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Efficiency Factors for Natural Contrasts in Partially Confounded Factorial Designs

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Abstract

With reference to a partially confounded design for a 3^n factorial experiment, an explicit expression is derived for the efficiency factors of natural contrasts of the form linear, linear$\times$linear, linear$\times$quadratic, etc. This expression involves the harmonic mean of the efficiency factors for pencils. It is also shown that such a neat result does not exist for general s-level factorials where $s > 3$. Nevertheless, the case of such general s is also explored.

MSC: 62K15

Keywords: Efficiency factor, harmonic mean, natural contrasts, pencil.

1. Introduction and preliminaries

Factorial experiments, introduced and popularized by Fisher (1935) have not only a rich theoretical foundation but also immense applications in almost all areas of human endeavor. Early important contributions to this area are due to Yates (1937) and Bose (1947), while informative accounts of the subsequent developments are available e.g., in Raktoe, Hedayat and Federer (1981), Gupta and Mukerjee (1989), Dean and Voss (1999), Hinkelmann and Kempthorne (2005), Bailey (2008) and Wu and Hamada (2009).

Notwithstanding the availability of a vast literature on factorial experiments as indicated above, it appears that there exists a gap which impacts even the standard text book level treatment of the subject. This concerns partial confounding, a topic that even a first course on factorial designs dwells on, at least for 2- and 3-level factorials. While for 2-level factorials, the existing theory is intuitively clear because of a 1-1 correspondence between pencils (Bose, 1947) and the associated factorial effects, the lack of a 1-1 correspondence of this kind hinders such a simple interpretation in the case of 3-level factorials. This motivates the present article where we investigate the relationship between the efficiency factors for natural contrasts as defined below and those for pencils in a partially confounded 3-level design.

We begin with some preliminaries in order to specify the problem considered here. Consider a 3^n factorial experiment involving n factors $F_1, \ldots, F_n$, each at three levels, 0, 1 and 2. The treatment combinations are coded as $\boldsymbol{x} = x_1 \ldots x_n$, where for $1 \le i \le n$, $x_i \in \{0, 1, 2\}$. The objects of interest in a factorial experiment are *factorial effects*, namely the main effects and interactions. Consider a factorial effect, say the one involving factors $F_1, F_2, \ldots, F_g$ and denoted by $F_1 \times F_2 \times \cdots \times F_g$, $1 \le g \le n$. In the literature including standard textbooks, the 2^g independent treatment contrasts belonging to $F_1 \times F_2 \times \cdots \times F_g$ are represented via 2^{g-1} components $F_1 F_2^{b_2} \cdots F_g^{b_g}$, where $b_i = 1$ or 2 for each i, such that any component $F_1 F_2^{b_2} \cdots F_g^{b_g}$ accounts for two independent treatment contrasts, namely those among the three mutually exclusive and exhaustive sets of treatment combinations, as given by

$$V_j(\boldsymbol{b}) = \{\boldsymbol{x} = x_1 \ldots x_n : x_1 + b_2 x_2 + \cdots + b_g x_g = j \bmod 3\},\ j = 0, 1, 2, \tag{1}$$

where $\boldsymbol{b} = (1, b_2, \ldots, b_g)$. These components, often called *orthogonal components*, are equivalent to *pencils* as discussed in depth by Bose (1947). It is well known that if a partially confounded 3^n factorial experiment is laid out in r replicates and a component $F_1 F_2^{b_2} \cdots F_g^{b_g}$ of the factorial effect $F_1 \times F_2 \times \cdots \times F_g$ is confounded in r^* of these, then the loss of information on any treatment contrast belonging to this component is r^*/r, or equivalently, the efficiency factor for any such contrast equals $(r - r^*)/r$.

Components of the form $F_1 F_2^{b_2} \cdots F_g^{b_g}$ are, however, essentially mathematical tools for constructing confounded designs and lack direct statistical interpretation. As a result, efficiency factors for treatment contrasts belonging to these components, as indicated above, are of rather limited statistical interest. On the other hand, with quantitative factors, attention is typically focused from a statistical perspective on *natural treatment contrasts*, such as the linear $\times$ linear $\times$ linear, linear $\times$ linear $\times$ quadratic, etc. in the context of a three-factor interaction. Thus it is important to know the efficiency factors for these natural contrasts in a partially confounded design. For example, if in a partially confounded 3^3 factorial design, the four components $F_1F_2F_3, F_1F_2F_3^2, F_1F_2^2F_3$ and $F_1F_2^2F_3^2$ of the three-factor interaction are confounded in r_1, r_2, r_3 and r_4 replicates respectively, then what can be said about the efficiency factors for the aforesaid natural treatment contrasts belonging to this interaction? Even though this is of compelling interest to a statistician, it seems that this point has not been addressed in the existing literature, even at an advanced level. We aim at filling this gap.

Given the unified treatment of partial confounding for $s(\ge 3)$-level factorials in the literature, the reader may wonder at this stage why we are focusing specifically on three-level factorials instead of looking at s-level factorials in general, where $s \ge 3$ is a prime or prime power. This is because, some what counter intuitively, there is an intrinsic difference between three-level factorials and $s(> 3)$-level factorials for the problem considered here. In the next section, this difference is indicated and we will return to this point in more detail in Section 4. It will be seen that three-level factorials allow more comprehensive results than the $s(> 3)$-level ones do. In a sense, this is reassuring because typically the former are of much more practical interest than the latter.

