

ON THE CHARACTERISTIC ROOTS OF THE INFORMATION MATRIX OF 2^m BALANCED FACTORIAL DESIGNS OF RESOLUTION V , WITH APPLICATIONS

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0. Summary. The characteristic roots of the information matrix $(M)_T$ of a balanced 2^m fractional factorial design T are obtained, when the parameters to be estimated include the general mean μ , the main effect A_i , and the two-factor interaction $A_i A_j$ (briefly, A_{ij}), the remaining effects being assumed negligible. (If $(M)_T$ is nonsingular, T is a design of resolution V .) It is well known that T depends on five nonnegative integers $(\mu_0, \mu_1, \mu_2, \mu_3, \mu_4)$, called its "index set." In Srivastava (1970), the special case when $\mu_0 = \mu_4$ and $\mu_1 = \mu_3$ was considered; in this paper, the theory is presented for the general case. As a by-product of this work, we obtain a class of useful necessary conditions on the set $(\mu_0, \mu_1, \mu_2, \mu_3, \mu_4)$ such that a design T with this index set may (combinatorially) exist. If $(M)_T$ is nonsingular, and $(V)_T = [(M)_T]^{-1}$, an explicit expression (as a function of the μ_i) has been obtained for $\text{tr}(V)_T$; similar expressions for $| (V)_T |$ and $\text{ch}_{\max}(V)_T$ can be easily written down using our results. One reason why $\text{tr}(V)_T$ (rather than the other two criteria) should be used for comparing balanced resolution V fractions is given. Finally, it is shown (through an example of a previously unknown design with resolution $V m = 7$) that for a given N (the number of runs), an (existing) optimal balanced design (optimal with respect to, say, the trace criterion) does not necessarily satisfy the restriction $(\mu_0 = \mu_4 \text{ and } \mu_1 = \mu_3)$, and may be distinct from the design which is optimal in the restricted class. (Scores of other such examples may be found in Srivastava and Chopra (1970a), where the results of this paper are used in a basic manner.) Thus the need for considering designs with general index sets (which is accomplished in the present paper) becomes obvious.

1. Introduction. The theory of fractional factorial designs has found increasing use in agriculture, biological and industrial experimentation. However, the basic problems in this area are still far from solved. For example, consider 2^m factorial designs of resolution V (a term introduced by Box and Hunter [1961]), i.e. in which μ , the A_i and the A_{ij} are all estimable, given that the rest of the effects are negligible. It is well known that a necessary and sufficient condition that the estimates of all of the above effects be mutually uncorrelated is that the design be an orthogonal array of strength 4. Orthogonal arrays were indeed introduced in this connection by C. R. Rao (1947), and later their combinatorial properties were studied by, among others, Bose and Bush (1952), and Seiden and Zemach (1966). It was found, however, that orthogonal arrays in general require too many observations to be widely useful as factorial designs. Thus, for example, when

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$m = 7$, an orthogonal array of strength 4 requires 64 observations, whereas a minimal design (see, for example, Srivastava and Bose (1965)) involves only 29 runs. Indeed, given m and N , one has almost always to look for a design which is not an orthogonal array. The class of "balanced designs" (defined in the next section) is the next wider class to be looked into. "Balanced" factorial designs, roughly speaking, possess the same advantages over "unbalanced" or "less balanced" ones, as a balanced incomplete block (BIB) design does over "unbalanced" or "partially balanced" designs. In particular, like BIB designs, they would provide great ease in the analysis and interpretation of results. "Balanced" designs were introduced first by Chakravarti (1956), who gave them the name "partially balanced array." However, we shall here call them "balanced arrays" (B-arrays), since they are a generalization of BIB rather than of PBIB designs. As we shall see, unlike orthogonal arrays, B-arrays (which reduce to orthogonal arrays for values of N for which the latter exist) permit economy in the number of observations, since they are available for every value of $N (\geq v)$, where $v (= 1 + m + \binom{m}{2})$ denotes the total number of factorial effects to be estimated. However, given a pair (m, N) , there are, in general, a large number of possible balanced 2^m resolution V designs with N runs. Out of these, one must choose a design which allows estimation of all the v effects (i.e., for which M is nonsingular), and furthermore which maximizes information in some sense. For the latter purpose, the popular optimality criteria (to be minimized) are $|V|$, $\text{tr} V$, and $\text{ch}_{\max} V$, where $V = M^{-1}$. All these criteria are functions of the characteristic roots of M . Thus in order to obtain a design which is optimal in the class of balanced designs (with given (m, N) , of course), the computation of the roots of M (as functions of the μ_i) is a basic first step. In Srivastava (1970), this was done for the special case when $\mu_0 = \mu_4$ and $\mu_1 = \mu_3$. But as pointed out in the summary, designs optimal in this subclass are generally not optimal in the entire class of balanced designs. The computation of the roots of M in the general case, though somewhat involved, has been carried out using the machinery of linear associative algebras corresponding to multidimensional partially balanced association schemes developed in Bose and Srivastava (1964a, b).

The results of this paper solve a major part of the analytical problem of the theory of optimal balanced resolution V designs. It also gives as a by-product some combinatorial existence conditions for B-arrays. However, to meet the further needs of this theory, some further combinatorial work has been started (Srivastava (1970b), Srivastava and Chopra (1970b, c)). Finally, using both the analytical and combinatorial results of these various papers, we have succeeded in finding optimal (w.r.t. the trace criterion) balanced 2^m resolution V designs, for $m = 4, 5, 6$ in Srivastava and Chopra (1970a). Work for larger values of m is in progress.

