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Efficiency Factors for Natural Contrasts

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Factorial experiments are an extremely important class of experiments with applications in many diverse areas. The literature on factorial experiments is very rich. The typical scenario in such experiments is that there is an output variable which depends on certain input variables, called *factors*. Each factor has two or more settings, these being called *levels*. A combination of the levels of all the factors is called a *treatment combination* and these treatment combinations are the treatments of the experiment. The interest centers around the effects of individual factors, called *main effects* and their possible inter-dependence, measured by *interactions*. A main effect or an interaction is called a *factorial effect*. Clearly, the total number of factorial effects in a factorial experiment involving n factors is $2^n - 1$.

A factorial experiment is called symmetric if all the factors have the same number of levels. With n factors each at $s \geq 2$ levels, a symmetric factorial experiment is denoted as an s^n experiment. In the context of symmetric factorial experiments, the notion of pencils, introduced by Bose (1947) plays a very important role. Consider an s^n factorial experiment involving the factors $F_1, \ldots, F_n$, where s is a prime or a prime power. The s levels of each factor may then be coded as $\rho_0, \rho_1, \ldots, \rho_{s-1}$, the elements of $GF(s)$, the Galois field of order s. As a result, the s^n treatment combinations can be represented by the s^n vectors of the form $\boldsymbol{z} = (z_1, \ldots, z_n)'$, where $z_i \in GF(s), 1 \leq i \leq n$. Equivalently, the treatment combinations are identified with the points of the finite n-dimensional affine geometry, $EG(n, s)$. Let $\mathcal{Z}$ denote the set of s^n treatment combinations, or equivalently, the set of points of $EG(n, s)$. For any $\boldsymbol{z} \in \mathcal{Z}$, let the effect of a treatment combination $\boldsymbol{z}$ be denoted by $\tau(\boldsymbol{z})$. Throughout, primes will denote transposition.

Let $\boldsymbol{a} = (a_1, \ldots, a_n)'$ be a fixed non-null vector over $GF(s)$. Then, it is easy to see that each of the sets

$$V_j(\boldsymbol{a}) = \{\boldsymbol{z} : \boldsymbol{z} \in \mathcal{Z}, \boldsymbol{a}'\boldsymbol{z} = \rho_j\}, 0 \leq j \leq s-1,$$

has cardinality s^{n-1} and, that these sets provide a partition of $\mathcal{Z}$. These sets are collectively called a parallel pencil of $(n-1)$-flats of $EG(n, s)$ and hence $\boldsymbol{a}$ itself is said to represent a *pencil*.

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Let

$$S_j(\boldsymbol{a}) = \sum_{\boldsymbol{z} \in V_j(\boldsymbol{a})} \tau(\boldsymbol{z}),\ 0 \le j \le s-1.$$

Then a treatment contrast is said to belong to the pencil $\boldsymbol{a}$ if it is of the form

$$L = \sum_{j=0}^{s-1} \ell_j S_j(\boldsymbol{a}),$$

where $\ell_0, \ldots, \ell_{s-1}$ are real numbers, not all zeros, satisfying $\sum_{j=0}^{s-1} \ell_j = 0$. Thus there are $s-1$ linearly independent treatment contrasts belonging to the pencil $\boldsymbol{a}$. The following are some important observations regarding the pencils, defined above:

• Two pencils, say $\boldsymbol{a}$ and $\boldsymbol{a}^*$, satisfying $\boldsymbol{a}^* = \lambda \boldsymbol{a}$ for some $\lambda (\neq 0) \in GF(s)$ induce the same partition of $\mathcal{Z}$. As such, pencils with proportional entries are considered identical and thus, there are $(s^n - 1)/(s-1)$ distinct pencils, no two of which are proportional.
• For any two distinct pencils $\boldsymbol{a}, \boldsymbol{b}$ and $0 \le j, j' \le s-1$, $|V_j(\boldsymbol{a}) \cap V_{j'}(\boldsymbol{b})| = s^{n-2}$, and
• treatment contrasts belonging to distinct pencils are mutually orthogonal.

Consider a typical factorial effect $F_{i_1} \times F_{i_2} \times \cdots \times F_{i_g}$. A pencil $\boldsymbol{a} = (a_1, \ldots a_n)'$ is said to belong to this factorial effect provided $a_i \neq 0$, if $i = i_1, \ldots, i_g$, and $a_i = 0$, otherwise. One can then show that

(a) there are $(s-1)^{g-1}$ distinct pencils belonging to $F_{i_1} F_{i_2} \cdots F_{i_g}$, and
(b) each of these pencils carry $s-1$ linearly independent contrasts.

