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On MV-optimality of resolvable designs from 2-level orthogonal arrays[1]

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Abstract

Affine resolvable designs with two blocks per replicate are combinatorially equivalent to orthogonal arrays with two levels. While affine designs are known to be Schur-optimal amongst all resolvable designs, their behavior with respect to the MV-optimality criterion has been little studied. Here it is shown that the MV-best affine designs must be MV-optimal for two and three replicates, but that MV-optimality need not hold for four replicates.

Key words: Resolvable block design; Optimal designs; Orthogonal array.

1 Introduction

An incomplete block design for v treatments in blocks of size k $(< v)$ is *resolvable* if the blocks can be partitioned into sets containing each treatment exactly once. Thus resolvable block designs are exactly those for which the blocks may be partitioned into replicates. Resolvable designs are used in a variety of fields for a variety of reasons as discussed in papers like Patterson and Silvey (1980) and Bailey, Monod, and Morgan (1995); also see the survey paper by Morgan (1996). Typically the number of replicates, r, employed is small while the number of treatments can be quite large.

[1]In honor of Professor Aloke Dey for his many contributions to the theory and application of orthogonal arrays

Now take any two blocks from different replicates of a resolvable design and calculate the number of treatments common to both. If this number is a constant, call it μ, independent of the pair of blocks chosen, then the design is said to be *affine resolvable*. Using s to denote the number of blocks per replicate, it follows that $v = \mu s^2$ and $k = \mu s$. Affine resolvable designs are known to be excellent resolvable designs from many statistical perspectives, as shown in the following result.

Theorem 1. *(Bailey, Monod, Morgan, 1995) In the class of all resolvable designs having the same v, r, and k, an affine resolvable design d minimizes $\sum_{i=1}^{v-1} f(z_{di})$ for every convex function f.*

The quantities z_{di} in Theorem 1 are the canonical variances of design d (see section 2). Thus A-optimality, D-optimality, and E-optimality are among the many standard optimalities enjoyed by affine resolvable designs. Not addressed by Theorem 1 is the behavior of affine resolvable designs with respect to the MV-optimality criterion. The MV-value of a design is the maximal variance of the $v(v-1)/2$ estimates of pairwise treatment contrasts; a design is MV-optimal if it minimizes the MV-value over all relevant competitors. Because the MV-value is not solely a function of the canonical variances, even global optimality for canonical variances (as given in Theorem 1) need not imply MV-optimality. Indeed it is easily shown that, despite having identical canonical variances, different affine resolvable designs for the same (v, r, k) can have different MV-values (see lemma 1 below).

Recently Morgan (2009) has undertaken a study to determine, among all affine resolvable designs with given (v, r, k), the best with respect to the MV criterion. This raises an important, and very interesting, question:

If design d is MV-best among affine resolvable designs, is it MV-best over all resolvable designs for the same (v, r, k)? (1)

The answer to question (1), as will be seen, is "sometimes."

Now consider the orthogonal arrays OA$(v, r, 2)$ for two symbols 1 and 2. Precisely, a $v \times r$ array of 1's and 2's is an OA if the pairs formed by the rows of any two columns are every ordered pair $(1, 1)$, $(1, 2)$, $(2, 1)$, and $(2,2)$ with equal frequency $v/4$. Writing $\mu = v/4$ for this count, Shrikhande and Bhagwandas (1969) established the equivalence of $\mathrm{OA}(v,r,2)$ and affine resolvable designs with $(v,r,k) = (4\mu, r, 2\mu)$ having $s = 2$ blocks per replicate. It is these designs that will be the focus here in addressing the question raised above, with special emphasis on small replication $r \leq 4$.

Interest in two-level orthogonal arrays as fractional factorial designs has been strong since their introduction by Rao (1947), with many notable advances having been achieved in the last two decades. Their importance is reflected in their central roles in both applied and more theoretical texts: see, for example, Dey (1985), Dey and Mukerjee (1999), or Wu and Hamada (2000). The use of orthogonal arrays and related combinatorial structures as resolvable designs, though having been paid less attention, is nonetheless a valuable statistical application, holding many unsolved problems.