2. Representation for contrasts and a useful result

In the context of a 3^n factorial experiment involving the factors $F_1, \ldots, F_n$, consider a component $F_1F_2^{b_2} \cdots F_g^{b_g}$ of the factorial effect $F_1 \times F_2 \times \cdots \times F_g$. In order to study the interplay between contrasts belonging to $F_1F_2^{b_2} \cdots F_g^{b_g}$ and what we have called natural contrasts here, we express these contrasts in a compact notation. Let $\tau(\boldsymbol{x})$ denote the treatment effect for the treatment combination $\boldsymbol{x} = x_1 \ldots x_n$, and $\boldsymbol{\tau}$ denote the $v \times 1$ vector with elements $\tau(\boldsymbol{x})$, arranged lexicographically, where $v = 3^n$ is the total number of treatment combinations. For example, if $n = 2$ then

$$\boldsymbol{\tau} = (\tau(00), \tau(01), \tau(02), \tau(10), \tau(11), \tau(12), \tau(20), \tau(21), \tau(22))',$$

with the prime denoting transposition.

We first present an expression for a complete set of orthonormal treatment contrasts belonging to $F_1F_2^{b_2} \cdots F_g^{b_g}$. Recall that the treatment contrasts belonging to this component are those among the three sets $V_j(\boldsymbol{b}),\ j = 0, 1, 2$, as shown in (1). Let $A(\boldsymbol{b})$ be a $3 \times v$ matrix with jth row representing the indicator function of $V_j(\boldsymbol{b})$, i.e., $A(\boldsymbol{b})$ is a matrix, with rows indexed by 0, 1, 2, and columns indexed by the lexicographically arranged treatment combinations, such that the $(j, \boldsymbol{x})$th element of $A(\boldsymbol{b})$ equals 1 if $\boldsymbol{x} \in V_j(\boldsymbol{b})$, and 0, otherwise. For example, if $n = 2$ and we are considering the component $F_1F_2^2$ of the interaction $F_1 \times F_2$, then $b_2 = 2$,

$$V_0(\boldsymbol{b}) = \{00, 11, 22\},\ V_1(\boldsymbol{b}) = \{02, 10, 21\},\ V_2(\boldsymbol{b}) = \{01, 12, 20\},$$

and

$$A(\boldsymbol{b}) = \begin{bmatrix} 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 1 & 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \end{bmatrix}.$$

In general, since the sets $V_j(\boldsymbol{b}),\ j = 0, 1, 2$, are disjoint and each of them has cardinality 3^{n-1}, we have

$$A(\boldsymbol{b})A(\boldsymbol{b})' = 3^{n-1}I_3,\ A(\boldsymbol{b})\mathbf{1}_v = 3^{n-1}\mathbf{1}_3,\ \mathbf{1}_3'A(\boldsymbol{b}) = \mathbf{1}_v', \tag{2}$$

where for a positive integer a, $\mathbf{1}_a$ is the $a \times 1$ vector of ones and I_a is the identity matrix of order a.

A complete set of orthonormal treatment contrasts belonging to $F_1F_2^{b_2} \cdots F_g^{b_g}$ is now given by $H(\boldsymbol{b})\boldsymbol{\tau}$, where

$$H(\boldsymbol{b}) = LA(\boldsymbol{b}), \tag{3}$$

L being any 2×3 matrix so chosen that

$$H(\boldsymbol{b})H(\boldsymbol{b})' = I_2 \ \text{ and } \ H(\boldsymbol{b})\mathbf{1}_v = \mathbf{0}. \tag{4}$$

In view of (2)–(4), then L must satisfy

$$LL' = 3^{-(n-1)} I_2,\ L\mathbf{1}_3 = \mathbf{0}. \tag{5}$$

Even though a matrix L satisfying (5) is non-unique, our results do not depend on the particular choice of L as long as (5) is satisfied.

Turning now to the natural contrasts introduced in Section 1, let

$$P = \begin{bmatrix} \frac{-1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{6}} & \frac{-2}{\sqrt{6}} & \frac{1}{\sqrt{6}} \end{bmatrix}. \tag{6}$$

The two rows of P, say $\boldsymbol{p}_1'$ and $\boldsymbol{p}_2'$, correspond to the linear and quadratic components of any three-level factor and, as a result, natural contrasts belonging to the factorial effect $F_1 \times F_2 \times \cdots \times F_g$ are of the form $\boldsymbol{c}'\boldsymbol{\tau}$, where

$$\boldsymbol{c} = \boldsymbol{c}_1 \otimes \boldsymbol{c}_2 \otimes \cdots \otimes \boldsymbol{c}_g \otimes \mathbf{1}_3 \otimes \cdots \otimes \mathbf{1}_3. \tag{7}$$

In (7), each $\boldsymbol{c}_i$ equals either $\boldsymbol{p}_1$ or $\boldsymbol{p}_2$ (i.e., the transpose of a row of P), $\otimes$ denotes Kronecker product, and $\mathbf{1}_3$ appears $n - g$ times (*cf.* Gupta and Mukerjee (1989, Ch. 2)). For instance, if $n = 3$ then $\boldsymbol{c}'\boldsymbol{\tau}$, with $\boldsymbol{c} = \boldsymbol{p}_1 \otimes \boldsymbol{p}_2 \otimes \mathbf{1}_3$, is the linear $\times$ quadratic contrast belonging to the interaction $F_1 \times F_2$.

We now have the following result which has been proved in the appendix.

