

ESTIMABILITY AND EFFICIENCY IN PROPORTIONAL FREQUENCY PLANS

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SUMMARY

This paper extends the calculus of factorial experiments to a fractional factorial set-up and examines critically the proportional frequency plans from the point of view of estimability and efficiency.

Introduction

Plackett [7] introduced the criterion of proportional frequency in a multifactor setting. It was contended by Addelman [1] that fractional factorial plans based on this criterion lead to orthogonal estimation of lower order factorial effects when higher order effects are absent. Lewis and John [4] and later, more rigorously, Mukerjee [5] had shown that the contention of Addelman regarding orthogonality in proportional frequency plans is not in general true and established, in the general case, the criterion of equal frequency (in terms of orthogonal arrays) as a necessary and sufficient condition for orthogonal fractional factorial plans.

Unfortunately, however, as shown in Mukerjee [5], especially in the asymmetric case, there are situations where orthogonal plans based on the equal frequency criterion are nonexistent. Hence in fractional experimentation under such circumstances one has no other alternative than to forgo orthogonality and search for possibly nonorthogonal plans. Since it is comparatively simpler to obtain proportional frequency plans (cf. Addelman [1], [2]) such plans may be considered in this context. But before the

proportional frequency plans are used, their worth with regard to estimability and efficiency should be critically reexamined particularly in view of the fact that the existing results on them appear to be incorrect. This paper makes a study in this line by extending the calculus of factorial experiments (cf. Kurkjian and Zelen [3]) to a fractional factorial set-up. Though the main emphasis will be on proportional frequency plans it is anticipated that the methods developed will be helpful in dealing with other problems in fractional replication as well.

2. Notations and Preliminaries

Consider a factorial experiment involving m factors F_1, \dots, F_m at s_1, \dots, s_m levels respectively ($s_j \geq 2, 1 \leq j \leq m$), there being $v = \prod_{j=1}^m s_j$

level combinations in all. Throughout this paper the v level combinations will be assumed to be lexicographically ordered (cf. Kurkjian and Zelen [3]). Let $\tau^{(v \times 1)}$ be the vector of treatment effects arranged lexicographically.

Let for $1 \leq j \leq m, I_j^{(s_j \times 1)} = (1, 1, \dots, 1)'$ and P_j be an $(s_j - 1) \times s_j$ matrix such that $(s_j^{-1} 1_j, P_j)$ is orthogonal. Let

$$P_j^{x_j} = s_j^{-\frac{1}{2}} 1_j' \text{ if } x_j = 0; = P_j \text{ if } x_j = 1. \quad (2.1)$$

Further let $\Omega = \{(x_1, \dots, x_m) : x_j = 0, 1 \forall j, \text{ not all } x_j\text{'s are zero}\}$. For any $x = (x_1, \dots, x_m) \in \Omega$, writing

$$P^x = \prod_{j=1}^m P_j^{x_j} = P_1^{x_1} \times \dots \times P_m^{x_m} \quad (2.2)$$

where \times denotes Kronecker product, it is easy to check that the $\prod (s_j - 1)^{x_j}$ linear functions $P^x \tau$ represent a complete set of orthonormal treatment contrasts belonging to the factorial effect $F_1^{x_1} \dots F_m^{x_m}$ (cf. Mukerjee [5]). Let for $1 \leq u \leq m$

$$J_u = \{(x_1, \dots, x_m) : (x_1, \dots, x_m) \in \Omega, \text{ at most } u \text{ of } x_1, \dots, x_m \text{ are } 1\},$$

$$P^{(u)'} = (\dots, P^{u'}, \dots), \bar{P}^{(u)'} = (\dots, P^{u'}, \dots), \quad (2.3)$$

P^x being included in $P^{(u)}$ ($\bar{P}^{(u)}$) if and only if $x \in J_u$ ($\Omega - J_u$).

In the factorial context it often happens that the higher order interactions, say those involving more than t factors, are absent i.e.

$$\bar{P}^{(t)} \tau = 0. \quad (2.4)$$

Then imposing the side restriction $\underline{\varepsilon}' \underline{\tau} = 0$, where $\underline{\varepsilon}^{(v \times 1)} = (1, 1, \dots, 1)'$ and following the line of Mukerjee [5] we have

$$\underline{\tau} = P^{(t)'} \underline{\tau}^* \tag{2.5}$$

where $\underline{\tau}^*$ is a vector of new parameters representing treatment effects under (2.4).