This accounts for a complete set of $(s-1)^g$ linearly independent contrasts belonging to $F_{i_1} \times F_{i_2} \times \cdots \times F_{i_g}$. For a summary of the important results in Bose (1947), see Dey and Mukerjee (2003).

There is another way to write down the contrasts belonging to factorial effects. Let Ω be the set of all binary n-tuples and $\Omega^* = \Omega \setminus \{0, 0, \ldots, 0\}$. It is easy to see that there is a 1–1 correspondence between Ω^* and the set of all factorial effects in the following sense.
• A factorial effect $F_{i_1} \ldots F_{i_g} (1 \le i_1 < \ldots < i_g \le n; 1 \le g \le n)$ corresponds to the element $\boldsymbol{x} = x_1 x_2 \ldots x_n$ of Ω^* such that $x_{i_1} = \ldots = x_{i_g} = 1$ and $x_u = 0$ for $u \neq i_1, \ldots, i_g$.
• Thus the $2^n - 1$ factorial effects may be represented by $F^{\boldsymbol{x}}, \boldsymbol{x} \in \Omega^*$.

For instance, if $n = 3$, then $\Omega^* = \{001, 010, 011, 100, 101, 110, 111\}$. The effect F^{100} represents the main effect of the first factor, F^{110} represents the 2-factor interaction of the first two factors, and so on.

Consider a symmetric factorial, s^n. Let $\mathbf{1}_s$ denote an $s \times 1$ vector of all ones and, for $1 \le i \le n$, let P_i be an $(s-1) \times s$ matrix such that

$$\begin{pmatrix} s^{-\frac{1}{2}}\mathbf{1}_s' \\ P_i \end{pmatrix}$$

is an orthogonal matrix.

For a pair of matrices $E = (e_{ij})$ and F, of orders $s \times t$ and $p \times q$, respectively, let $E \otimes F = (e_{ij}F)$ denote their tensor (Kronecker) product and for $\boldsymbol{x} \in \Omega^*$, let $\alpha(\boldsymbol{x}) = \prod_{i=1}^{n}(s-1)^{x_i}$. Note that $\alpha(\boldsymbol{x})$ is the number of linearly independent treatment contrasts belonging to the factorial effect $F^{\boldsymbol{x}}, \boldsymbol{x} \in \Omega^*$.

For each $\boldsymbol{x} = (x_1, \ldots, x_n) \in \Omega$, define the $\alpha(\boldsymbol{x}) \times s^n$ matrix

$$P^{\boldsymbol{x}} = P_1^{x_1} \otimes \cdots \otimes P_n^{x_n},$$

where for $1 \le i \le n$,

$$P_i^{x_i} = \begin{cases} s^{-1/2}\mathbf{1}_s' & \text{if} \quad x_i = 0 \\ P_i & \text{if} \quad x_i = 1. \end{cases}$$

Then one can show that for each $\boldsymbol{x}, \boldsymbol{y} \in \Omega^*, \boldsymbol{x} \neq \boldsymbol{y}$,

- (a) $P^{\boldsymbol{x}}(P^{\boldsymbol{x}})' = I_{\alpha(\boldsymbol{x})}$, and
- (b) $P^{\boldsymbol{x}}(P^{\boldsymbol{y}})' = \mathbf{O}$ (a null matrix).

By (a) above, $\text{Rank}(P^{\boldsymbol{x}}) = \alpha_{\boldsymbol{x}}$, which equals the number of linearly independent contrasts belonging to $F^{\boldsymbol{x}}$. Thus for each $\boldsymbol{x} \in \Omega^*$, the elements of $P^{\boldsymbol{x}}\boldsymbol{\tau}$ represent a *complete set* of orthonormal treatment contrasts belonging to the effect $F^{\boldsymbol{x}}$, where $\boldsymbol{\tau}$ denotes the $v \times 1$ vector with elements $\tau(\boldsymbol{z})$, arranged lexicographically and v is the total number of treatment combinations. Also by part (b), contrasts belonging to different factorial effects are mutually orthogonal. These orthonormal treatment contrasts are different from the contrasts represented by pencils. In particular, if one chooses the rows of the matrix P_i with entries as the orthogonal polynomial coefficients (suitably normalized), we get a set of contrasts, which we shall call as *natural contrasts.*

We now restrict attention to a 3^n factorial experiment (i.e., $s = 3$) involving n factors, $F_1, \ldots, F_n$ each at three levels, coded as 0, 1,2. There are

2^g independent treatment contrasts belonging to a factorial effect $F_1 \times F_2 \times \cdots \times F_g, 1 \leq g \leq n$, represented via 2^{g-1} components or, pencils $F_1F_2^{b_2} \cdots F_g^{b_g}$, where b_i =1 or 2 for each i, such that any component $F_1F_2^{b_2} \cdots F_g^{b_g}$ accounts for two independent contrasts.

