1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 \\
1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 \\
1 & 1 & -1 & -1 & 1 & 1 & -1 & -1 \\
1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 \\
1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
-1 & 1 & 1 & -1 & 1 & -1 & -1 & 1 \\
-1 & -1 & 1 & 1 & 1 & 1 & -1 & -1 \\
-1 & 1 & -1 & 1 & 1 & -1 & 1 & -1 \\
-1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 \\
-1 & 1 & 1 & -1 & -1 & 1 & 1 & -1 \\
-1 & -1 & 1 & 1 & -1 & -1 & 1 & 1 \\
-1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 \\
-1 & -1 & -1 & -1 & -1 & -1 & -1 & -1
\end{array}
\tag{13.3.2}
$$

Example 13.3.3. an $\mathrm{OA}(12,\ 2^{11}, 2)$:

$$
\begin{array}{rrrrrrrrrrr}
-1 & -1 & 1 & -1 & -1 & -1 & 1 & 1 & 1 & -1 & 1 \\
1 & -1 & -1 & 1 & -1 & -1 & -1 & 1 & 1 & 1 & -1 \\
-1 & 1 & -1 & -1 & 1 & -1 & -1 & -1 & 1 & 1 & 1 \\
1 & -1 & 1 & -1 & -1 & 1 & -1 & -1 & -1 & 1 & 1 \\
1 & 1 & -1 & 1 & -1 & -1 & 1 & -1 & -1 & -1 & 1 \\
1 & 1 & 1 & -1 & 1 & -1 & -1 & 1 & -1 & -1 & -1 \\
-1 & 1 & 1 & 1 & -1 & 1 & -1 & -1 & 1 & -1 & -1 \\
-1 & -1 & 1 & 1 & 1 & -1 & 1 & -1 & -1 & 1 & -1 \\
-1 & -1 & -1 & 1 & 1 & 1 & -1 & 1 & -1 & -1 & 1 \\
1 & -1 & -1 & -1 & 1 & 1 & 1 & -1 & 1 & -1 & -1 \\
-1 & 1 & -1 & -1 & -1 & 1 & 1 & 1 & -1 & 1 & -1 \\
1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1
\end{array}
\tag{13.3.3}
$$

Example 3.3.4. an OA$(18, 2 \times 3^7, 2)$:

$$\begin{array}{cccccccc}
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 1 & 1 & 1 & 1 & 1 \\
0 & 0 & 2 & 2 & 2 & 2 & 2 & 2 \\
0 & 1 & 0 & 0 & 1 & 1 & 2 & 2 \\
0 & 1 & 1 & 1 & 2 & 2 & 0 & 0 \\
0 & 1 & 2 & 2 & 0 & 0 & 1 & 1 \\
0 & 2 & 0 & 1 & 0 & 2 & 1 & 2 \\
0 & 2 & 1 & 2 & 1 & 0 & 2 & 0 \\
0 & 2 & 2 & 0 & 2 & 1 & 0 & 1 \\
1 & 0 & 0 & 2 & 2 & 1 & 1 & 0 \\
1 & 0 & 1 & 0 & 0 & 2 & 2 & 1 \\
1 & 0 & 2 & 1 & 1 & 0 & 0 & 2 \\
1 & 1 & 0 & 1 & 2 & 0 & 2 & 1 \\
1 & 1 & 1 & 2 & 0 & 1 & 0 & 2 \\
1 & 1 & 2 & 0 & 1 & 2 & 1 & 0 \\
1 & 2 & 0 & 2 & 1 & 2 & 0 & 1 \\
1 & 2 & 1 & 0 & 2 & 0 & 1 & 2 \\
1 & 2 & 2 & 1 & 0 & 1 & 2 & 0
\end{array} \tag{13.3.4}$$

13.4 Regular fractional factorial designs

The difference between regular and nonregular designs lies in their construction. Design 13.3.1 is constructed in the following simple manner. The first three columns in this design consist of all the eight treatment combinations of the first three factors. Column 4 is the Hadamard product of the first two columns, column 5 is the Hadamard product of the second and third columns, and column 6 is the Hadamard product of the first three columns. If each row (treatment combination) is denoted by $(x_1, \cdots, x_6)$, where $x_i = 1$ or -1, then the eight treatment combinations in the design satisfy

$$x_4 = x_1x_2,\ x_5 = x_2x_3, x_6 = x_1x_2x_3. \tag{13.4.1}$$

In other words, since the design has $8 = 2^3$ runs, we first write down all the combinations of three factors (in this case, factors 1, 2, and 3); these factors are called *basic factors*. Then we use $(13.4.1)$ to define three additional factors, called *added factors*.