Consider an arrangement of the v level combinations in an (unblocked) completely randomised design such that for $1 \leq i \leq v$, the i th level combination is replicated r_i times.

Let $\mathbf{r}^{(v \times 1)} = (r_1, \dots, r_v)'$, $\mathbf{r}^s = \text{Diag}(r_1, \dots, r_v)$, $n = \sum_{i=1}^v r_i (> 0)$, $\mathbf{T}^{(v \times 1)}$ = vector of observed treatment totals, $\mathbf{G} = \underline{\varepsilon}' \mathbf{T}$

$$\mathbf{C} = \mathbf{r}^s - n^{-1} \mathbf{r} \mathbf{r}', \tag{2.6}$$

$$\mathbf{Q} = \mathbf{T} - n^{-1} \mathbf{G} \mathbf{r}.$$

Then following Mukerjee [5], assuming the usual fixed effects linear model with a constant error variance (σ^2 , say) under the reparametrized set-up (2.5), the reduced normal equations are found to be

$$P^{(t)} \mathbf{C} P^{(t)'} P^{(t)} \underline{\tau} = P^{(t)} \mathbf{Q}. \tag{2.7}$$

3. Estimability in Proportional Frequency Plans

Consider an unblocked m factor design in which the i th level combination is replicated $r_i (> 0)$ times, $1 \leq i \leq v$. Let for $1 \leq j_1 < \dots < j_a \leq m$, $1 \leq q \leq m$, $0 \leq i_{j_l} \leq s_{j_l} - 1$ ($1 \leq l \leq q$), $n_{i_{j_1} \dots i_{j_q}}^{(j_1 \dots j_q)}$ represent the number of times the level combination $(i_{j_1}, \dots, i_{j_q})$ of the factors F_{j_1}, \dots, F_{j_q} occur among the level combinations included in the experiment. The chosen level combinations will be defined to represent a proportional frequency plan of strength $d (< m)$ if for every j_1, \dots, j_a and every i_{j_1}, \dots, i_{j_d} [$1 \leq j_1 < \dots < j_a \leq m$; $0 \leq i_{j_l} \leq s_{j_l} - 1$ ($1 \leq l \leq d$)]

$$n_{i_{j_1}, \dots, i_{j_d}}^{(j_1 \dots j_a)} = n^{-(a-1)} \prod_{l=1}^d n_{i_{j_l}}^{(j_l)} > 0, \tag{3.1}$$

where $n = \sum r_i (> 0)$. In this section we shall study the worth of such plans from the point of view of estimability.

For $1 \leq j \leq m$, let $D_j = \text{Diag}(n_0^{(j)}, \dots, n_{s_j-1}^{(j)})$,

$$\mathbf{n}^{(j)} = (n_0^{(j)}, \dots, n_{s_j-1}^{(j)})'$$

$$V_j = n^{-1}D_j, T_j = n^{-2} \mathbf{n}^{(j)} \mathbf{n}^{(j)'}, I_j = I^{(s_j \times s_j)} \quad (3.2)$$

$$\varepsilon_j^{x_j} = 1_j \text{ if } x_j = 0; = I_j \text{ if } x_j = 1,$$

$$V_j^{(x_j, y_j)} = n^{-1}D_j \text{ if } x_j = y_j = 1; = n^{-1} \mathbf{n}^{(j)} \text{ if } x_j = 1, y_j = 0; \\ = n^{-1} \mathbf{n}^{(j)'} \text{ if } x_j = 0, y_j = 1; = 1 \text{ if } x_j = y_j = 0$$

$$T_j^{(x_j, y_j)} = n^{-2} \mathbf{n}^{(j)} \mathbf{n}^{(j)'} \text{ if } x_j = y_j = 1; = V_j^{(x_j, y_j)} \text{ otherwise.}$$

It is easy to check that for $1 \leq j \leq m; x_j = 0, 1; y_j = 0, 1,$

$$\varepsilon_j^{x_j} V_j \varepsilon_j^{y_j} = V_j^{(x_j, y_j)}, \varepsilon_j^{x_j} T_j \varepsilon_j^{y_j} = T_j^{(x_j, y_j)} \quad (3.3)$$