These contrasts are those among the three mutually exclusive and exhaustive sets of treatment combinations, given by

$$V_j(\boldsymbol{b}) = \{\boldsymbol{z} = z_1 \ldots z_n : z_1 + \sum_{j=2}^{g} b_j z_j = j \bmod 3\}, j = 0, 1, 2,$$

where $\boldsymbol{b} = (1, b_2, \ldots, b_g)$ and $\boldsymbol{z} = (z_1 \ldots z_n)$ is a typical treatment combination. These components, which are equivalent to pencils, are called *orthogonal components.*

Example 1. Consider a 3^3 experiment involving the factors F_1, F_2 and F_3. The orthogonal components belonging to the 3-factor interaction effect $F_1 \times F_2 \times F_3$ are $F_1F_2F_3,\ F_1F_2F_3^2,\ F_1F_2^2F_3$ and $F_1F_2^2F_3^2$. The sets $V_j(\boldsymbol{b})$ for the component $F_1F_2F_3^2$ are

$$\begin{aligned} V_0(112) &= \{000, 011, 022, 101, 112, 120, 202, 210, 221\}, \\ V_1(112) &= \{002, 010, 021, 100, 111, 122, 201, 212, 220\}, \\ V_2(112) &= \{001, 012, 020, 102, 110, 121, 200, 211, 222\}. \end{aligned}$$

The sets $V_j(\boldsymbol{b})$ for the other components can be obtained in a similar fashion.

In a factorial experiment, the number of treatment combinations increases rapidly with increase in the number of factors, n, and therefore, further blocking of treatment combinations into blocks of smaller sizes within each replicate becomes necessary to reduce the experimental error. The consequence of such blocking is that some factorial effects become identical to certain block contrasts and are therefore no longer estimable. Such factorial effects are said to be *confounded with blocks.* If a factorial effect is confounded in all the replicates, then it is said to be *totally confounded*; otherwise, the effect is said to be *partially confounded.* It is known that if a partially confounded 3^n factorial experiment is laid out in r replicates and a component $F_1F_2^{b_2} \cdots F_g^{b_g}$ of the factorial effect $F_1 \times F_2 \times \cdots \times F_g$ 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 $F_1F_2^{b_2}\cdots F_g^{b_g}$ are, however, essentially mathematical tools for constructing confounded designs and lack direct statistical interpretation. In contrast, 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. Such contrasts are important e.g., in the context of fitting orthogonal polynomial models; see Raktoe *et al.* (1981) for more details on this.

Let

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

The two rows of P, say $\boldsymbol{p}_1'$ and $\boldsymbol{p}_2'$, correspond to the linear and quadratic components of any 3-level factor. Then, the 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

$$\boldsymbol{c}' = \boldsymbol{c}_1' \otimes \boldsymbol{c}_2' \otimes \cdots \otimes \boldsymbol{c}_g' \otimes \mathbf{1}_3' \otimes \cdots \otimes \mathbf{1}_3'. \tag{2}$$

In (2), each $\boldsymbol{c}_i'$ equals either $\boldsymbol{p}_1'$ or $\boldsymbol{p}_2'$ and $\mathbf{1}_3$ appears $n-g$ times. For example, let $n=3$ and let the factors be F_1, F_2 and F_3. Consider the 2-factor interaction $F_1 \times F_2$. 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 (written as $F_{1L}F_{2Q}$) belonging to this interaction. It is important to know the efficiency factors for these natural contrasts in a partially confounded design. While this problem is important from a statistical perspective, somewhat surprisingly it was not addressed in the literature till it was tackled by Dey and Mukerjee (2012). In what follows, we describe some of their results. For details and proofs, the original paper may be consulted.

In the context of a 3^n experiment, consider a component $F_1F_2^{b_2}\cdots F_g^{b_g}$ of the factorial effect $F_1 \times F_2 \times \cdots \times F_g$. As before, with $\tau(\boldsymbol{z})$ denoting the effect of the treatment combination $\boldsymbol{z} = z_1 \ldots z_n$, let $\boldsymbol{\tau}$ denote the $v \times 1$ vector with elements $\tau(\boldsymbol{z})$, arranged lexicographically, where $v = 3^n$ is the total number of treatment combinations.