2. Preliminaries. The runs or assemblies of a 2^m factorial will be written $(j_1, \dots, j_m)'$, where j_r , the level of the r th factor, equals 0 or 1. Let T be a fraction with N runs; then T can be expressed as a $(0, 1)$ matrix of size $(m \times N)$ whose columns denote runs. We shall consider the situation where three factor and higher

order effects are assumed negligible; the vector of unknown parameters is then $\mathbf{L}(v \times 1)$, where

$$(2.1) \quad \mathbf{L}' = (\mu; A_1, \dots, A_m; A_{12}, A_{13}, \dots, A_{1m}, A_{23}, A_{24}, \dots, A_{m-1,m}) \\ = (\{\mu\}; \{A_i\}; \{A_{ij}\}), \text{ say.}$$

Consider a resolution V design T . Let $(\mathbf{L})_T$ denote the best linear unbiased estimate (BLUE) of \mathbf{L} based on T , and let $(V)_T$ be the variance-covariance matrix of $(\mathbf{L})_T$. In this paper, we study the case where T has the property of being "balanced," i.e. $(V)_T$ must be such that $\text{Var}(\hat{A}_i)$, $\text{Var}(\hat{A}_{ij})$, $\text{Cov}(\hat{\mu}, \hat{A}_i)$, $\text{Cov}(\hat{\mu}, \hat{A}_{ij})$, $\text{Cov}(\hat{A}_i, \hat{A}_j)$, $\text{Cov}(\hat{A}_i, \hat{A}_{ij})$, $\text{Cov}(\hat{A}_i, \hat{A}_{kl})$, $\text{Cov}(\hat{A}_{ij}, \hat{A}_{ik})$, and $\text{Cov}(\hat{A}_{ij}, \hat{A}_{kl})$ are independent of i, j, k, l (assumed to be all distinct; $i, j, k, l = 1, \dots, m$). Now suppose the normal equations are of the form (see, for example, Bose and Srivastava (1964a)) $M\hat{\mathbf{L}} = \mathbf{z}$. Then the "normal equations" matrix (also called "information" matrix) $M = (M)_T$ is $v \times v$, and its rows and columns correspond respectively to the elements of \mathbf{L} . It is well known that a necessary and sufficient condition for T to be balanced is that M have only five distinct elements $\gamma_i (i = 1, \dots, 5)$ as indicated below:

$$(2.2) \quad \gamma_1 = N = \varepsilon(\mu, \mu) = \varepsilon(A_i, A_i) = \varepsilon(A_{ij}, A_{ij}), \quad \gamma_2 = \varepsilon(\mu, A_i) = \varepsilon(A_j, A_{ij}) \\ \gamma_3 = \varepsilon(\mu, A_{ij}) = \varepsilon(A_i, A_j) = \varepsilon(A_{ik}, A_{jk}), \quad \gamma_4 = \varepsilon(A_i, A_{jk}), \\ \gamma_5 = \varepsilon(A_{ij}, A_{kl}),$$

where $i, j, k, l (= 1, \dots, m)$ are all distinct, and for $x, y \in L$, $\varepsilon(x, y)$ denotes the element of M in the cell corresponding to (x, y) . It is further known (see, for example, Srivastava (1970a)) that the above condition for T to be balanced is equivalent to requiring that T be a "Balanced array (B-array) of strength 4." For the reader's convenience, we define this concept here.

DEFINITION 1. $T(m \times N)$ is said to be a balanced array (B-array) of strength 4, and index set $\mu' = (\mu_0, \mu_1, \mu_2, \mu_3, \mu_4)$, if every subarray T_0 of T is such that every $(0, 1)$ vector (of size 4×1) with weight $i (i = 0, 1, 2, 3, 4)$ occurs exactly μ_i as a column of T_0 . (Here, "the weight of a $(0, 1)$ vector" means the number of ones in the vector.)

For a balanced array T , it is shown in Srivastava (1970a) that

$$(2.3) \quad \gamma_1 = N = \mu_0 + 4\mu_1 + 6\mu_2 + 4\mu_3 + \mu_4, \quad \gamma_5 = \mu_0 - 4\mu_1 + 6\mu_2 - 4\mu_3 + \mu_4, \\ \gamma_2 = (\mu_4 - \mu_0) + 2(\mu_3 - \mu_1), \quad \gamma_4 = (\mu_4 - \mu_0) - 2(\mu_3 - \mu_1), \\ \gamma_3 = \mu_4 - 2\mu_2 + \mu_0.$$

Finally, in what follows, we would consider M in the partitioned form (recall Bose and Srivastava (1964a), Srivastava (1970a)):

$$(2.4) \quad M = \begin{bmatrix} M_{00} & M_{01} & M_{02} \\ & M_{11} & M_{12} \\ \text{Sym.} & & M_{22} \end{bmatrix}$$

where the partition corresponds to $\{\mu\}$, $\{A_i\}$, $\{A_{ij}\}$. Thus M_{00} is (1×1) , M_{12} is $m \times \binom{m}{2}$, M_{22} is $\binom{m}{2} \times \binom{m}{2}$, etc. and $M_{20} = M'_{02}$, etc.

It can be easily checked that if an array T is of strength 4, then it is also of strength $t_1 \leq 4$. For purposes of illustration, we now present a B-array of strength 4.

EXAMPLE 1. Below, we present a B-array with $m = 7$, $N = 44$, $t = 4$, and index set $\mu' = (3, 2, 3, 3, 3)$. Notice that the array can also be considered as a fractional factorial design of the 2^7 type with 44 assemblies (treatment combinations). Here the rows correspond to factors and the columns to assemblies. Thus the seventh assembly below is a factor-level combination in which the fourth factor is at level 1, and all the others are at level 0.