For, $x, y \in \Omega$, define

$$\varepsilon^x = \prod_{j=1}^m \varepsilon_j^{x_j}, V^{(x, y)} = \prod_{j=1}^m V_j^{(x_j, y_j)}, T^{(x, y)} = \prod_{j=1}^m T_j^{(x_j, y_j)} \quad (3.4)$$

By (3.2), (3.3), it is immediate that for $x, y \in \Omega$,

$$\varepsilon^{x'} \left(\prod_{j=1}^m V_j \right) \varepsilon^y = V^{(x, y)}, \varepsilon^{x'} \left(\prod_{j=1}^m T_j \right) \varepsilon^y = T^{(x, y)}. \quad (3.5)$$

Theorem 3.1. *If the chosen level combinations form a proportional frequency plan of strength $2g (\leq m)$ then all contrasts belonging to effects involving g or less factors are estimable when all effects involving more than g factors are absent.*

Proof. Because of the reduced normal equations (2.7) (here $g = t$) we only have to show that $P^{(g)} CP^{(g)'}$ is positive definite under the given condition. Now if the chosen level combinations form a proportional frequency plan (i.e. if (3.1) holds with $d = 2g$) proceeding as in the proof of Lemma 2.2 of Mukerjee [5] by showing that the corresponding elements of the two sides are equal, we have for any $x, y \in J_g$

$$\varepsilon^{x'} C \varepsilon^y = n[V^{(x, y)} - T^{(x, y)}],$$

i.e. by (3.5)

$$\varepsilon^{x'} C \varepsilon^y = n \varepsilon^{x'} G \varepsilon^y, \quad (3.6)$$

where by (3.2)

$$G = \prod_{j=1}^m (n^{-1}D_j) - \left\{ \prod_{j=1}^m (n^{-1}\mathbf{n}^{(j)}) \right\} \left\{ \prod_{j=1}^m (n^{-1}\mathbf{n}^{(j)'}) \right\}, \text{ i.e.}$$

$$G = \text{Diag}(a_1, \dots, a_v) - aa', \quad (3.7)$$

where $\mathbf{a} = (a_1, \dots, a_v)' = \prod_{j=1}^m (n^{-1} \mathbf{n}^{(j)})$. Since the chosen level combinations form a proportional frequency plan of strength $2g$, by (3.1), $n_{i_j}^{(j)} > 0 \forall i_j, j$. Hence $a_i > 0, i = 1, 2, \dots, v$.

By (2.1), (2.2), (3.4), for any $x \in \Omega$, there exists matrix L_x such that $P^x = L_x e^{x'}$. Hence by (3.6), under the given conditions for $x, y \in J_g, P^x C P^{y'} = n P^x G P^{y'}$, so that by (2.3)

$$P^{(g)} C P^{(g)'} = n P^{(g)} G P^{(g)'}. \tag{3.8}$$

By (2.1), (2.2), (2.3) $P^{(g)} \left(\prod_{j=1}^m \mathbf{1}_j \right) = 0$ and $P^{(g)} P^{(g)'} = I$. Further $a_i > 0, i = 1, 2, \dots, v$. Hence by (3.7) and some standard steps in matrix algebra, it is evident that $P^{(g)} G P^{(g)'}$ (and hence $P^{(g)} C P^{(g)'}$, by (3.8) is positive definite.

Q.E.D.

One would naturally like to investigate the possible extension of the above theorem to the case $g < t$ i.e. to examine whether all contrasts belonging to effects involving g or less factors are estimable when all effects involving more than t factors are absent given that the chosen level combinations form a proportional frequency plan of strength $(g + t)$.

If $g < t$, by (2.3), (2.5), the reduced normal equations (2.7) can be written as

$$\begin{bmatrix} P^{(g)} C P^{(g)'} & P^{(g)} \bar{C} \bar{P}^{(g,t)'} \\ \bar{P}^{(g,t)} C \bar{P}^{(g)'} & \bar{P}^{(g,t)} C \bar{P}^{(g,t)'} \end{bmatrix} \begin{bmatrix} P^{(g)} \underline{\tau} \\ \bar{P}^{(g,t)} \underline{\tau} \end{bmatrix} = \begin{bmatrix} P^{(g)} Q \\ \bar{P}^{(g,t)} Q \end{bmatrix} \tag{3.9}$$

where $\bar{P}^{(g,t)'} = (\dots, P^x, \dots)$, P^x being included in $\bar{P}^{(g,t)}$ if and only if $x \in J_t - J_g$. Since here we are interested in estimating the elements of $P^{(g)} \underline{\tau}$ the problem reduces to examine whether, given that the chosen level combinations form a proportional frequency plan of strength $(g + t)$, it is necessarily true that

$$\text{row space } (I^*, 0) \subset \text{row space } (P^{(t)} C P^{(t)'}) \tag{3.10}$$

where I^* is identity matrix of order v_1 , 0 is null matrix of order $v_1 \times (v_2 - v_1)$ and v_1, v_2 denote respectively the number of rows in $P^{(g)}, P^{(t)}$.