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 treatment combinations, such that the $(j, \boldsymbol{z})$th element of $A(\boldsymbol{b})$ equals 1 if $\boldsymbol{z} \in V_j(\boldsymbol{b})$, and 0, otherwise. Since the sets $V_j(\boldsymbol{b}),\ j = 0, 1, 2,$ are disjoint and each of them has cardinality 3^{n-1}, we have

$$\begin{aligned} A(\boldsymbol{b})A(\boldsymbol{b})' &= 3^{n-1}I_3,\ A(\boldsymbol{b})\mathbf{1}_v = 3^{n-1}\mathbf{1}_3, \\ \mathbf{1}_3'A(\boldsymbol{b}) &= \mathbf{1}_v', \end{aligned}$$

where 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

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

L being any 2×3 matrix so chosen that

$$H(\boldsymbol{b})H(\boldsymbol{b})' = I_2, \quad H(\boldsymbol{b})\mathbf{1}_v = \mathbf{0}.$$

Then L must satisfy

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

Even though a matrix L satisfying the above is non-unique, our results do not depend on the particular choice of L. We now show that any natural contrast $\boldsymbol{c}'\boldsymbol{\tau}$ belonging to a factorial effect $F_1\times F_2\times\cdots\times F_g$ can be expressed as a linear combination of all the contrasts belonging to the 2^{g-1} orthogonal components, $F_1F_2^{b_2}\cdots F_g^{b_g}$.

Let $q=2^{g-1}$ and let the orthogonal components $F_1F_2^{b_2}\cdots F_g^{b_g}$ be denoted by $C_1,\ldots,C_q$. Also, for $1\le j\le q$, let H_j be the $H(\boldsymbol{b})$ matrix corresponding to C_j, so that $H_j\boldsymbol{\tau}$ gives a complete set of orthonormal treatment contrasts belonging to C_j.

Let $H = (H_1' \; H_2' \; \cdots H_q')'$ be a matrix with $2q=2^g$ rows. 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. Thus, for a natural contrast $\boldsymbol{c}'\boldsymbol{\tau}$, $\boldsymbol{c}'$ must belong to the row space of $H \Leftrightarrow \boldsymbol{c}'=\boldsymbol{\xi}'H$ for some vector $\boldsymbol{\xi}$. Since $HH'=I_{2q}$, we have $\boldsymbol{c}'H'=\boldsymbol{\xi}'$, i.e., $\boldsymbol{c}'=\boldsymbol{c}'H'H=\sum_{j=1}^{q}\boldsymbol{c}'H_j'H_j$, so that

$$\boldsymbol{c}'\boldsymbol{\tau}=\sum_{j=1}^{q}\boldsymbol{c}'H_j'H_j\boldsymbol{\tau}.$$

We now have the following results, proved by Dey and Mukerjee (2012).

Theorem 1. *If $H(\boldsymbol{b})$ and $\boldsymbol{c}$ are as defined earlier, then*

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

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 (2). Then the efficiency factor for $\boldsymbol{c}'\boldsymbol{\tau}$ is given by*

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

From Theorem 2, we see that the efficiency factor for every natural contrast belonging to a factorial effect equals the simple harmonic mean of the component-wise efficiency factors, $(r - r_j)/r$. 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.

So far, we have restricted attention to 3-level symmetric factorials. What happens if $s > 3$? As seen earlier, for a general s-level factorial design, where s is a prime or prime power, any factorial effect, say $F_1 \times F_2 \times \ldots \times F_g$, can be represented via $(s-1)^{g-1}$ components, each carrying $s - 1$ independent treatment contrasts. As before, 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, $1 \leq j \leq q$, 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 efficiency factor for $\boldsymbol{c}'\boldsymbol{\tau}$ can be shown to be (see Dey and Mukerjee (2012) for details)

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

where

$$W(\boldsymbol{c}, j) = \frac{\boldsymbol{c}' H_j' H_j \boldsymbol{c}}{\boldsymbol{c}'\boldsymbol{c}}, \; 1 \leq j \leq q.$$

Thus, for $s > 3$, we see somewhat counter-intuitively that though the efficiency factor of a natural contrast is again a harmonic mean of component-wise efficiency factors, this mean is now a weighted one. The weights depend on the particular natural contrast chosen and the orthogonal component. As such, given the total number of replicates r and the replicates $r_1, \ldots, r_q$ where the components $C_1, \ldots, C_q$ are confounded, respectively ($q = (s-1)^{g-1}$ here), typically no choice of $r_1, \ldots, r_q$ can simultaneously maximize the efficiency factor of a natural contrast belonging to a factorial effect and one has to be proceed separately for each such contrast based on explicit calculation of the weights.

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