Note that $(13.4.1)$ is equivalent to

$$x_1x_2x_4 = 1, x_2x_3x_5 = 1 \text{ and } x_1x_2x_3x_6 = 1. \tag{13.4.2}$$

If $x_1x_2x_4$, $x_2x_3x_5$ and $x_1x_2x_3x_6$ are all equal to 1, then their products $(x_1x_2x_4)(x_2x_3x_5)$ $= x_1x_3x_4x_5$, $(x_1x_2x_4)(x_1x_2x_3x_6) = x_3x_4x_6$, $(x_2x_3x_5)(x_1x_2x_3x_6) = x_1x_5x_6$ and $(x_1x_2x_4)(x_2x_3x_5)(x_1x_2x_3x_6) = x_2x_4x_5x_6$ are also equal to 1. Thus the eight treatment combinations in this fraction are solutions of the following system of equations

$$1 = x_1x_2x_4 = x_2x_3x_5 = x_1x_2x_3x_6 = x_1x_3x_4x_5 = x_3x_4x_6 = x_1x_5x_6 = x_2x_4x_5x_6. \tag{13.4.3}$$

Suppose the two levels are represented by the two elements 0 and 1 of $\mathbb{Z}_2$. Specifically we replace 1 and -1 with 0 and 1, respectively. Then $(13.4.2)$ is equivalent to

$$x_1 + x_2 + x_4 = 0, x_2 + x_3 + x_5 = 0 \text{ and } x_1 + x_2 + x_3 + x_6 = 0. \tag{13.4.4}$$

In other words, the eight treatment combinations in this fraction are the solutions of a system of three independent linear equations. They are those in the principal block when the 64 treatment combinations in a complete 2^6 factorial are divided into eight blocks of size eight by confounding the interactions of factors 1, 2, 4, factors 2, 3, 5 and factors 1, 2, 3, 6. These eight treatment combinations also constitute a three-dimensional subspace of EG$(6,2)$ when each treatment combination is considered as a point in EG$(6,2)$. In general, when s is a prime or prime power, subspaces (or flats) of EG(n,s) are called *regular* fractional factorial designs. This implies that the run size of a regular design must be a power of s. Construction and properties of regular designs will be discussed in more details in Handout #14.

13.5 Hadamard matrices

Design 13.3.3 can be constructed from a Hadamard matrix of order 12. A Hadamard matrix of order N is an $N \times N$ matrix $\boldsymbol{H}$ of 1's and -1's such that

$$\boldsymbol{H}^T\boldsymbol{H} = N\boldsymbol{I}_N,$$

where $\boldsymbol{I}_N$ is the identity matrix of order N. If we multiply all the entries in the same row or the same column of a Hadamard matrix by -1, then the resulting matrix is still a Hadamard matrix. Therefore, without loss of generality, we may assume that all the entries in the first row and/or the first column of $\boldsymbol{H}$ are equal to 1.

We have the following equivalence between a Hadamard matrix of order N and an OA$(N, 2^{N-1}, 2)$.

Theorem 13.5.1. Suppose $\boldsymbol{H}$ is a Hadamard matrix of order $N > 2$ such that all the entries in the first column are equal to 1. Then the matrix obtained by deleting the first column of $\boldsymbol{H}$ is an OA$(N, 2^{N-1}, 2)$. Conversely, adding a column of 1's to an OA$(N, 2^{N-1}, 2)$ results in a Hadamard matrix of order N.