Theorem 1. *If $H(\boldsymbol{b})$ and $\boldsymbol{c}$ are as given by (3) and (7), then*

$$\frac{\boldsymbol{c}'H(\boldsymbol{b})'H(\boldsymbol{b})\boldsymbol{c}}{\boldsymbol{c}'\boldsymbol{c}} = \frac{1}{2^{g-1}}.$$

Theorem 1 will play a crucial role in studying the efficiency factors for the natural contrasts in a partially confounded 3^n factorial design. Such a neat result does not hold for general $s(> 3)$-level factorials, where the counterpart of the ratio considered in Theorem 1 depends on the specific factorial effect component $F_1 F_2^{b_2} \cdots F_g^{b_g}$ and the specific natural contrast $\boldsymbol{c}'\boldsymbol{\tau}$. Remark A.1 in the appendix explains where the arguments leading to Theorem 1 break down for general $s > 3$.

3. Efficiency factors for natural contrasts

With reference to a partially confounded 3^n factorial design, consider any particular factorial effect, say $F_1 \times F_2 \times \cdots \times F_g$, as represented by the 2^{g-1} components $F_1 F_2^{b_2} \cdots F_g^{b_g}$, where $b_i = 1$ or 2 for each i, $2 \le i \le g$. For notational simplicity, let $q = 2^{g-1}$ and denote these components by $C_1, \ldots, C_q$. Let H_j denote the $H(\boldsymbol{b})$ matrix (see (3)) for C_j, so that $H_j\boldsymbol{\tau}$ gives a complete set of orthonormal treatment contrasts belonging to C_j, $1 \le j \le q$. Thus, for example, the interaction $F_1\times F_2\times F_3$ is represented by $q=4$ components, $C_1=F_1F_2F_3,\ C_2=F_1F_2F_3^2,\ C_3=F_1F_2^2F_3$ and $C_4=F_1F_2^2F_3^2$, and $H_1,\ldots,H_4$ are the $H(\boldsymbol{b})$ matrices for $C_1,\ldots,C_4$, respectively. In view of (4) and the fact that treatment contrasts belonging to different components are mutually orthogonal, we have

$$H_jH_j'=I_2,\ \ H_jH_k'=\mathbf{0},\ 1\le j,k\le q,\ j\ne k. \tag{8}$$

Now, suppose the partially confounded factorial design is laid out in r replicates. Let the components $C_1,\ldots,C_q$ of the factorial effect $F_1\times F_2\times\cdots\times F_g$ be confounded in $r_1,\ldots,r_q$ (≥ 0) replicates, respectively. The possibility of more than one of $C_1,\ldots,C_q$ being confounded in the same replicate is allowed here. However, we assume that $r_j<r,\ 1\le j\le q$, so as to ensure that none of $C_1,\ldots,C_q$ is completely confounded; otherwise, not all contrasts belonging to $F_1\times\cdots\times F_g$ remain estimable, which is unwarranted if this factorial effect is of interest. Then, writing $H_j\hat{\boldsymbol{\tau}}$ for the best linear unbiased estimator (BLUE) of $H_j\boldsymbol{\tau}$, standard arguments yield

$$\mathrm{Disp}(H_j\hat{\boldsymbol{\tau}})=\frac{\sigma^2}{r-r_j}I_2,\ \ \mathrm{Cov}(H_j\hat{\boldsymbol{\tau}},H_k\hat{\boldsymbol{\tau}})=0, 1\le j,k\le q, j\ne k, \tag{9}$$

where σ^2 is the constant error variance, $\mathrm{Disp}(\cdot)$ stands for the dispersion matrix and Cov (,) denotes the covariance. The truth of (9) is evident from (8) noting that $H_j\hat{\boldsymbol{\tau}}$ is the mean of the corresponding observational contrasts from the $r-r_j$ replicates where component C_j remains unconfounded. We are now in a position to present the main result of this paper.

Theorem 2. *Let $\boldsymbol{c}'\boldsymbol{\tau}$ be any natural contrast belonging to the factorial effect $F_1\times\cdots\times F_g$, where $\boldsymbol{c}$ is given by (7). Then the efficiency factor for $\boldsymbol{c}'\boldsymbol{\tau}$ is given by*

$$\mathrm{Eff}(\boldsymbol{c})=\left(\frac{1}{q}\sum_{j=1}^{q}\frac{r}{r-r_j}\right)^{-1}.$$

Proof. Define the matrix H, with $2q$ rows, as

$$H=(H_1'\ H_2'\ \cdots H_q')'.$$

Since H incorporates the matrix H_j corresponding to every component C_j of $F_1\times\cdots\times F_g$, the rows of H span the coefficient vectors of all treatment contrasts belonging to this factorial effect. In particular, for the natural contrast $\boldsymbol{c}'\boldsymbol{\tau}$ under consideration here, $\boldsymbol{c}'=\boldsymbol{\xi}'H$ for some vector $\boldsymbol{\xi}$. As $HH'=I_{2q}$ by (8), this implies that $\boldsymbol{c}'H'=\boldsymbol{\xi}'$, i.e., $\boldsymbol{c}'=\boldsymbol{c}'H'H=\sum_{j=1}^{q}\boldsymbol{c}'H_j'H_j$, so that the BLUE of $\boldsymbol{c}'\boldsymbol{\tau}$ is given by $\boldsymbol{c}'\hat{\boldsymbol{\tau}}=\sum_{j=1}^{q}\boldsymbol{c}'H_j'H_j\hat{\boldsymbol{\tau}}$. Consequently, by (9) and Theorem 1, the variance of this BLUE is

$$\mathrm{Var}(\boldsymbol{c}'\hat{\boldsymbol{\tau}})=\sigma^2\sum_{j=1}^{q}\frac{1}{r-r_j}\boldsymbol{c}'H_j'H_j\boldsymbol{c}=\sigma^2\frac{\boldsymbol{c}'\boldsymbol{c}}{q}\sum_{j=1}^{q}\frac{1}{r-r_j}, \tag{10}$$

because $q = 2^{g-1}$ and each H_j equals some $H(\boldsymbol{b})$.