TABLE 1

Balanced array with 7 rows, 44 columns, strength 4, and index set (3, 2, 3, 3, 3)

0 0 0	1 0 0 0	1 0 0 0	1 1 1 0 0 0	1 1 1 0 0 0
0 0 0	0 1 0 0	0 1 0 0	1 0 0 1 1 0	1 0 0 1 1 0
0 0 0	0 0 1 0	0 0 1 0	0 1 0 1 0 1	0 1 0 1 0 1
0 0 0	0 0 0 1	0 0 0 1	0 0 1 0 1 1	0 0 1 0 1 1
1 0 0	0 0 0 0	1 1 1 1	0 0 0 0 0 0	1 1 1 1 1 1
0 1 0	0 0 0 0	1 1 1 1	1 1 1 1 1 1	0 0 0 0 0 0
0 0 1	0 0 0 0	1 1 1 1	1 1 1 1 1 1	1 1 1 1 1 1
1 1 1 0 0 0	1 1 0 0	1 1 1 0	1 1 1 0	1 1 1
1 0 0 1 1 0	1 1 0 1	1 1 0 1	1 1 0 1	1 1 1
0 1 0 1 0 1	1 0 1 1	1 0 1 1	1 0 1 1	1 1 1
0 0 1 0 1 1	0 1 1 1	0 1 1 1	0 1 1 1	1 1 1
1 1 1 1 1 1	1 1 1 1	0 0 0 0	0 0 0 0	0 1 1
1 1 1 1 1 1	0 0 0 0	1 1 1 1	0 0 0 0	0 1 1
0 0 0 0 0 0	0 0 0 0	0 0 0 0	1 1 1 1	0 1 1

3. Derivation of the characteristic polynomial. We have

$$(3.1) \quad |M - \delta I| = \begin{bmatrix} M^* - \delta I & M_0 \\ M'_0 & M_{11} - \delta I \end{bmatrix}, \quad \text{where}$$

$$(3.1a) \quad M_0 = \begin{bmatrix} M_{01} \\ M_{21} \end{bmatrix}, \quad M^* = \begin{bmatrix} M_{00} & M_{02} \\ M_{20} & M_{22} \end{bmatrix},$$

and where I is the identity matrix of appropriate size. Hence

$$(3.2) \quad \begin{aligned} |M - \delta I| &= |M^* - \delta I| |(M_{11} - \delta I) - [M_{10} M_{12}] [M^* - \delta I]^{-1} [M'_{01} M'_{21}]'| \\ &= |M^* - \delta I| |(M_{11} - \delta I) - (M_{10} Q_{00} M_{01} + M_{12} Q_{20} M_{01} \\ &\quad + M_{10} Q_{02} M_{21} + M_{12} Q_{22} M_{21})| \end{aligned}$$

where

$$(3.3) \quad [M^* - \delta I]^{-1} = \begin{bmatrix} Q_{00} & Q_{02} \\ Q_{21} & Q_{22} \end{bmatrix} \text{ say.}$$

Since $[M^* - \delta I][M^* - \delta I]^{-1} = I$, we get

$$(3.4) \quad (M_{00} - \delta I)Q_{00} + M_{02}Q_{20} = I, (M_{00} - \delta I)Q_{02} + M_{02}Q_{22} = 0, \\ M_{20}Q_{00} + (M_{22} - \delta I)Q_{20} = 0, M_{20}Q_{02} + (M_{22} - \delta I)Q_{22} = I.$$

From the above we get

$$(3.5a) \quad Q_{02} = -(M_{00} - \delta I)^{-1}M_{02}Q_{22}.$$

$$(3.5b) \quad Q_{22} = [(M_{22} - \delta I) - M_{20}(M_{00} - \delta I)^{-1}M_{02}]^{-1}.$$

$$(3.5c) \quad Q_{00} = (M_{00} - \delta I)^{-1} + (M_{00} - \delta I)^{-1}M_{02}Q_{22}M_{20}(M_{00} - \delta I)^{-1}.$$

Throughout this paper, I will denote a matrix (of appropriate size) each of whose elements is one. Now, since $(M_{00} - \delta I)$ is scalar, the matrix $M_{20}(M_{00} - \delta I)^{-1}M_{02}$ is a multiple of J . Thus, from Bose and Srivastava (1964b), it follows that Q_{22} belongs to the linear associative algebra L_5 (corresponding to the general triangular association scheme). Using the tables of characteristic roots of the association matrix corresponding to the algebra L_5 , it can be checked that (cf. Srivastava (1970a)) the (possibly) distinct roots of Q_{22} are $(\pi_1 - \delta)^{-1}$, $(\pi_2 - \delta)^{-1}$, $(\pi_3 - \delta)^{-1}$ with respective multiplicities 1, $m-1$, and m' , where

$$(3.5d) \quad \pi_1 = \gamma_1 + 2(m-2)\gamma_3 + m''\gamma_5, \quad \pi_2 = \gamma_1 + (m-4)\gamma_3 - (m-3)\gamma_5, \\ \pi_3 = \gamma_1 - 2\gamma_3 + \gamma_5, \\ m' = m(m-3)/2, \quad m'' = (m-2)(m-3)/2.$$

Also, as in Bose and Srivastava (1964b), let B_{22}^α ($\alpha = 0, 1, 2$) denote the association matrix for L_5 . Then, from the theory in that paper, it follows that there exists a vector of constants $\mathbf{q}'_{22} = (q_0, q_1, q_2)$ such that

$$(3.6) \quad Q_{22} = \sum_{\alpha=0}^2 q_\alpha M_{22}^\alpha.$$

Now the vector of roots of Q_{22} is \mathbf{q}_{22} where

$$(3.7) \quad \Delta \mathbf{q}_{22} = [(\pi_1^* - \delta)^{-1}, (\pi_2^* - \delta)^{-1}J_{1, m-1}, (\pi_3^* - \delta)^{-1}J_{1, m'}] = \mathbf{q}^*, \text{ say,}$$

and where Δ' is given by equation (ii), page 162 (Bose and Srivastava (1964b)). Thus we obtain

$$(3.8) \quad \mathbf{q}_{22} = (\Delta' \Delta)^{-1} \Delta' \mathbf{q}^*, \quad \text{where } \Delta' \Delta = \text{diag} \left(\binom{m}{2}, 6\binom{m}{3}, 6\binom{m}{4} \right)$$

$$q_0 = \binom{m}{2}^{-1} [(\pi_1^* - \delta)^{-1} + (m-1)(\pi_2^* - \delta)^{-1} + m'(\pi_3^* - \delta)^{-1}]$$

$$(3.9) \quad q_1 = \frac{1}{6}\binom{m}{3}^{-1} [2(m-2)(\pi_1^* - \delta)^{-1} + (m-1)(m-4)(\pi_2^* - \delta)^{-1} \\ - 2m'(\pi_3^* - \delta)^{-1}]$$

$$q_2 = \frac{1}{6}\binom{m}{4}^{-1} [m''(\pi_1^* - \delta)^{-1} - (m-1)(m-3)(\pi_2^* - \delta)^{-1} + m'(\pi_3^* - \delta)^{-1}].$$