Proof. It is trivial that an OA$(N, 2^{N-1}, 2)$ supplemented by a column of 1's is a Hadamard matrix. Thus it is enough to prove the converse. Suppose $\boldsymbol{H}$ is a Hadamard matrix such that all the entries in the first column are equal to 1. Let $\boldsymbol{h}_i = [h_{1i}, \cdots, h_{Ni}]^T$ and $\boldsymbol{h}_j = [h_{1j}, \cdots, h_{Nj}]^T$ be the ith and jth columns of $\boldsymbol{H}$, where $i \neq 1$, $j \neq 1$ and $i \neq j$. We need to show that each of $(1,\, 1)$, $(1,\, -1)$, $(-1,\, 1)$ and $(\,-1, -1)$ appears $N/4$ times among the N pairs $(h_{1i}, h_{1j}), \cdots, (h_{Ni}, h_{Nj})$. Suppose $(1,\, 1)$ appears a times, (1, $-1)$ appears b times, $(-1,\, 1)$ appears c times, and $(-1,\, -1)$ appears d times. Then since $\boldsymbol{h}_i$ is orthogonal to $\boldsymbol{h}_j$, and they are both orthogonal to the column of 1's, we have

$$a + b + c + d = N,$$

$$a + b - c - d = 0,$$

$$a - b + c - d = 0,$$

and

$$a - b - c + d = 0.$$

Solving these equations, we have $a = b = c = d$. $\square$

We shall call an OA$(N, 2^{N-1}, 2)$ constructed from a Hadamard matrix of order N as described in Theorem 13.5.1 a Hadamard design. Design 13.3.3 can be obtained by deleting a column of 1's from a Hadamard matrix of order 12. In view of Corollary 13.2.5, all Hadamard designs are saturated.

An immediate consequence of Theorem 13.5.1 is that if there exists a Hadamard matrix of order $N > 2$, then N must be a multiple of 4. Hadamard designs are not regular when N is not a power of 2; when N is a power of 2, they may or may not be regular.

The following are Hadamard matrices of orders 1 and 2:

$$\boldsymbol{P}_1 = [1],$$

$$\boldsymbol{P}_2 = \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}.$$

It has been conjectured that a Hadamard matrix of order N exists for every N that is a multiple of 4. This is called the *Hadamard conjecture*.

It is easy to see that if $\boldsymbol{H}$ and $\boldsymbol{K}$ are Hadamard matrices of orders m and n, respectively, then the Kronecker product $\boldsymbol{H} \otimes \boldsymbol{K}$ is a Hadamard matrix of order mn. Applying this result to $\boldsymbol{P}_2$ repeatedly, we conclude that there exists a Hadamard matrix of order 2^n for every positive integer n.

Remark 13.5.2. As shown in Section 9.6 in Handout #9, the $2^n - 1$ columns of the n-fold Kronecker product

$$\begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix} \otimes \cdots \otimes \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix},$$

except the first one, constitute an orthogonal basis of $\mathbb{R}^{2^n} \ominus G_0$, representing the various factorial effects in a 2^n complete factorial. Notice that the Hadamard design obtained by deleting the first column of $\begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix} \otimes \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix} \otimes \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix}$ is the same as the array in $(9.6.3)$ after the seven columns of the array are rearranged in the lexicographic order (1, 2, 12, 3, 13, 23, 123). In fact, the regular fractional factorial design in Example 13.3.1 consists of six of these seven columns. It can be seen from $(13.4.1)$ that the construction of this design amounts to using interaction contrasts of the basic factors to define the added factors. This construction will be treated in more details in Handout #14.

Although the Hadamard conjecture has not been proved, so far no counterexamples have been found, and Hadamard matrices have been constructed for many orders that are multiples of four. This provides more flexibility than regular designs in terms of the run sizes. Plackett and Burman (1946) were the first to propose the use of Hadamard designs in factorial experiments. The Hadamard designs constructed in their paper are referred to as *Plackett-Burman designs*.

A method of constructing Hadamard matrices used by Plackett and Burman was due to Paley (1933). Suppose N is a multiple of 4 such that $N-1$ is an odd prime power. Let $q = N-1$ and let $\alpha_1 = 0, \alpha_2, \cdots, \alpha_q$ denote the elements of $GF(q)$. Define a function $\chi : GF(q) \to \{0,\ 1,\ -1\}$ by

$$\chi(\beta) = \begin{cases} 1, & \text{if } \beta = y^2 \text{ for some } y \in GF(q), \\ 0, & \text{if } \beta = 0, \\ -1, & \text{otherwise.} \end{cases}$$