2 MV properties of ARDs based on OA$(v, r, 2)$

The variances of elementary treatment contrasts, also called *pairwise variances* when scaled by the plot variance σ^2, are easily determined for affine resolvable designs. For any binary block design d, let λ_{dij} be the number of blocks containing both treatments i and j, called a treatment concurrence count.

Lemma 1. *(Bailey, Monod, Morgan, 1995) When using an affine resolvable design d, the pairwise variance $p_{dij} = \mathrm{Var}_d(\widehat{\tau_i - \tau_j})/\sigma^2$ is a linear function of λ_{dij}. Specifically,*

$$p_{dij} = \frac{2[r - \lambda_{dij} + k(r-1)]}{kr(r-1)}. \tag{2}$$

More generally for block design d with $v \times bk$ treatment/plot incidence matrix A_d and $b \times bk$ block/plot incidence matrix L, the pairwise variances are calculated as

$$p_{dij} = e'_{ij} C_d^{+} e_{ij} \tag{3}$$

where e_{ij} is the $v \times 1$ vector with 1 in position i, -1 in position j, and 0 otherwise; $C_d = A_d'(I - L(L'L)^{-1}L')A_d$ is the treatments information matrix; and C_d^+ is the Moore-Penrose inverse of C_d. The $v-1$ largest eigenvalues of C_d^+ are the canonical variances mention in section 1. Equation (3) is derived in Dey (1986, page 59).

So long as one is only discussing affine resolvable designs, lemma 1 says the pairwise variances are completely determined by the treatment concurrences, with MV-value found from the smallest concurrence. For other resolvable designs this is not generally true, and because direct calculation of (3) is usually not feasible other than on a case-by-case basis (though see Theorem 2 below), other methods are needed for evaluating MV-values. One of these is the bound of the next lemma.

Lemma 2. *(Jacroux, 1983) When using a resolvable design d having r replicates in blocks of size k, the pairwise variance p_{dij} must satisfy*

$$p_{dij} \geq \frac{2k}{r(k-1) + \lambda_{dij}} \tag{4}$$

Now consider an arbitrary resolvable design for two or three replicates having two blocks per replicate. Let B_{fg} be the g^{th} block in replicate f. With no loss of generality it may be assumed that $B_{11} \cap B_{21} = S_1$ is a nonempty subset of the treatments, and write $S_2 = B_{11} \cap B_{22}$ for the treatments in B_{11} other than those in S_1. Then $B_{12} = S_3 \cup S_4$ where $S_3 = B_{12} \cap B_{21}$ and $S_4 = B_{12} \cap B_{22}$ (see Figure 1). The first two replicates are determined by the numbers of treatments v_e in the sets S_e, $e = 1, 2, 3, 4$. A third replicate can now be described in terms of subsets of the S_e: let S_{em} be the subset of S_e that occurs in block m of the third replicate. With v_{em} the size of S_{em}, any three-replicate resolvable design with two blocks per replicate is determined by the v_e and the v_{em}. Thus Figure 1 displays the general form for the designs in question.

Theorem 2. *The affine resolvable design having $r = 2$ replicates of $v = 4\mu$ treatments in blocks of size $k = 2\mu$ is MV-optimal over all resolvable designs for these values of (v, r, k).*

Proof. The information matrix for a resolvable design d in this class

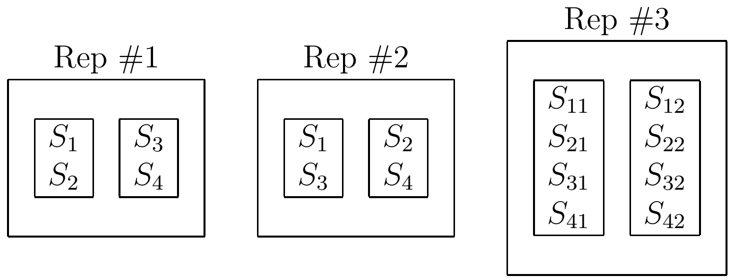

Figure 1: Resolvable design with three replicates, two blocks per replicate

is the partitioned matrix

$$C_d = \begin{pmatrix} 2(I - \frac{1}{k}J) & -\frac{1}{k}J & -\frac{1}{k}J & 0 \\ -\frac{1}{k}J & 2(I - \frac{1}{k}J) & 0 & -\frac{1}{k}J \\ -\frac{1}{k}J & 0 & 2(I - \frac{1}{k}J) & -\frac{1}{k}J \\ 0 & -\frac{1}{k}J & -\frac{1}{k}J & 2(I - \frac{1}{k}) \end{pmatrix}$$