Furthermore, from (3.5a, b, c), we get

$$(3.10) \quad Q_{02} = -(\gamma_1 - \delta)^{-1} \gamma_3 [q_0 + 2(m-2)q_1 + m''q_2] \mathbf{J}' = q_{02} \mathbf{J}', \quad \text{say, where} \\ q_{02} = -(\gamma_1 - \delta)^{-1} \gamma_3 [q_0 + 2(m-2)q_1 + m''q_2]$$

$$(3.11) \quad Q_{00} = (\gamma_1 - \delta)^{-1} - (\gamma_1 - \delta)^{-1} q_{02} \gamma_3 m_2 = q_{00}, \quad \text{say.}$$

Therefore we have

$$(3.12) \quad M_{10} Q_{00} M_{01} = q_{00} \gamma_2^2 \mathbf{J}_{mm},$$

$$(3.13) \quad (M_{10} Q_{02} M_{21})' = M_{12} Q_{20} M_{01} = M_{12} q_{02} \mathbf{J} \gamma_2 \mathbf{J}' = \gamma_2 q_{02} M_{12} \mathbf{J}_{mm} \\ = \gamma_2 q_{02} (m-1) [\gamma_2 + \frac{1}{2}(m-2) \gamma_4] \mathbf{J}_{mm},$$

$$M_{12} Q_{22} M_{21} = \xi_1 I + \xi_2 (J - I) \quad \text{where}$$

$$\xi_1 = (m-1) \gamma_2 \zeta_1 + \frac{(m-1)(m-2)}{2} \gamma_4 \zeta_2,$$

$$(3.14) \quad \xi_2 = \gamma_2 \zeta_1 + (m-2) \gamma_4 \zeta_1 + (m-2) \gamma_2 \zeta_2 + \frac{(m-2)(m-3)}{2} \gamma_4 \zeta_2,$$

$$\zeta_1 = q_0 \gamma_2 + (m-2) q_1 \gamma_2 + (m-2) q_1 \gamma_4 + \frac{(m-2)(m-3)}{2} q_2 \gamma_4,$$

$$\zeta_2 = q_0 \gamma_4 + 2q_1 \gamma_2 + 2(m-3) q_1 \gamma_4 + (m-3) q_2 \gamma_2 \\ + \frac{(m-3)(m-4)}{2} q_2 \gamma_4.$$

Substituting from (3.12)–(3.14), and $M_{11} = \gamma_1 I + (J - I) \gamma_3$ in (3.1), we obtain $|M - \delta I| = |M^* - \delta I| |\sigma_0 I + \sigma_1 J|$, where

$$(3.15) \quad \sigma_0 = (\gamma_1 - \gamma_3 - \delta) - (\xi_1 - \xi_2),$$

$$(3.16) \quad \sigma_1 = \gamma_3 - q_{00} \gamma_2^2 - 2(m-1) q_{02} \gamma_2 \left(\gamma_2 + \frac{m-2}{2} \gamma_4 \right) - \xi_2.$$

Now $|\sigma_0 I + \sigma_1 J| = (\sigma_0 + m \sigma_1) \sigma_0^{m-1}$. Thus it can be easily checked that

$$(3.17) \quad |M - \delta I| = [\sigma_0 (\pi_2^* - \delta)]^{m-1} (\pi_3^* - \delta)^{m'} (\sigma_0 + m \sigma_1) [(\gamma_1 - \delta) (\pi_1^* - \delta) \\ - m_2 \gamma_3^2].$$

Now we shall express σ_0 and hence $(\xi_1 - \xi_2)$ as a linear combination of $(\pi_1^* - \delta)^{-1}$, $(\pi_2^* - \delta)^{-1}$, $(\pi_3^* - \delta)^{-1}$. From (3.14), we have

$$(3.18) \quad \xi_1 - \xi_2 = (m-2) (\gamma_2 - \gamma_4) (\zeta_1 - \zeta_2) = (m-2) (\gamma_2 - \gamma_4)^2 [q_0 + (m-4) q_1 \\ - (m-3) q_2].$$

Let

$$(3.19) \quad q_0 + (m-4) q_1 - (m-3) q_2 = x_1 (\pi_1^* - \delta)^{-1} + x_2 (\pi_2^* - \delta)^{-1} + x_3 (\pi_3^* - \delta)^{-1}.$$

Substituting the values of q_0, q_1 , and q_2 from (3.9), and comparing both sides, we will have after some simplification, $x_1 = 0, x_2 = 1$, and $x_3 = 0$. Thus

$$(3.20) \quad \xi_1 - \xi_2 = (m-2)(\gamma_2 - \gamma_4)^2(\pi_2^* - \delta)^{-1}.$$