Let $\boldsymbol{A}$ be the $q \times q$ matrix $[a_{ij}]$, where $a_{ij} = \chi(\alpha_i - \alpha_j)$ for $i,j = 1, 2, \cdots, q$, and

$$\boldsymbol{P}_N = \begin{bmatrix} 1 & -\mathbf{1}_q^T \\ \mathbf{1}_q & \boldsymbol{A} + \boldsymbol{I}_q \end{bmatrix}, \tag{13.5.1}$$

where $\mathbf{1}_q$ is the $q \times 1$ vector of 1's and $\boldsymbol{I}_q$ is the identity matrix of order q. Then $\boldsymbol{P}_N$ is a Hadamard matrix. For a proof see Hedayat, Sloane and Stufken (1999). We shall call the OA$(N, 2^{N-1}, 2)$ obtained by deleting the first column of $(13.5.1)$ the *Paley design* of order N.

There is also a connection between Hadamard matrices and balanced incomplete block designs (BIBD). Suppose $\boldsymbol{H}$ is a Hadamard matrix of order N. Without loss of generality, assume that all the entries in the first row and first column of $\boldsymbol{H}$ are equal to 1. Delete the first row and first column from $\boldsymbol{H}$; then we have an $(N-1) \times (N-1)$ matrix $\boldsymbol{H}^*$ of 1's and -1's. Define a block design d with $N-1$ treatments and $N-1$

blocks such that the ith treatment appears in the j th block once if the (i,j)th entry of $\boldsymbol{H}^*$ is equal to 1; otherwise, it does not appear. Then d is a balanced incomplete block design. The block size is $N/2-1$ since there are $N/2-1$ 1's in each column of $\boldsymbol{H}^*$. Conversely, given a balanced incomplete block design d with $N-1$ treatments and $N-1$ blocks of size $N/2-1$, write down an $(N-1)\times(N-1)$ *incidence matrix* $\boldsymbol{H}^*$ of 1's and -1's such that the (i,j)th entry of $\boldsymbol{H}^*$ is equal to 1 if and only if the ith treatment appears in the jth block of d. Supplement $\boldsymbol{H}^*$ by a row and column of 1's; then we obtain an $N\times N$ matrix which can be shown to be a Hadamard matrix.

For example, the OA$(12,2^{11},2)$ displayed in $(13.3.3)$ can be constructed by applying the method described in the previous paragraph to a balanced incomplete block design with 11 treatments and 11 blocks of size 5. The first 11 rows of the array come from the incidence matrix of the BIBD which can be developed from the initial block $\{1,3,4,5,9\}$ in a cyclic manner. Thus the associated incidence matrix is a circulant matrix. One row of 1's is then added at the bottom to produce an orthogonal array. If we also add a column of 1's, then a Hadamard matrix of order 12 is obtained.

13.6 Foldover designs

The orthogonal array displayed in $(13.3.2)$ has strength three. One can see that the first eight rows of this design constitute the Hadamard matrix $\begin{bmatrix}1 & -1\\ 1 & 1\end{bmatrix}\otimes\begin{bmatrix}1 & -1\\ 1 & 1\end{bmatrix}\otimes\begin{bmatrix}1 & -1\\ 1 & 1\end{bmatrix}$, which is also the OA$(8,2^7,2)$ in $(9.6.3)$ supplemented by a column of 1's after the other columns are rearranged in lexicographic order. The last eight rows of array $(13.3.2)$ are obtained from the first eight rows by interchanging the two levels. We say that array $(13.3.2)$ is the *foldover* of (the rearranged) array $(9.6.3)$. In general, given an OA$(N,2^n,t)$ $\boldsymbol{X}$ where the two levels are represented by 1 and -1, the following array is called the foldover of $\boldsymbol{X}$:

$$\tilde{\boldsymbol{X}}=\begin{bmatrix}\mathbf{1} & \boldsymbol{X}\\ -\mathbf{1} & -\boldsymbol{X}\end{bmatrix}, \tag{13.6.1}$$

where **1** is the $N\times 1$ vector of 1's. The foldover design is of size $2N$ and has $n+1$ two-level factors Compared with the original design, one factor is added and the run size is doubled.

The method of foldover was first proposed by Box and Wilson (1951) for regular fractional factorial designs. The following result for general two-level orthogonal arrays is due to Seiden and Zemach (1966).

Theorem 13.6.1. The foldover of a two-level orthogonal array of even strength t has strength $t+1$.

Theorem 13.6.1 follows from the following lemma.