with partition sizes v_1, v_2, v_3, v_4; J is the all ones matrix. It is easily verified that the following matrix, found as $C_d^+ = (C_d + \frac{1}{k}J)^{-1} - \frac{1}{4k}J$, is the Moore-Penrose inverse of C_d:

$$C_d^+ = \begin{pmatrix} \frac{1}{2}[I + \frac{(v_1+v_4)}{v(v-v_1-v_4)}J] & -\frac{1}{2v}J & -\frac{1}{2v}J & -\frac{(2v-v_1-v_4)}{2v(v-v_1-v_4)}J \\ -\frac{1}{2v}J & \frac{1}{2}[I + \frac{(v_2+v_3)}{v(v-v_2-v_3)}J] & -\frac{(2v-v_2-v_3)}{2v(v-v_2-v_3)}J & -\frac{1}{2v}J \\ -\frac{1}{2v}J & -\frac{(2v-v_2-v_3)}{2v(v-v_2-v_3)}J & \frac{1}{2}[I + \frac{(v_2+v_3)}{v(v-v_2-v_3)}J] & -\frac{1}{2v}J \\ -\frac{(2v-v_1-v_4)}{2v(v-v_1-v_4)}J & -\frac{1}{2v}J & -\frac{1}{2v}J & \frac{1}{2}[I + \frac{(v_1+v_4)}{v(v-v_1-v_4)}J] \end{pmatrix}$$

Then for $i \in S_1$ and $j \in S_4$, the pairwise variance p_{dij}, using (3) and the fact that $v_1 = v_4$, is $p_{dij} = 1 + \frac{2}{v-2v_1}$. Similarly for $i \in S_2$ and $j \in S_3$, using $v_2 = v_3 = \frac{v}{2} - v_1$, $p_{dij} = 1 + \frac{1}{v_1}$. All other pairwise variances are smaller than these. The maximum of these two larger variances is minimized when $v_1 = v_2 = v_3 = v_4 = v/4$, in which case d is affine.

The proof of Theorem 2 goes through even when affineness is not possible.

Corollary 1. *The resolvable design having $r = 2$ replicates of $v = 4\mu + 2$ treatments in blocks of size $k = 2\mu + 1$, specified by $v_1 = v_4 = (v-2)/4$ and $v_2 = v_3 = (v+2)/4$, is MV-optimal over all resolvable designs for these values of (v, r, k).*

Any resolvable design $(v, r, k = v/2)$ can be converted into a $v \times r$ two-level array A as follows:

$$A_{ij} = \begin{cases} 1 \text{ if treatment } i \text{ is in block 1 of the } j^{th} \text{ replicate,} \\ 2 \text{ if treatment } i \text{ is in block 2 of the } j^{th} \text{ replicate.} \end{cases}$$

If the resolvable design is affine, then A is an orthogonal array; this is the equivalence mentioned in section 1. The design of corollary 1 corresponds to a balanced array (Chakravarti, 1956), proven type-1 optimal as a resolvable design in corollary 21 of Morgan and Reck (2007).

For three replicate designs as in Figure 1, the MV-best affine design, call it d^*, is specified (up to isomorphism) by $v_1 = v_2 = v_3 = v_4 = v/4$ and $v_{11} = v_{22} = v_{32} = v_{41} = 0$, $v_{12} = v_{21} = v_{31} = v_{42} = v/4$ (Morgan, 2009). Design d^* has $\lambda_{d^*ij} = 3$ for $v(v-4)/32$ pairs $i < j$, and all other $\lambda_{d^*ij} = 1$.