Similarly it can be checked that

$$(3.21) \quad \xi_2 = \frac{m-1}{2m} [2\gamma_2 + (m-2)\gamma_4]^2 - \frac{m-2}{m} (\gamma_2 - \gamma_4)^2(\pi_2^* - \delta)^{-1},$$

$$(3.22) \quad q_0 + 2(m-2)q_1 + m''q_2 = (\pi_1^* - \delta)^{-1}.$$

Thus, from (3.10), (3.11), and (3.15), we have

$$(3.23) \quad q_{02} = \gamma_3(\gamma_1 - \delta)^{-1}(\pi_1^* - \delta)^{-1},$$

$$(3.24) \quad q_{00} = (\gamma_1 - \delta)^{-1} + \binom{m}{2}\gamma_3^2(\gamma_1 - \delta)^{-2}(\pi_1^* - \delta)^{-1},$$

$$(3.25) \quad \sigma_1 = \gamma_3 - \gamma_2^2(\gamma_1 - \delta)^{-1} - \gamma_2^2\gamma_3^2\binom{m}{2}(\gamma_1 - \delta)^{-2}(\pi_1^* - \delta)^{-1} \\ + (m-1)\gamma_2(2\gamma_2 + \overline{m-2}\gamma_4)\gamma_3(\gamma_1 - \delta)^{-1}(\pi_1^* - \delta)^{-1} - \frac{m-1}{2m} \\ \cdot (2\gamma_2 + \overline{m-2}\gamma_4)^2(\pi_1^* - \delta)^{-1} + \frac{m-2}{m} (\gamma_2 - \gamma_4)^2(\pi_2^* - \delta)^{-1},$$

$$(3.26) \quad \sigma_0 = (\gamma_1 - \gamma_3 - \delta) - (\gamma_2 - \gamma_4)^2(m-2)(\pi_2^* - \delta)^{-1}.$$

Using (3.25) and (3.26), and simplifying, we get

$$(3.27) \quad (\sigma_0 + m\sigma_1)[(\gamma_1 - \delta)(\pi_1^* - \delta) - \binom{m}{2}\gamma_3^2] \\ = \gamma_1^2\pi_1^* - \gamma_1^2\delta - 2\gamma_1\delta\pi_1^* + 2\gamma_1\delta^2 + \delta^2\pi_1^* - \delta^3 - \binom{m}{2}\gamma_1\gamma_3^2 \\ + \binom{m}{2}\gamma_3^2\delta + \gamma_1\gamma_3(m-1)\pi_1^* + (m-1)\gamma_3\delta^2 \\ - \gamma_3(m-1)(\gamma_1 + \pi_1^*)\delta - \binom{m}{2}(m-1)\gamma_3^3 - m\gamma_2^2\pi_1^* + m\gamma_2^2\delta \\ + m(m-1)\gamma_2\gamma_3(2\gamma_2 + \overline{m-2}\gamma_4) - \frac{m-1}{2} [2\gamma_2 + (m-2)\gamma_4]^2\gamma_1 \\ + \frac{m-1}{2} [2\gamma_2 + (m-2)\gamma_4]^2\delta.$$

Now, from (3.5d), we have finally

$$(3.28) \quad (\sigma_0 + m\sigma_1)[(\gamma_1 - \delta)(\pi_1^* - \delta) - \binom{m}{2}\gamma_3^2] = -\delta^3 + c_1\delta^2 - c_2\delta + c_3, \quad \text{where}$$

$$(3.29a) \quad c_1 = 3\gamma_1 + (3m-5)\gamma_3 + m''\gamma_5.$$

$$(3.29b) \quad c_2 = 3\gamma_1^2 + 2\gamma_1\gamma_3(3m-5) + 2m''\gamma_1\gamma_5 + \frac{(m-1)(3m-8)}{2} \gamma_3^2 + m''(m-1)\gamma_3\gamma_5 \\ - m\gamma_2^2 - \frac{m-1}{2} (2\gamma_2 + \overline{m-2}\gamma_4)^2$$

$$\begin{aligned}
 (3.29c) \quad c_3 = & \gamma_1^3 - \binom{m}{2}(m-1)\gamma_3^3 + \frac{(m-1)(3m-8)}{2} \gamma_1\gamma_3^2 + (3m-5)\gamma_1^2\gamma_3 \\
 & + m''\gamma_1^2\gamma_5 + m''(m-1)\gamma_1\gamma_3\gamma_5 - m\gamma_1\gamma_2^2 - mm''\gamma_2^2\gamma_5 + 2m\gamma_2^2\gamma_3 \\
 & + m(m-1)(m-2)\gamma_2\gamma_3\gamma_4 - \frac{m-1}{2} \gamma_1(2\gamma_2 + \overline{m-2\gamma_4})^2.
 \end{aligned}$$

Therefore the characteristic polynomial of M is given by

$$\begin{aligned}
 (3.30) \quad |M - \delta I| = & (-\delta^3 + c_1\delta^2 - c_2\delta + c_3) \cdot (\gamma_1 - 2\gamma_3 + \gamma_5 - \delta)^{m'} \\
 & \cdot [\delta^2 - \delta(2\gamma_1 + \overline{m-5\gamma_3} - \overline{m-3\gamma_5}) + (\gamma_1 - \gamma_3)(\gamma_1 - \overline{m-3\gamma_5} \\
 & + \overline{m-4\gamma_3}) - (\gamma_2 - \gamma_4)^2(m-2)]^{m-1}.
 \end{aligned}$$

In order to get the characteristic polynomial of M^{-1} , change δ to $1/\delta$ in (3.30). Thus we have

$$\begin{aligned}
 (3.31) \quad |M^{-1} - \delta I| = & (c_3\delta^3 - c_2\delta^2 + c_1\delta - 1)(\delta\gamma_1 - 2\gamma_3 + \gamma_5 - 1)^{m'} \\
 & \cdot (c_5\delta^2 - c_4\delta + 1)^{m-1}
 \end{aligned}$$

where

$$\begin{aligned}
 (3.32) \quad c_4 = & 2\gamma_1 + (m-5)\gamma_3 - (m-3)\gamma_5, \\
 c_5 = & (\gamma_1 - \gamma_3)(\gamma_1 - \overline{m-3\gamma_5} + \overline{m-4\gamma_3}) - (\gamma_2 - \gamma_4)^2(m-2).
 \end{aligned}$$

Now, we need the following theorem, which can be easily established.