On the other hand, for an unconfounded (complete block) 3^n factorial design in r replicates, $\mathrm{Var}(\boldsymbol{c}'\hat{\boldsymbol{\tau}}) = \sigma_1^2(\boldsymbol{c}'\boldsymbol{c})/r$, where σ_1^2 is the error variance in such a complete block design. The result now follows from (10). $\square$

Remark 1. Clearly, the efficiency factor for any treatment contrast belonging to the component C_j of the factorial effect $F_1 \times \cdots \times F_g$ equals $(r - r_j)/r$, i.e., the proportion of replicates where C_j remains unconfounded. Theorem 2 shows that the efficiency factor for *every* natural contrast belonging to this factorial effect equals the simple harmonic mean of these component-wise efficiency factors. Thus given r and $r_1 + \cdots + r_q$, the efficiency factors for all such natural contrasts are *simultaneously* maximized if and only if $r_1, \ldots, r_q$ are as nearly equal as possible, i.e., if and only if no two of $r_1, \ldots, r_q$ differ by more than unity. It will be seen in the next section that this kind of simultaneous maximization of efficiency factors for all natural contrasts belonging to the same factorial effect is not possible for $s(> 3)$-level factorials. $\square$

Example 1. Consider a partially confounded 3^3 factorial design such that every replicate consists of nine blocks, each of size three. The confounding pattern is one in which there are
(i) r_1 replicates where the components $F_1F_2^2, F_1F_3^2, F_2F_3^2, F_1F_2F_3$ are confounded,
(ii) r_2 replicates where the components $F_1F_2^2, F_1F_3, F_2F_3, F_1F_2F_3^2$ are confounded,
(iii) r_3 replicates where the components $F_1F_2, F_1F_3^2, F_2F_3, F_1F_2^2F_3$ are confounded,
(iv) r_4 replicates where the components $F_1F_2, F_1F_3, F_2F_3^2, F_1F_2^2F_3^2$ are confounded.

The total number of replicates is $r = r_1 + \cdots + r_4$. Clearly, each main effect contrast has efficiency factor 1, while by Theorem 2, the efficiency factor for any natural contrast belonging to an interaction equals, say,

$$\mathrm{Eff}_{12} = \left[\frac{1}{2}\left(\frac{r}{r_1 + r_2} + \frac{r}{r_3 + r_4}\right)\right]^{-1}, \quad \mathrm{Eff}_{13} = \left[\frac{1}{2}\left(\frac{r}{r_1 + r_3} + \frac{r}{r_2 + r_4}\right)\right]^{-1},$$

$$\mathrm{Eff}_{23} = \left[\frac{1}{2}\left(\frac{r}{r_1 + r_4} + \frac{r}{r_2 + r_3}\right)\right]^{-1}, \qquad \mathrm{Eff}_{123} = \left(\frac{1}{4}\sum_{j=1}^{4}\frac{r}{r - r_j}\right)^{-1},$$

according as whether the contrast belongs to $F_1 \times F_2$, $F_1 \times F_3$, $F_2 \times F_3$ or $F_1 \times F_2 \times F_3$, respectively. As noted in Remark 1, all natural contrasts belonging to the same interaction have the same efficiency factor. Note that, given $r = r_1 + \cdots + r_4$, the necessary and sufficient conditions for the maximization of $\mathrm{Eff}_{12}, \mathrm{Eff}_{13}, \mathrm{Eff}_{23}$ and Eff_{123} are given respectively, by
(a) $|r_1 + r_2 - r_3 - r_4| \leq 1$,
(b) $|r_1 + r_3 - r_2 - r_4| \leq 1$,
(c) $|r_1 + r_4 - r_2 - r_3| \leq 1$, and
(d) $|r_j - r_k| \leq 1$ for every $j \neq k$.

For instance, with $r = 3$, these conditions are all met if $r_1 = r_2 = r_3 = 1, r_4 = 0$, while with $r = 4$ or 5, the same happens if $r_1 = \cdots = r_4 = 1$ or $r_1 = r_2 = r_3 = 1, r_4 = 2$, respectively. $\square$

4. Case of $s(> 3)$-level factorials

For a general s-level factorial design, where s is a prime or prime power, it is well-known (Bose, 1947) that any factorial effect, say $F_1 \times F_2 \times \ldots \times F_g$, can be represented via $(s-1)^{g-1}$ components or pencils, each carrying $s-1$ independent treatment contrasts. As in Section 3, denote these components by $C_1, \ldots, C_q$, and let $H_j \boldsymbol{\tau}$ represent a complete set of orthonormal treatment contrasts belonging to C_j, $1 \le j \le q$, where now $q = (s-1)^{g-1}$. Suppose the design in laid out in r replicates and let C_j be confounded in r_j of these. Then for any natural contrast $\boldsymbol{c}'\boldsymbol{\tau}$ belonging to $F_1 \times F_2 \times \cdots \times F_g$, the first equation in (10) continues to hold as before, i.e.,

$$\mathrm{Var}(\boldsymbol{c}'\hat{\boldsymbol{\tau}}) = \sigma^2 \sum_{j=1}^{q} \frac{1}{r - r_j} \boldsymbol{c}' H_j' H_j \boldsymbol{c}. \tag{11}$$