Lemma 3. *The design d^* is the only resolvable design d for $(v, r, k) = (4\mu, 3, 2\mu)$ having no λ_{dij} equal to zero.*

Proof. Let d be an arbitrary resolvable design for $(v, r, k) = (4\mu, 3, 2\mu)$, i.e. d has form displayed in Figure 1. There is no loss of generality in assuming $v_1 = |S_1| \geq v/4$ (if $v_1 < v/4$ then reverse the blocks in the second replicate and interchange subscripts $e = 1$ and $e = 2$ on the S_e and S_{em}). If d has all $\lambda_{dij} > 0$ then each treatment in S_1 (S_2) is in at least one block with each treatment of S_4 (respectively S_3). Inspection of Figure 1 shows that this implies $\lambda_{d0} = 0$ where

$$\begin{aligned} \lambda_{d0} &\equiv \#\{(i,j) : \lambda_{dij} = 0 \text{ and } i < j\} \\ &= v_{11}v_{42} + v_{12}v_{41} + v_{21}v_{32} + v_{22}v_{31} \end{aligned} \tag{5}$$

Each of the eight terms v_{em} in (5) is a nonnegative integer, so $\lambda_{d0} = 0$ says at least one of the two terms in each product is zero. If $v_{11} = 0$ then $v_{12} = v_1 - v_{11} = v_1 \geq v/4 \Rightarrow v_{41} = 0 \Rightarrow v_{42} = v_4 - v_{41} = v_4 = v_1$. But $v/2 = |B_{32}| \geq v_{12} + v_{42} = v_1 + v_4 \geq v/4 + v/4 = v/2 \Rightarrow v_{12} = v_{42} = v/4 = v_1 = v_4 \Rightarrow v_{21} = v_{31} = v/4 = v_2 = v_3$; this is d^*. A parallel argument reaches the same conclusion if $v_{12} = 0$. If both $v_{11} > 0$ and $v_{12} > 0$ then $v_{41} = v_{42} = 0 \Rightarrow v_4 = 0$, contradicting $v_1 = v_4$.

Theorem 3. *The affine resolvable design d^* is uniquely MV-optimal over all resolvable designs for $(v, r, k) = (4\mu, 3, 2\mu)$.*

Proof. Putting $\lambda_{d^*ij} = 1$ for $r = 3$, $k = v/2$ in (2), the MV-value for d^* is $\mathrm{MV}_{d^*} = 2(v+2)/3v$. For any other resolvable design d, lemma 3 says $\lambda_{dij} = 0$ for some i, j, so by (4),

$$\mathrm{MV}_d \geq \frac{v}{3(\frac{v}{2}-1)} > \frac{2(v+2)}{3v} = \mathrm{MV}_{d^*}$$

as claimed.

The positive results of Theorems 2 and 3 do not carry through for four replicates. For $(v, r, k) = (4\mu, 4, 2\mu)$ and $v \equiv 4 \pmod 8$ every affine resolvable design has at least $(v-6)/2$ pairs $i < j$ such that $\lambda_{dij} = 0$ (Morgan, 2009). Thus from (3) the MV-value is $\mathrm{MV}_{\mathrm{ARD}} = (3v+8)/6v$. This is bested by the design $\tilde{d}$ constructed like this: the first three replicates are as in Figure 1 with $v_1 = v_2 = v_3 = v_4 = v/4$ and $v_{11} = v_{41} = (v+4)/8$, $v_{21} = v_{31} = (v-4)/8$; the fourth replicate has one block consisting of S_1 and S_4, and one block consisting of S_2 and S_3.

The information matrix for $\tilde{d}$ is easily worked out; needed here is an expression for that matrix amenable to calculating the MV-value. Write $A_1 = c_1c_1'$ for $c_1 = \frac{1}{2}(1, -1, -1, 1)'$, $A_2 = c_2c_2'$ for $c_2 = \frac{1}{\sqrt{v_{21}}}(0'_{v_{11}}, 1'_{v_{21}})'$, and $A_3 = c_3c_3'$ for $c_3 = \frac{1}{\sqrt{v_{11}}}(1'_{v_{11}}, 0'_{v_{21}})'$. Now define four orthogonal, $v \times v$ projection matrices $P_1, \ldots, P_4$ by

$$P_1 = I_4 \otimes (I - A_2 - A_3) + (I - A_1) \otimes (A_2 + A_3 - \frac{4}{v}J),\ P_2 = A_1 \otimes A_2,$$

$$P_3 = (I - A_1 - \frac{1}{4}J_4) \otimes \frac{4}{v}J,\ P_4 = A_1 \otimes A_3$$