THEOREM 3.1. Consider the polynomial $x^3 + a_2x^2 + a_1x + a_0$. A necessary and sufficient condition that this polynomial has three nonnegative real zeros, is that one of the following conditions must hold: (i) $a_0 = a_1 = a_2 = 0$, (ii) $a_0 = a_1 = 0$, $a_2 < 0$, (iii) $a_0 = 0$, $a_1 > 0$, $a_2 < 0$, and (iv) $a_0 < 0$, $a_1 > 0$, $a_2 < 0$. (Notice that these conditions imply: $a_0 \leq 0$, $a_1 \geq 0$, $a_2 \leq 0$).

The above result is made use of in

THEOREM 3.2. Let T be a BA with m constraints, two symbols and of strength 4. Let $(\mu_0, \mu_1, \mu_2, \mu_3, \mu_4)$ be the index set of parameters for this array. Then a set of necessary conditions that T exists are

$$(3.33) \quad \gamma_1 - 2\gamma_3 + \gamma_5 \geq 0 \quad \text{which implies that } \mu_2 \geq 0;$$

$$(3.34a) \quad 2\gamma_1 + (m-5)\gamma_3 - (m-3)\gamma_5 \geq 0, \quad \text{or equivalently}$$

$$(3.34b) \quad (m-1)\mu_1 + (m-1)\mu_3 \geq 2(m-5)\mu_2;$$

$$(3.35a) \quad (\gamma_1 - \gamma_3)[\gamma_1 - (m-3)\gamma_5 + (m-4)\gamma_3] - (m-2)(\gamma_2 - \gamma_4)^2 \geq 0,$$

or equivalently

$$(3.35b) \quad (m-4)\mu_2^2 \leq \mu_2(\mu_1 + \mu_3) + (m-2)\mu_1\mu_3;$$

$$(3.36) \quad 3\gamma_1 + (3m-5)\gamma_3 + \frac{(m-2)(m-3)}{2} \gamma_5 \geq 0;$$

$$(3.37) \quad 3\gamma_1^2 - (3m-2)\gamma_2^2 + \frac{(m-1)(3m-8)}{2} \gamma_3^2 - \frac{(m-1)(m-2)^2}{2} \gamma_4^2 \\ + 2(3m-5)\gamma_1\gamma_3 + (m-2)(m-3)\gamma_1\gamma_5 - 2(m-1)(m-2)\gamma_2\gamma_4 \\ + \frac{(m-1)(m-2)(m-3)}{2} \gamma_3\gamma_5 \geq 0;$$

$$(3.38) \quad \gamma_1^3 - \frac{m(m-1)^2}{2} \gamma_3^3 + (3m-5)\gamma_1^2\gamma_3 + \frac{(m-2)(m-3)}{2} \gamma_1^2\gamma_5 \\ + \frac{(m-1)(3m-8)}{2} \gamma_1\gamma_3^2 + \frac{(m-1)(m-2)(m-3)}{2} \gamma_1\gamma_3\gamma_5 \\ - (3m-2)\gamma_1\gamma_2^2 - \frac{(m-1)(m-2)^2}{2} \gamma_1\gamma_4^2 - 2(m-1)(m-2)\gamma_1\gamma_2\gamma_4 \\ + 2m\gamma_2^2\gamma_3 - \frac{m(m-2)(m-3)}{2} \gamma_2^2\gamma_5 + m(m-1)(m-2)\gamma_2\gamma_3\gamma_4 \geq 0.$$

PROOF. The above conditions are easily established by applying Theorem 3.1 to the various factors of the characteristic polynomial in (3.31).

We now obtain an expression for $\text{tr} V_T$, which equals $\text{tr} M^{-1}$. The trace of a matrix equals the sum of its characteristic roots. From (3.31) it can easily be seen that M^{-1} will not have more than six distinct characteristic roots. Let these be $\delta_1, \delta_2, \delta_3, \delta_4, \delta_5$, and δ_6 . Then, again from (3.21) we see that three of the six roots are with multiplicity 1 each, two are with multiplicity $m-1$ each, and one is with multiplicity m' . Therefore

$$\text{tr} M^{-1} = (\delta_1 + \delta_2 + \delta_3) + (m-1)(\delta_4 + \delta_5) + m'\delta_6.$$

But, from (3.31), we have

$$(3.39) \quad \delta_1 + \delta_2 + \delta_3 = \frac{c_2}{c_3}, \quad \delta_4 + \delta_5 = \frac{c_4}{c_5}, \quad \delta_6 = \frac{1}{\gamma_1 - 2\gamma_3 + \gamma_5}$$

where the c_i 's have been defined in (3.29) and (3.32). Hence we get

THEOREM 3.3.

$$(3.40) \quad \text{tr} M^{-1} \equiv \text{tr} V_T = \frac{c_2}{c_3} + \frac{(m-1)c_4}{c_5} + \frac{m'}{16\mu_2}.$$

It can be shown that for any array T (considered as a fractional design), a necessary condition for nonsingularity of $(M)_T$ is that T contains at least v_m distinct columns. Also in that case $(M)_T$ is positive definite. This gives

THEOREM 3.4. *Consider the array T of Theorem 3.2. A necessary and sufficient condition that L is estimable from T (taken as a fraction), is that (3.33)–(3.38) be satisfied with strict inequality in each case. Also then the number of distinct columns in T is at least v_m .*

We finally establish

THEOREM 3.5. *There exists a B -array T of strength 4 for any m (≥ 4) and any $N \geq v_m$, where v_m is the number of effects to be estimated (i.e. $v_m = 1 + m + m(m-1)/2$).*

PROOF. In [Srivastava and Bose (1965)], a fraction for 2^m factorial is presented, in which v_m effects of interest are estimable, under the assumption that third and higher order interactions are negligible. This fraction is a B -array with v_m assemblies. Enlarging this array by the addition of $(N - v_m)$ runs, each run being $(0, 0, \dots, 0)'$ (say), obviously gives a balanced fraction of resolution V with N runs.