Therefore, as in Theorem 2, the efficiency factor for $\boldsymbol{c}'\boldsymbol{\tau}$ equals

$$\mathrm{Eff}(\boldsymbol{c}) = \left(\sum_{j=1}^{q} \frac{r}{r - r_j} W(\boldsymbol{c}, j) \right)^{-1}, \tag{12}$$

where

$$W(\boldsymbol{c}, j) = \frac{\boldsymbol{c}' H_j' H_j \boldsymbol{c}}{\boldsymbol{c}'\boldsymbol{c}}, \ 1 \le j \le q. \tag{13}$$

Let $H = [H_1' \ H_2' \ \cdots H_q']'$. Since $\boldsymbol{c}' = \boldsymbol{c}' H' H$ as in Theorem 2, then by (13), $\sum_{j=1}^{q} W(\boldsymbol{c}, j) = \boldsymbol{c}' H' H \boldsymbol{c} / \boldsymbol{c}'\boldsymbol{c} = 1$. Hence by (12), $\mathrm{Eff}(\boldsymbol{c})$ is again a harmonic mean of the component-wise efficiency factors $(r - r_j)/r$. But this harmonic mean is now weighted and, in contrast to Theorem 1, the weights $W(\boldsymbol{c}, j)$ depend on $\boldsymbol{c}'\boldsymbol{\tau}$ and C_j, for $s > 3$. So, unlike in Theorem 2, $\mathrm{Eff}(\boldsymbol{c})$ in (12) depends on $\boldsymbol{c}$. As a result, given r and $r_1 + \cdots + r_q$, typically no choice of $r_1, \ldots, r_q$ can simultaneously maximize $\mathrm{Eff}(\boldsymbol{c})$ for all natural contrasts belonging to $F_1 \times F_2 \times \cdots \times F_g$. Rather, one has to proceed separately for each such contrast based on explicit calculation of the $W(\boldsymbol{c}, j)$. We conclude with an example that illustrates these points.

Example 2. Consider a partially confounded 5^2 factorial design such that every replicate confounds a component of the two-factor interaction $F_1 \times F_2$ and hence consists of five blocks, each of size five. For $1 \le j \le 4$, suppose there are r_j replicates where the component $C_j = F_1 F_2^j$ of $F_1 \times F_2$ is confounded. The total number of replicates is $r = r_1 + \cdots + r_4$.

Clearly, then each main effect contrast has efficiency factor 1. We next consider the natural contrasts belonging to $F_1 \times F_2$. Let

$$P = \begin{bmatrix} \frac{-2}{\sqrt{10}} & \frac{-1}{\sqrt{10}} & 0 & \frac{1}{\sqrt{10}} & \frac{2}{\sqrt{10}} \\ \frac{2}{\sqrt{14}} & \frac{-1}{\sqrt{14}} & \frac{-2}{\sqrt{14}} & \frac{-1}{\sqrt{14}} & \frac{2}{\sqrt{14}} \\ \frac{-1}{\sqrt{10}} & \frac{2}{\sqrt{10}} & 0 & \frac{-2}{\sqrt{10}} & \frac{1}{\sqrt{10}} \\ \frac{1}{\sqrt{70}} & \frac{-4}{\sqrt{70}} & \frac{6}{\sqrt{70}} & \frac{-4}{\sqrt{70}} & \frac{1}{\sqrt{70}} \end{bmatrix}.$$

The four rows of P, say $\boldsymbol{p}_1', \boldsymbol{p}_2', \boldsymbol{p}_3'$ and $\boldsymbol{p}_4'$, correspond respectively, to the linear, quadratic, cubic and quartic components of a five-level factor. Hence, as in (7), any natural contrast belonging to $F_1 \times F_2$ is of the form $\boldsymbol{c}'\boldsymbol{\tau}$, where $\boldsymbol{c} = \boldsymbol{p}_k \otimes \boldsymbol{p}_m [= \boldsymbol{c}(km)$, say], for some $1 \leq k, m \leq 4$. For instance, $\boldsymbol{c}(11)'\boldsymbol{\tau}$ is the linear $\times$ linear contrast, $\boldsymbol{c}(32)'\boldsymbol{\tau}$ is the cubic $\times$ quadratic contrast, and so on.

One can now explicitly write down the matrices H_j corresponding to the components $C_j (= F_1 F_2^j)$ in the same manner as in (3), and then employ (13) to calculate the weights $W(\boldsymbol{c}, j)$, for every natural contrast $\boldsymbol{c}'\boldsymbol{\tau}$ and every j, $1 \leq j \leq 4$. These weights, shown in Table 1, depend on $\boldsymbol{c}'\boldsymbol{\tau}$ and j. Hence given $r = r_1 + \cdots + r_4$, no choice of r_1, r_2, r_3, r_4 can simultaneously maximize the efficiency factors for all the natural contrasts $\boldsymbol{c}(km)'\boldsymbol{\tau}$. For example, if $r = r_1 + \cdots + r_4 = 4$, then using the $W(\boldsymbol{c}, j)$ values from Table 1 in (12), the optimal choices of (r_1, r_2, r_3, r_4) which uniquely maximize $\mathrm{Eff}(\boldsymbol{c})$ for various $\boldsymbol{c}$ turn out to be as follows:

(i) $\boldsymbol{c} = \boldsymbol{c}(11), \boldsymbol{c}(13), \boldsymbol{c}(31), \boldsymbol{c}(33)$: optimal $(r_1, r_2, r_3, r_4) = (1, 1, 1, 1)$.
(ii) $\boldsymbol{c} = \boldsymbol{c}(12), \boldsymbol{c}(21), \boldsymbol{c}(22), \boldsymbol{c}(34), \boldsymbol{c}(43), \boldsymbol{c}(44)$: optimal $(r_1, r_2, r_3, r_4) = (0, 2, 2, 0)$.
(iii) $\boldsymbol{c} = \boldsymbol{c}(14), \boldsymbol{c}(23), \boldsymbol{c}(24), \boldsymbol{c}(32), \boldsymbol{c}(41), \boldsymbol{c}(42)$: optimal $(r_1, r_2, r_3, r_4) = (2, 0, 0, 2)$.