Readers can check that $C_{\tilde{d}} = \sum_{i=1}^4 e_{\tilde{d}i}P_i$ where $e_{\tilde{d}1} = 4$, $e_{\tilde{d}2} = 3 + \frac{4}{v}$, $e_{\tilde{d}3} = 3$, and $e_{\tilde{d}4} = 3 - \frac{4}{v}$. Because the P_i are orthogonal projectors, this is the spectral decomposition of $C_{\tilde{d}}$ and the $e_{\tilde{d}i}$ are the eigenvalues of $C_{\tilde{d}}$ with multiplicities equal to the ranks of the S_i. The Moore-Penrose inverse of $C_{\tilde{d}}$ is simply $C_{\tilde{d}}^+ = \sum_{i=1}^4 z_{\tilde{d}i}P_i$ where the $z_{\tilde{d}i} = e_{\tilde{d}i}^{-1}$ are the canonical variances. The largest pairwise variance, easily found from direct inspection of $C_{\tilde{d}}^+$, occurs for any pair i, j such that $i \in S_{11} \cup S_{41}$ and $j \in S_{22} \cup S_{32}$. Its value $\mathrm{MV}_{\tilde{d}}$ simplifies to

$$\mathrm{MV}_{\tilde{d}} = \frac{(3v-2)(3v+4)}{6v(3v-4)} < \frac{(3v+8)}{6v} = \mathrm{MV}_{\mathrm{ARD}},$$

establishing the final result of this section.

Theorem 4. *The MV-best affine resolvable design for* $(v, r, k) = (4\mu, 4, 2\mu)$ *with odd* μ *is never MV-optimal over all resolvable designs for these values of* (v, r, k).

3 Discussion and conjecture

It has been shown that the MV-best affine resolvable designs based on 2-level orthogonal arrays are MV-optimal resolvable designs for two and three replicates, but need not be so for four replicates. At the other extreme for r, the maximal replication for affine resolvable designs with two blocks per replicate is $v - 1$, corresponding to a saturated orthogonal array (equivalently, a Hadamard matrix of order v). These $(v-1)$-replicate designs are BIBDs and so are MV-optimal over more than just resolvable designs. This with the similar result for $r = v - 2$ is stated as Theorem 5.

Theorem 5. *An affine resolvable design with* r *replicates in blocks of size* $k = v/2$ *is MV-optimal over all block designs with* $(b, k) = (2r, v/2)$, *for* $r = v - 1$ *and for* $r = v - 2$.

Proof. The result for BIBDs is well known. Deleting any one replicate from the $(v-1)$-replicate design gives d with all $\lambda_{dij} \in \{\frac{v}{2} - 1, \frac{v}{2} - 2\}$. This is a group divisible design having $\lambda_2 = \lambda_1 + 1$, MV-optimal over the full class by the unnumbered theorem on page 144 of Takeuchi (1961).

While Theorems 2, 3, 4 and 5 provide some answers to the main question in (1), there is still much to be done. In the spirit of Professor Dey's tireless educational and research efforts in experimental design, here is a list of specific problems suggested by the work here:

- Are the non-affine designs $\tilde{d}$ for $v \equiv 4 \pmod 8$ and $(r, k) = (4, \frac{v}{2})$ in fact MV-optimal resolvable designs? Notably, these designs correspond to neither orthogonal nor balanced arrays.
- Are the MV-best affine resolvable designs for $v \equiv 0 \pmod 8$ and $(r, k) = (4, \frac{v}{2})$, identified in Morgan (2009), MV-optimal over all resolvable designs?

- The MV-best affine resolvable designs for $(r,k) = (5, \frac{v}{2})$ have also been identified in Morgan (2009). Which of these, if any, are MV-optimal resolvable designs?

My conjectures for the answers to the first two questions are both *yes*. For the third, I suspect the answer is yes only for those designs with all $\lambda_{dij} \geq 1$.

More broadly, other than for simple cases like BIBDs and the one-replicate deletions in Theorem 5, little seems to be known about MV-optimality in the important class of resolvable designs. There are many interesting combinatorial questions tied to the MV-problem, including the relevance of balanced arrays or other generalizations of orthogonal arrays that may prove to be useful in this context. The challenging problem of MV-optimal resolvable designs is wide open.

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