Before closing this section we may remark that from (3.31), we find that V may have six (possibly) distinct roots with multiplicities 1, 1, 1, $m-1$, $m-1$, and $m(m-3)/2$ which are widely different. This implies that $\text{Ch}_{\max} V$ may not give as good an “overall” view of a fraction as $\text{tr} V$. Since the argument of Srivastava (1970a) against $|V|$ still stands, $\text{tr} V$ may usually be preferred over $|V|$ and $\text{Ch}_{\max} V$ for comparison of balanced resolution V designs.

4. Optimal arrays. We now consider the array (T^* , say) for the case $m = 7$, $N = 44$ already given in Example 1. Here $v_m = 29$, so that the design allows fifteen degrees of freedom for error, which is neither too large nor too small. Thus, from this point of view, this design should be of practical use. The smallest orthogonal array available for this problem involves sixty-four assemblies, so that the present one cuts this number down to about two-thirds. This exemplifies the economy that one might achieve by using B -arrays.

It is easily checked that, we shall have in this case $\gamma_1 = N = 44$, $\gamma_2 = -\gamma_4 = 2$, $\gamma_3 = 0$, $\gamma_5 = 4$. From Theorem 3.3, after some calculations, we then obtain $\text{trace}(V_T) = 0.73$. Now, of course, for $m = 7$, $t = 4$, $N = 44$, an orthogonal array does not exist. On the other hand, if an orthogonal array T^+ with N assemblies and strength 4 does exist for a 2^m factorial, then clearly, $\text{trace}(V_T +) = v_m N^{-1}$. Thus the ratio

$$(4.1) \quad (\text{tr} V_T +) / (\text{tr} V_T) = v_m [N \text{tr}(V_T)]^{-1} = R, \text{ say,}$$

measures, in a sense, the relative efficiency (w.r.t. the ‘trace criterion’) of a 2^m fractional factorial design T (with N assemblies, and of resolution V). Now suppose, among all designs within a certain class C , a design T minimizes (say) the trace of the covariance matrix. Then the “absolute efficiency” (w.r.t. trace criterion) of T within the class C is indeed one. Thus, for the array of Example 1, $R \cong 29/(44 \times 0.73) \cong 0.91$, while its absolute efficiency within the class of balanced designs with $N = 44$, $m = 7$ and resolution V , is one. Now if for some m and N

(say $m = m_0$, $N = N_0$), an orthogonal array does exist, then it coincides with the optimal B-array, and we get $R = R(m_0, N_0) = 1$. Hence, for a given m_0 and N_0 , what R measures is in a sense "the non-orthogonality inherent in the pair (m_0, N_0) ". We may remark here, that in Srivastava and Chopra (1968e), optimal balanced designs of resolution V for $m \leq 6$, and various practical values of N have been tabulated, and the value of R is high (> 0.85) in the majority of cases.

In Srivastava (1970), a B-array with $m = 7$, $N = 44$, $t = 4$ and index set $(4, 3, 2, 3, 4)$ was presented, and was shown to be optimal w.r.t. the trace criterion within the subclass of B-arrays for which $\mu_0 = \mu_4$ and $\mu_1 = \mu_3$. Now, for a B-array to be orthogonal, we must have $\mu_0 = \mu_4 = \mu_1 = \mu_3 = \mu_2$. Also, orthogonal arrays (when they exist) have $R = 1$. From this, one might conjecture, that in the general class of B-arrays (for fixed m and N), arrays having $\mu_0 = \mu_4$ and $\mu_1 = \mu_3$ (when they exist) will be better (say, w.r.t. the trace criterion) than arrays not having this property. Although some very special modified versions of this conjecture are proved in Chopra (1967), this conjecture itself is false. The counter example is provided by the array T^* in Example 1, since for the array T^{**} in Srivastava (1970), we have $\text{tr}V_{T^{**}} = 0.75$, while $\text{tr}V_{T^*} = 0.73$.

Finally, we may remark that it can be shown that T^* is the *unique* optimal B-array in the sense that the only other array T_1 with the same (m, N, t) and trace $V_{T_1} = \text{tr}V_T$ is such that T_1 is obtainable from T^* by merely interchanging the symbols zero and one. In practical situations, the choice between T^* and T_1 may be dictated by physical considerations. Otherwise, one may choose between T^* and T_1 by randomization, assigning probability $(1/2)$ to each.

5. Proof of the optimality of the design of Example 1. In the following discussion, we shall consider B-arrays $T(7 \times N)$ of strength 4, and index set $(\mu_0, \mu_1, \mu_2, \mu_3, \mu_4)$. Also we write $\mu' = \mu_1 + \mu_3$, and $\mu'' = \mu_0 + \mu_4$.

THEOREM 5.1. *For $\mu_2 \geq 4$, we must have $N \geq 45$.*

PROOF. (i) $\mu_2 = 6$. Here, (3.34b) implies $\mu' \geq 4$. Hence, by (2.3), $N \geq 52$. (ii) $\mu_2 = 5$. (3.34b) gives $\mu' \geq 3$. But $\mu' = 3$ (with, of course, $\mu_1 \geq 0$, $\mu_3 \geq 0$) is ruled out by (3.35b). Thus $\mu' \geq 4$, and hence $N \geq 46$. (iii) $\mu_2 = 4$. As in (ii), (3.34b), (3.35b) imply $\mu' \geq 5$. Now, when $\mu' = 5$ and $\mu'' = 0$, (3.37) is not satisfied. Thus either $\mu' > 5$, or $\mu' = 5$ and $\mu'' > 0$. In both cases, we have $N \geq 45$. (iv) $\mu_2 \geq 7$. Here (3.34b), (2.3) give $N \geq 62$. This completes the proof.

Now, from (3.40), for the design T^* of Example 1, we have $\text{tr}V_{T^*} = 0.73$. In order to prove that for any B-array T with $N = 44$, we must have $\text{tr}V_T \geq \text{tr}V_{T^*}$, we can (in view of Theorem 5.1 and Theorem 3.4) restrict attention to arrays T with $1 \leq \mu_2 \leq 3$.