Table 1: Weights $W(\boldsymbol{c}, j)$ in Example 2

$\boldsymbol{c}$	$W(\boldsymbol{c}, 1)$	$W(\boldsymbol{c}, 2)$	$W(\boldsymbol{c}, 3)$	$W(\boldsymbol{c}, 4)$
$\boldsymbol{c}(11), \boldsymbol{c}(33)$	0.3000	0.2000	0.2000	0.3000
$\boldsymbol{c}(12), \boldsymbol{c}(21), \boldsymbol{c}(34), \boldsymbol{c}(43)$	0.3571	0.1429	0.1429	0.3571
$\boldsymbol{c}(13), \boldsymbol{c}(31)$	0.2000	0.3000	0.3000	0.2000
$\boldsymbol{c}(14), \boldsymbol{c}(23), \boldsymbol{c}(32), \boldsymbol{c}(41)$	0.1429	0.3571	0.3571	0.1429
$\boldsymbol{c}(22), \boldsymbol{c}(44)$	0.4796	0.0204	0.0204	0.4796
$\boldsymbol{c}(24), \boldsymbol{c}(42)$	0.0204	0.4796	0.4796	0.0204

Thus a clear-cut recommendation about the choice of (r_1, r_2, r_3, r_4) is not possible. One may go by the natural contrasts which are of greater interest than others in a given context – e.g., if those in (i) above are of greatest interest, then taking $(r_1, r_2, r_3, r_4) = (1, 1, 1, 1)$ is sensible. However, this may seriously curtail the best achievable efficiency factors for the contrasts in (ii) and (iii). Thus with $(r_1, r_2, r_3, r_4) = (1, 1, 1, 1)$, the efficiency factor for $\boldsymbol{c}(km)'\boldsymbol{\tau}$, where

$k, m \in \{2,4\}$, will be less than that under the corresponding optimal (r_1, r_2, r_3, r_4) by as much as about 22%.

Other approaches include choosing (r_1, r_2, r_3, r_4) so as to maximize the average or minimum efficiency factor over all natural contrasts, even though the results so obtained will not be as strong as those discussed earlier for three-level designs. $\square$

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Appendix: Proof of Theorem 1

By (6), $PP' = I_2$ and $P\mathbf{1}_3 = \mathbf{0}$. Since each $\boldsymbol{c}_i$ in (7) equals the transpose of a row of P, we get

$$\boldsymbol{c}_i'\boldsymbol{c}_i = 1, \boldsymbol{c}_i'\mathbf{1}_3 = 0, \ 1 \le i \le g. \tag{A.1}$$

We will now prove Theorem 1 through a sequence of lemmas. For each i, write the 3×1 vector $\boldsymbol{c}_i$ explicitly as $\boldsymbol{c}_i = (c_i(0), c_i(1), c_i(2))'$.

Lemma A.1. *For $1 \le i \le g$ and any fixed integers $j_0, j_1, j_2 \in \{0,1,2\}, \ j_0 \neq 0$,*

$$\begin{aligned} \sum_{j=0}^{2} c_i((j-j_1)/j_0)c_i((j-j_2)/j_0) &= 1, \text{ if } j_1 = j_2, \\ &= -\frac{1}{2}, \text{ otherwise,} \end{aligned}$$

where $(j-j_1)/j_0$ and $(j-j_2)/j_0$ are reduced mod 3.

Proof. As j equals 0, 1 and 2, so does each of $(j-j_1)/j_0$ and $(j-j_2)/j_0$ (mod 3), possibly in a different order. Hence if $j_1 = j_2$, then the sum under consideration equals $\boldsymbol{c}_i'\boldsymbol{c}_i$ and the result follows from (A.1). On the other hand, for any $j_1 \neq j_2$ and $j_0 \neq 0$, one can check that

$$\begin{aligned} \sum_{j=0}^{2} c_i((j-j_1)/j_0)c_i((j-j_2)/j_0) &= c_i(0)c_i(1) + c_i(0)c_i(2) + c_i(1)c_i(2) \qquad \text{(A.2)} \\ &= \tfrac{1}{2}\{(\boldsymbol{c}_i'\mathbf{1}_3)^2 - \boldsymbol{c}_i'\boldsymbol{c}_i\} = -\tfrac{1}{2}, \end{aligned}$$

using (A.1) again. $\square$

With reference to the factorial effect component $F_1F_2^{b_2}\ldots F_g^{b_g}$ considered in Theorem 1, write $b_1 = 1$. For $1 \le u \le g$, $j \in \{0,1,2\}$, let

$$\Omega(u) = \{\boldsymbol{x}(u) = x_1 \ldots x_u : x_i = 0, 1 \text{ or } 2, \ 1 \le i \le u\}, \tag{A.3}$$

$$\Gamma(u,j) = \{\boldsymbol{x}(u) = x_1 \ldots x_u : \boldsymbol{x}(u) \in \Omega(u) \text{ and } b_1x_1 + \cdots + b_ux_u = j \pmod 3\}, \tag{A.4}$$

and

$$\phi_u = \sum_{j=0}^{2} \left[\sum_{\boldsymbol{x}(u) \in \Gamma(u,j)} \left\{ \prod_{i=1}^{u} c_i(x_i) \right\} \right]^2, \tag{A.5}$$

where the second sum in (A.5) is over $\boldsymbol{x}(u) \in \Gamma(u,j)$. Then the following lemma holds.