The answer, however, will, in general, be in the negative as the following example illustrates.

Example 3.1. Consider the following plan of a $3^2 \times 2^2$ factorial (the level combinations are written as columns) which is easily seen to be a proportional frequency plan of strength 3.

0 0 0 1 0 1 1 1 0 0 0 1 0 1 1 1 0 0 0 2 0 2 2 2 0 0 0 2 0 2 2 2
 0 0 1 0 1 0 1 1 0 0 2 0 2 0 2 2 0 0 1 0 1 0 1 1 0 0 2 0 2 0 2 2
 0 1 0 0 1 1 0 1 0 1 0 0 1 1 0 1 0 1 0 0 1 1 0 1 0 1 0 0 1 1 0 1
 0 1 1 1 0 0 0 1 0 1 1 1 0 0 0 1 0 1 1 1 0 0 0 1 0 1 1 1 0 0 0 1

with $g = 1, t = 2$, it may be checked that (3.10) does not hold. The process which involves actual computation of $P^{(t)} CP^{(t)'}$ is lengthy and is not shown here. Thus though the chosen level combinations form a proportional frequency plan of strength 3, it is not possible to estimate all main effect contrasts even when all interactions involving more than two factors are absent.

Thus it is seen that further extension of Theorem 3.1 in the line contemplated above is not possible. As such the use of proportional frequency plans should be as envisaged in Theorem 3.1.

4. Analysis and Efficiency

We now consider in brief the analysis of such plans. Consider a proportional frequency plan of strength $2g$. Then by (2.7) (with $g = t$), (3.8) and Theorem 3.1, assuming the absence of all interactions involving more than g factors

$$P^{(g)}\hat{\xi} = (P^{(g)} CP^{(g)'})^{-1} P^{(g)}Q, \tag{4.1}$$

so that

$$\text{Disp } (P^{(g)}\hat{\xi}) = \sigma^2(P^{(g)} CP^{(g)'})^{-1} = \sigma^2 n^{-1} (P^{(g)} GP^{(g)'})^{-1}. \tag{4.2}$$

As such the sum of squares (SS) due to $P^{(g)}\hat{\xi}$ is given by

$$n^{-1} Q' P^{(g)'} (P^{(g)} GP^{(g)'})^{-1} P^{(g)}Q.$$

The error SS is obtained by subtracting this from the total SS. For any $x \in J_g, P^x\hat{\xi}$, $\text{Disp } (P^x\hat{\xi})$ may be obtained from appropriate subvector and submatrix of (4.1), (4.2) respectively. It should be noted that the plan under study is nonorthogonal so that separate ANOVA tables would be required for various factorial effects.

We can derive a lower bound for the average efficiency of such plans.

It is easy to check that $\times_{j=1}^m (nD_j^{-1}) = (H, \text{ say})$ is a generalised inverse of G . Hence by (4.2) after some simplification we have

$$\text{Disp } (P^{(g)}\hat{\xi}) = \sigma^2 n^{-1} \begin{bmatrix} P^{(g)} HP^{(g)'} - P^{(g)} H\bar{P}^{(g)'} \\ HP^{(g)'} \end{bmatrix} \bar{P}^{(g)} (H\bar{P}^{(g)'})^{-1} \bar{P}^{(g)} \tag{4.3}$$

It is difficult to have a compact expression for $\text{Trace } [\text{Disp } (P^{(g)}\hat{\xi})]$. How-

ever, noting that the second term within square brackets on the right hand side of (4.3) is nonnegative definite, by (2.3),

$$\begin{aligned} \text{Trace [Disp } (P^{(g)}\hat{\Sigma})] &\leq \sigma^2 n^{-1} \text{Trace } (P^{(g)} HP^{(g)'}) \\ &= \sigma^2 n^{-1} \text{Trace } (HP^{(g)' } P^{(g)}) = \sigma^2 n^{-1} \sum_{x \in J_g} \text{Trace } (HP^{x'} P^x) \end{aligned} \quad (4.4)$$