Lemma 13.6.2. Suppose $\boldsymbol{X}$ is an OA$(N, 2^n, t)$ with $n \geq t+1$ in which the two levels are denoted by 1 and -1. Let $\boldsymbol{Y}$ be an $N \times (t+1)$ submatrix of $\boldsymbol{X}$. Then there exist two nonnegative integers α and β with $\alpha + \beta = N/2^t$ such that all the vectors $\boldsymbol{x} = (x_1, x_2, \cdots, x_{t+1})$ with $x_1 x_2 \cdots x_{t+1} = 1$, where $x_i = 1$ or -1, appear α times as row vectors of $\boldsymbol{Y}$, and each of those with $x_1 x_2 \cdots x_{t+1} = -1$ appears β times.

Proof. For each $\boldsymbol{x} = (x_1, \cdots, x_{t+1})$ with $x_i = 1$ or -1, let $f(\boldsymbol{x})$ be the number of times $\boldsymbol{x}$ appears as row vectors of $\boldsymbol{Y}$. Then since $\boldsymbol{X}$ has strength t, we have

$$f(x_1, \cdots, x_t, x_{t+1}) + f(x_1, \cdots, x_t, -x_{t+1}) = \lambda.$$

Also,

$$f(x_1, \cdots, -x_t, -x_{t+1}) + f(x_1, \cdots, x_t, -x_{t+1}) = \lambda.$$

It follows from these two equations that $f(x_1, \cdots, x_t, x_{t+1}) = f(x_1, \cdots, -x_t, -x_{t+1})$. Repeating the same argument, we see that any two rows $\boldsymbol{x}$ and $\boldsymbol{y}$ differing in an even number of components appear the same number of times as row vectors of $\boldsymbol{Y}$. Thus all the vectors $\boldsymbol{x} = (x_1, x_2, \cdots, x_{t+1})$ with $x_1 x_2 \cdots x_{t+1} = 1$ appear the same number of times, say α times, as row vectors of $\boldsymbol{Y}$, and each of those with $x_1 x_2 \cdots x_{t+1} = -1$ also appears the same number of times, say β times. Since $\boldsymbol{X}$ has strength t, we have $\alpha + \beta = N/2^t$. $\square$

Now we prove Theorem 13.6.1. Let $\boldsymbol{X}$ be an OA$(N, 2^n, t)$, where t is even, and let $\tilde{\boldsymbol{Y}}$ be a $2N \times (t+1)$ submatrix of $\tilde{\boldsymbol{X}}$. If $\tilde{\boldsymbol{Y}}$ contains the first column of $\tilde{\boldsymbol{X}}$ as displayed in (13.6.1), then since $\boldsymbol{X}$ has strength t, it is clear that all the $(t+1)$-tuples of 1's and -1's appear the same number of times as row vectors of $\tilde{\boldsymbol{Y}}$. Suppose

$$\tilde{\boldsymbol{Y}} = \begin{bmatrix} \boldsymbol{Y} \\ -\boldsymbol{Y} \end{bmatrix},$$

where $\boldsymbol{Y}$ is an $N \times (t+1)$ submatrix of $\boldsymbol{X}$. Then by Lemma 13.6.2, there exists a nonnegative integer α such that each $\boldsymbol{x} = (x_1, x_2, \cdots, x_{t+1})$ appears either α or $N/2^t - \alpha$ times as a row vector of $\boldsymbol{Y}$. Since $t+1$ is odd, if $\boldsymbol{x}$ appears α times, then $-\boldsymbol{x}$ must appear $N/2^t - \alpha$ times. It follows that if $\boldsymbol{x}$ appears α times in $\boldsymbol{Y}$, then it appears $N/2^t - \alpha$ times in $-\boldsymbol{Y}$, and thus appears $\alpha + (N/2^t - \alpha) = N/2^t$ times in $\tilde{\boldsymbol{Y}}$. $\square$

It is also clear from the above proof why the foldover method does not increase the strength when it is applied to an orthogonal array of odd strength.

Corollary 13.2.5 shows that an OA$(N, 2^n, 2)$ must have $N \geq n+1$ and an OA$(N, 2^n, 3)$ must have $N \geq 2n$. It follows from Theorem 13.6.1 that the foldover of a saturated two-level orthogonal array of strength two achieves the lower bound on the run size of an orthogonal array of strength three.