Lemma A.2. *For* $1 \le u \le g$, $\phi_u = (3/2)^{u-1}$.

Proof. For $u = 1$, the result is evident from (A.1), (A.4), (A.5) and the fact that $b_1 = 1$. Next let $u \ge 2$. As $b_u \ne 0$, then by (A.3) and (A.4), $\Gamma(u,j)$ consists of u-tuples $\boldsymbol{x}(u)(= x_1 \ldots x_u)$ satisfying

$$\boldsymbol{x}(u-1)(= x_1 \ldots x_{u-1}) \in \Omega(u-1) \;\text{ and }\; x_u = (j - b[\boldsymbol{x}(u-1)])/b_u \bmod 3,$$

where

$$b[\boldsymbol{x}(u-1)] = b_1x_1 + \cdots + b_{u-1}x_{u-1} \bmod 3. \tag{A.6}$$

Therefore, by (A.5),

$$\phi_u = \sum_{j=0}^{2} \left[\sum_{\boldsymbol{x}(u-1) \in \Omega(u-1)} \left\{ \prod_{i=1}^{u-1} c_i(x_i) \right\} c_u((j - b[\boldsymbol{x}(u-1)])/b_u) \right]^2. \tag{A.7}$$

But by (A.3), (A.4), $\Omega(u-1)$ is the union of $\Gamma(u-1,k)$, $k \in \{0,1,2\}$, and by (A.6), $b[\boldsymbol{x}(u-1)] = k$ for $\boldsymbol{x}(u-1) \in \Gamma(u-1,k)$. Hence (A.7) yields

$$\begin{aligned}
\phi_u &= \sum_{j=0}^{2} \left[\sum_{k=0}^{2} \sum_{\boldsymbol{x}(u-1) \in \Gamma(u-1,k)} \left\{ \prod_{i=1}^{u-1} c_i(x_i) \right\} c_u((j-k)/b_u) \right]^2 \\
&= \sum_{j=0}^{2} \sum_{k=0}^{2} \sum_{m=0}^{2} \sum_{\boldsymbol{x}(u-1) \in \Gamma(u-1,k)} \sum_{\boldsymbol{y}(u-1) \in \Gamma(u-1,m)} \left\{ \prod_{i=1}^{u-1} c_i(x_i)c_i(y_i) \right\} \times \\
&\quad c_u((j-k)/b_u)c_u((j-m)/b_u),
\end{aligned} \tag{A.8}$$

where the sum over $\boldsymbol{y}(u-1)(= y_1 \ldots y_{u-1})$ is analogous to that over $\boldsymbol{x}(u-1)$. Since by Lemma A.1,

$$\sum_{j=0}^{2} c_u((j-k)/b_u)c_u((j-m)/b_u) = \frac{3}{2}\delta_{km} - \frac{1}{2},$$

where δ_{km} equals 1 if $k = m$, and 0 otherwise, from (A.8) we get

$$\begin{aligned}
\phi_u &= \sum_{k=0}^{2}\sum_{m=0}^{2}\sum_{\boldsymbol{x}(u-1)\in\,\Gamma(u-1,k)}\ \sum_{\boldsymbol{y}(u-1)\in\,\Gamma(u-1,m)}\left\{\prod_{i=1}^{u-1} c_i(x_i)c_i(y_i)\right\}\times \\
&\quad \left(\tfrac{3}{2}\delta_{km}-\tfrac{1}{2}\right) \\
&= \tfrac{3}{2}\sum_{k=0}^{2}\sum_{\boldsymbol{x}(u-1)\in\,\Gamma(u-1,k)}\ \sum_{\boldsymbol{y}(u-1)\in\,\Gamma(u-1,k)}\left\{\prod_{i=1}^{u-1} c_i(x_i)c_i(y_i)\right\} \\
&\quad -\tfrac{1}{2}\sum_{k=0}^{2}\sum_{m=0}^{2}\sum_{\boldsymbol{x}(u-1)\in\,\Gamma(u-1,k)}\ \sum_{\boldsymbol{y}(u-1)\in\,\Gamma(u-1,m)}\left\{\prod_{i=1}^{u-1} c_i(x_i)c_i(y_i)\right\} \qquad \text{(A.9)} \\
&= \tfrac{3}{2}\sum_{k=0}^{2}\left[\sum_{\boldsymbol{x}(u-1)\in\,\Gamma(u-1,k)}\left\{\prod_{i=1}^{u-1} c_i(x_i)\right\}\right]^2 \\
&\quad -\tfrac{1}{2}\left[\sum_{k=0}^{2}\sum_{\boldsymbol{x}(u-1)\in\,\Gamma(u-1,k)}\left\{\prod_{i=1}^{u-1} c_i(x_i)\right\}\right]^2 \\
&= \tfrac{3}{2}\phi_{u-1}-\tfrac{1}{2}\left[\sum_{\boldsymbol{x}(u-1)\in\,\Omega(u-1)}\left\{\prod_{i=1}^{u-1} c_i(x_i)\right\}\right]^2,
\end{aligned}$$