By (2.1), (2.2), for any $x \in \Omega$, $P^{x'} P^x = \prod_{j=1}^m W_j^{x_j}$, where for $1 \leq j \leq m$,

$$\begin{aligned} W_j^{x_j} &= I_j - s_j^{-1} \mathbf{1}_j \mathbf{1}_j' \text{ if } x_j = 1, \\ &= s_j^{-1} \mathbf{1}_j \mathbf{1}_j' \quad \text{if } x_j = 0. \end{aligned}$$

Hence writing for $x \in \Omega$, $\alpha(x) = \prod_{j=1}^m (s_j - 1)^{x_j}$

$$\begin{aligned} \text{Trace } (HP^{x'} P^x) &= \text{Trace } \left[\left\{ \prod_{j=1}^m (nD_j^{-1}) \right\} P^{x'} P^x \right] \\ &= n^m \alpha(x) \nu^{-1} \sum_{i_1=0}^{s_1-1} \dots \sum_{i_m=0}^{s_m-1} (n_{i_1}^{(1)} \dots n_{i_m}^{(m)})^{-1} = n^m \alpha(x) \nu^{-1} \prod_{j=1}^m \\ &\quad \left\{ \sum_{i_j=0}^{s_j-1} n_{i_j}^{(j)-1} \right\}. \end{aligned}$$

Thus by (4.4),

$$\begin{aligned} \text{Trace [Disp } (P^{(g)}\hat{\Sigma})] &\leq \sigma^2 n^{m-1} \left[\prod_{j=1}^m \left\{ \sum_{i_j=0}^{s_j-1} n_{i_j}^{(j)-1} \right\} \right] \\ &\quad \left\{ \sum_{x \in J_g} \alpha(x) \right\} \nu^{-1} \end{aligned} \quad (4.5)$$

Since $\text{Disp } (P^{(g)}\hat{\Sigma})$ is a square matrix of order $\sum_{x \in J_g} \alpha(x)$, by (4.5), average variance of the elements of $P^{(g)}\hat{\Sigma}$

$$\leq \sigma^2 n^{m-1} \nu^{-1} \prod_{j=1}^m \left\{ \sum_{i_j=0}^{s_j-1} n_{i_j}^{(j)-1} \right\} \quad (4.6)$$

As shown in Mukerjee [6] for any given n , an equal frequency plan

(based on orthogonal array with variable symbols) if it exists is universally optimal with

$$\text{Disp } P^{(g)}\hat{\xi} = \sigma^2 n^{-1} \nu I \quad (4.7)$$

where I is identity matrix of appropriate order. For any particular n , even if an equal frequency does not exist we shall define the relative efficiency of any other plan relative to a hypothetical equal frequency plan for the sake of definiteness. Thus by (4.6), (4.7), the average relative efficiency of a plan based on a proportional frequency criterion (of strength $2g$) is at least

$$\nu^2 n^{-m} \prod_{j=1}^m \left\{ \sum_{i_j=0}^{s_j-1} n_{i_j}^{(j)} - 1 \right\}^{-1} \quad (4.8)$$

The smaller the scatter of $n_{i_j}^{(j)}$, $i_j = 0, 1, \dots, s_j - 1$, for different j , the greater the value of (4.8). Hence in the construction of proportional frequency plans, $n_0^{(j)}, \dots, n_{s_j-1}^{(j)}$ should be as nearly equal as possible for each j .

5. Concluding Remarks

The discussion in section 3 following the proof of Theorem 3.1 indicates that if all effects involving more than t factors are absent and it is desired to keep all effects involving $g (< t)$ factors estimable using a proportional frequency plan, a plan of strength $(g + t)$ will not necessarily serve the purpose. The authors have, however, come across examples, obtained by hit and trial, which suggest that in such situations a proportional frequency plan of strength $(g + t)$ may be helpful provided $n_0^{(j)} = n_1^{(j)} = \dots = n_{s_j-1}^{(j)}$ holds for some j 's. This leads one to think in terms of some 'mixture' of proportional and equal frequency plans. It is intended to take up these developments in a subsequent communication.

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