THEOREM 5.2. *If the index set μ' of T is such that (i) $\mu_2 = 1$, or (ii) $\mu_2 = 2$, $\mu' \neq 6$, or (iii) $\mu_2 = 3$, $\mu' \neq 5$ holds, then $\text{tr}V_T \geq \text{tr}V_{T^*}$.*

PROOF. (i) $\mu_2 = 1$. Using (3.40), we find that $\text{tr}V_T \geq (6C_4/C_5) + (7/8\mu_2) \geq 7/8 \geq \text{tr}V_{T^*}$. (ii) $\mu_2 = 2$. Here, (3.34b), (3.35b), (3.36) give $7 \geq \mu' \geq 3$. Also, since

$\mu_2 = 2$, $N = 44$, we have (for fixed μ') $\mu'' = 32 - 4\mu'$, $C_4 = 8(3\mu' - 4)$, and $C_5 = 16\{(5\mu'^2 + 8\mu' - 48) - 5(\mu_3 - \mu_1)^2\}$. For given μ' , the ratio C_4/C_5 is least when $(\mu_3 - \mu_1)$ equals 0 (μ' even) or ± 1 (μ' odd). Using this fact, it can be easily checked, that when $\mu' = 3, 4$, or 5 , the bound $6C_4/C_5 + 14/16\mu_2 \geq \text{tr}V_{T^*}$. Finally, when $\mu' = 7$, we show that there does not exist any m -rowed B-array with $m \geq 5$, $\mu_2 = 2$. It is enough to prove this for $m = 5$, since the result for general m is clearly implied by this. Now, suppose a 5-row array T^- exists with $\mu_2 = 2$, $\mu' = 7$. Let d be the number of times the vector $(1, 1, 1, 1, 1)'$ occurs as a column of T^- . Then it can be checked that if $\mathbf{v}(5 \times 1)$ has k zeros and $(5 - k)$ ones ($k = 0, 1, \dots, 5$) in it, then \mathbf{v} must occur as a column of T^- exactly

$$\mu_{4-k+1} - \mu_{4-k+2} + \dots + (-1)^{k+1}\mu_4 + (-1)^kd$$

times. This gives

$$\min(\mu_4, \mu_4 - \mu_3 + \mu_2, \mu_4 - \mu_3 + \mu_2 - \mu_1 + \mu_0) \geq d \geq \max(0, \mu_4 - \mu_3, \mu_4 - \mu_3 + \mu_2 - \mu_1),$$

which in turn implies, for example, $\mu'' + \mu_2 \geq \mu'$. This is not satisfied by $\mu' = 7$, $\mu_2 = 2$, $N = 44$, (since then, $\mu'' = 4$). (iii) $\mu_2 = 3$. By (3.34b), (3.35b), (3.36), we have $4 \leq \mu' \leq 6$. However, $\mu' = 6$ implies $\mu'' + \mu_2 < \mu'$. Hence, we have to consider only $\mu' = 4$. However, in this case, it is easily seen that $6C_4/C_5 + 14/16\mu_2 > \text{tr}V_{T^*}$.

THEOREM 5.3. *For $m = 7$, $N = 44$, the array T^* and the array obtained from T^* by interchanging one and zero provide the optimal balanced designs of resolution V .*

PROOF. In view of the preceding results of this section, we need to consider only the competing arrays T with (i) $\mu_2 = 2$, $\mu' = 6$, or (ii) $\mu_2 = 3$, $\mu' = 5$. As in the last theorem, we can check that $6C_4/C_5 + 14/16\mu_2 > \text{tr}V_{T^*}$, for case (i) if $|\mu_3 - \mu_1| \geq 4$, and for case (ii) if $|\mu_3 - \mu_1| \geq 2$. Thus we are left with arrays T with (α) $\mu_2 = 2$, $\mu' = 6$, $\mu_3 - \mu_1 = 0$ or ± 2 , and (β) $\mu_2 = 3$, $\mu' = 5$, $\mu_3 - \mu_1 = \pm 1$. There are 21 sets of values of μ' (apart from an interchange of 0 and 1 in an array) whose parameters satisfy one of the two conditions (α) or (β). Of these, three values of μ' (namely, $(8, 3, 2, 3, 0)$, $(0, 4, 2, 2, 8)$ and $(1, 4, 2, 2, 7)$) are rejected because of the combinatorial inequalities involving d in the proof of the last theorem. The remaining 18 values of μ' can be directly substituted in (3.40), and the fact that $\mu' = (3, 3, 3, 2, 3)$ (which corresponds to T^* , or $\mu' = (3, 2, 3, 3, 3)$ which corresponds to the array obtained by interchanging 0 and 1 in T^*) gives rise to the minimum value for $\text{tr}V$ may be verified. This completes the proof.

We would like to stress that there is an alternative combinatorial proof using which, the direct verification of only two (instead of the present 18) arrays need be done. However, such a proof, because of its different nature, is out of place here. On the other hand, the reader will observe that there are hundreds of values of μ' satisfying the necessary condition $N = 44 = \mu_0 + 4\mu_1 + 6\mu_2 + 4\mu_3 + \mu_4$. If only

the value of $\text{tr}V$ (at (3.40)) were used and the development of this section ignored, one would have to substitute each such value of μ' in (3.40), and compare the resulting values of $\text{tr}V$. The amount of resulting computations would be tens of times more compared to that needed for the above 18 arrays. This shows the usefulness of Theorem 3.2 other than that for obtaining (3.40). Finally, if the development in the whole paper is completely ignored, one would have to calculate $\text{tr}V_T$ starting from scratch (say from Bose and Srivastava (1964a)) for each μ' (with $N = 44$). Even on very fast computers (like CDC 6400), this would take dozens of hours (compared to about an hour needed on a desk calculator for comparing the above 18 arrays using (3.40))!

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