recalling (A.5) and the fact that the union of $\Gamma(u-1,k), k \in \{0,1,2\}$, equals $\Omega(u-1)$. Now, by (A.1) and (A.3),

$$\sum_{\boldsymbol{x}(u-1)\in\,\Omega(u-1)}\left\{\prod_{i=1}^{u-1} c_i(x_i)\right\} = \sum_{x_1=0}^{2}\cdots\sum_{x_{u-1}=0}^{2}\left\{\prod_{i=1}^{u-1} c_i(x_i)\right\} = \prod_{i=1}^{u-1}(\boldsymbol{c}_i'\boldsymbol{1}_3) = 0.$$

Therefore, (A.9) yields $\phi_u = \frac{3}{2}\phi_{u-1}$, for $u \geq 2$. Since $\phi_1 = 1$, the result now follows using a recursive argument. □

Lemma A.3. *If $A(\boldsymbol{b})$ is as defined in Section 2 and $\boldsymbol{c}$ is given by (7), then*

$$\boldsymbol{c}'A(\boldsymbol{b})'A(\boldsymbol{b})\boldsymbol{c} = 3^{2(n-g)}(3/2)^{g-1}.$$

Proof. By (1) and (A.4), the set $V_j(\boldsymbol{b})$ consists of n-tuples $\boldsymbol{x}(= x_1 \dots x_n)$ such that $\boldsymbol{x}(g)(= x_1 \dots x_g) \in \Gamma(g,j)$ and $x_i \in \{0,1,2\}$, $g+1 \leq i \leq n$. Hence from (7) and the definition of $A(\boldsymbol{b})$, the jth element of $A(\boldsymbol{b})\boldsymbol{c}$ is given by

$$\sum_{\boldsymbol{x}\in\,V_j(\boldsymbol{b})}\left\{\prod_{i=1}^{g} c_i(x_i)\right\} = 3^{n-g}\sum_{\boldsymbol{x}(g)\in\,\Gamma(g,j)}\left\{\prod_{i=1}^{g} c_i(x_i)\right\},\ j = 0,1,2.$$

Thus recalling (A.5), $\boldsymbol{c}'A(\boldsymbol{b})'A(\boldsymbol{b})\boldsymbol{c} = 3^{2(n-g)}\phi_g$, and the result follows invoking Lemma A.2. □

Proof of Theorem 1. By (7) and (A.1),

$$\boldsymbol{c}'\boldsymbol{c} = 3^{n-g}, \quad \boldsymbol{c}'\mathbf{1}_v = 0. \tag{A.10}$$

Also, by (5), the 3×3 matrix

$$\begin{bmatrix} 3^{-1/2}\mathbf{1}_3' \\ 3^{(n-1)/2}L \end{bmatrix}$$

is orthogonal. Therefore, $L'L = 3^{-(n-1)}(I_3 - \frac{1}{3}\mathbf{1}_3\mathbf{1}_3')$. Consequently, by (2) and (3), $H(\boldsymbol{b})'H(\boldsymbol{b}) = 3^{-(n-1)}\{A(\boldsymbol{b})'A(\boldsymbol{b}) - \frac{1}{3}\mathbf{1}_v\mathbf{1}_v'\}$. Hence invoking (A.10) and Lemma A.3,

$$\boldsymbol{c}'H(\boldsymbol{b})'H(\boldsymbol{b})\boldsymbol{c} = 3^{-(n-1)}\boldsymbol{c}'A(\boldsymbol{b})'A(\boldsymbol{b})\boldsymbol{c} = 3^{n-g}/2^{g-1} = 2^{-(g-1)}(\boldsymbol{c}'\boldsymbol{c}),$$

and the result follows. □

Remark A.1. Theorem 1 cannot be extended to general s-level factorials, where $s > 3$ is a prime or prime or prime power, because Lemma A.1, which is crucial in proving this theorem, allows no such extension. To see this, take for example, $s = 5$ and consider the vector

$$\tilde{\boldsymbol{c}} = (\tilde{c}(0), \tilde{c}(1), \ldots, \tilde{c}(4))' = \frac{1}{\sqrt{10}}(-2, -1, 0, 1, 2),$$

which corresponds to the normalized linear component of a five-level factor. As in (A.1), $\tilde{\boldsymbol{c}}'\tilde{\boldsymbol{c}} = 1$ and $\tilde{\boldsymbol{c}}'\mathbf{1}_5 = 0$. But unlike in Lemma 1, the value of the sum $\sum_{j=0}^{4} \tilde{c}((j - j_1)/j_0)\tilde{c}((j - j_2)/j_0)$, where $j_0, j_1, j_2 \in \{0, 1, 2, 3, 4\}$, $j_0 \neq 0$ and $(j - j_1)/j_0$ and $(j - j_2)/j_0$ are reduced mod 5, depends on the specific choice of j_1 and j_2 when $j_1 \neq j_2$; e.g., with $j_0 = 1$, this sum equals 0 for $j_1 = 0$ and $j_2 = 1$, and $-\frac{1}{2}$ for $j_1 = 0$ and $j_2 = 2$. This happens because a counterpart of (A.2) cannot hold in general for $s > 3$, since the two sides of such a counterpart would involve s and $s(s-1)/2$ terms, while $s < s(s-1)/2$ for $s > 3$. □

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