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OPTIMAL RESOLVABLE DESIGNS WITH MINIMUM PV ABERRATION

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Abstract: Amongst resolvable incomplete block designs, affine resolvable designs are optimal in many conventional senses. However, different affine resolvable designs for the same numbers of treatments and replicates, and the same block size, can differ in how well they estimate elementary treatment contrasts. An aberration criterion is employed to distinguish the best of the affine resolvable designs for this task. Methods for constructing the best designs are detailed and an extensive online catalog is compiled.

Key words and phrases: Affine resolvable block design, design optimality, orthogonal array, pairwise variance aberration.

1. Introduction

An oft-sought property of incomplete block designs is resolvability: 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. The sets of this partition may be used to accommodate a second blocking factor, orthogonal to treatments, and containing the first. Quite naturally, the sets, or "large" blocks, are termed replicates, the number of which is denoted by r. Examples of the use of resolvable designs are abundant and may be found in several of the papers cited forthwith.

One special class of resolvable designs has received special attention, for good reason. Suppose any two blocks from distinct replicates of a resolvable design intersect in the same number of treatments, call this number μ. Such a design is said to be *affine resolvable* (Bose (1942)). Using s to denote the number of small blocks per replicate in a resolvable design, and b the total number of small blocks, then $v = ks$ and $b = rs$. For an affine resolvable design, the number μ is necessarily $\mu = k/s$, and so $v = \mu s^2$ and $k = \mu s$. That k is a multiple of s is the limitation imposed by affineness relative to all resolvable designs. The advantage gained is a host of very nice statistical properties.

Bailey, Monod and Morgan (1995) established Schur-optimality of affine resolvable designs amongst all resolvable designs with the same v, r, and k. Thus an affine resolvable design minimizes (i) the average variance of any complete set of orthonormal treatment contrasts, which is proportional to the average variance of the $v(v-1)/2$ pairwise treatment contrasts (i.e., is A-optimal); (ii) the largest variance over all normalized treatment contrasts (i.e., is E-optimal); (iii) the volume of the confidence ellipsoid for any $v-1$ orthonormal treatment contrasts (i.e., is D-optimal). Moreover, the treatment contrasts estimation space is especially simple for an affine resolvable design, there being just two canonical efficiency factors 1 and $(r-1)/r$.

Given these excellent statistical properties, one might think that every affine resolvable design with the same v, r, and k should be equally efficacious. Inspection of the variances of the elementary treatment contrasts, however, shows this notion to be false, for the distribution of these variances depends on the particular affine resolvable design selected. The purpose of this paper is to identify the best of the affine resolvable designs for estimation of elementary contrasts. Section 2 formalizes the notion of "best," provides two representations of affine resolvable designs useful in finding best designs, and constructs a family of best designs based on orthogonal Latin squares. Section 3 provides a full solution in up to five replicates having two blocks per replicate. The known best designs for up to 200 treatments are compiled in an online catalog, as discussed in Section 4. Section 5 includes additional discussion and examples.

2. Minimum PV Aberration

Though not generally partially balanced, affine resolvable designs share an important property with the partially balanced incomplete block designs. This property, stated next as a lemma, is the key to ordering the designs in terms of how well they estimate elementary contrasts. For a given affine resolvable design, let λ_{ij} be the number of small blocks containing both treatments i and j. For any resolvable design write p_{ij} for the pairwise variance $\mathrm{VAR}(\widehat{\tau_i - \tau_j})$.

Lemma 1. (Bailey, Monod and Morgan (1995)) *The pairwise variance p_{ij} when using an affine resolvable design is a linear function of λ_{ij}. Specifically,*

$$p_{ij} = \frac{2[r - \lambda_{ij} + k(r-1)]}{kr(r-1)}\sigma^2, \tag{2.1}$$

where σ^2 is the plot variance.

The best affine resolvable design for estimating elementary treatment contrasts is one that, in some appropriate sense, makes the $v(v-1)/2$ quantities p_{ij} in (2.1) small. Lemma 1 says that, equivalently, the quantities λ_{ij} should be made large in a correspondingly appropriate sense. Since every resolvable design has $\sum_i \sum_{j>i} \lambda_{ij} = bk(k-1)/2$, the average pairwise variance for every affine resolvable design is the same (and, as mentioned in Section 1, is minimal over all resolvable designs). If the collection of p_{ij} (or λ_{ij}) for an affine design is thought of as a uniform distribution on its points, then the problem is one of selecting among distributions with the same mean. The statistically meaningful route is to consider the tails of these distributions. Specifically, minimizing the number of poorly estimated elementary contrasts is achieved by selecting a design for which the left tail of its λ_{ij} distribution is dominant in a natural sense. This motivates the following definition.

Definition 1. For any affine resolvable design d, let $\eta_{du} = |(i,j) : i < j$ and $\lambda_{ij} = u|$ and write $\eta_d = (\eta_{d0}, \eta_{d1}, \ldots, \eta_{dr})$. Design d_1 is said to have smaller *pairwise variance aberration* (shortly, *PV-aberration*) than design d_2 if, for some t, $\eta_{d_1t} < \eta_{d_2t}$ and $\eta_{d_1u} = \eta_{d_2u}$ for $u < t$. If no affine design has smaller PV-aberration than d, then d has *minimum PV-aberration*.

If a design has minimum PV-aberration, then it minimizes the maximal p_{ij}, that is, it is MV-optimal amongst all affine resolvable competitors. Minimal PV-aberration is generally stronger than MV-optimality, however, for it examines more than just the largest p_{ij}. When there are several MV-optimal designs, minimizing PV-aberration selects among them according to the next largest pairwise variance, then the next, and so on, sequentially on the ordered p_{ij}.

The task of determining the best affine resolvable design for pairwise comparisons has been translated into a study of the η_{du}, beginning with η_{d0}. Needed now is a description of affine resolvable designs that lends itself to evaluating these quantities. Two such descriptions will be given here, beginning with the sometimes useful connection to orthogonal arrays.

Bailey, Monod and Morgan (1995) constructed affine resolvable designs based on orthogonal arrays of strength two as follows. Begin with an orthogonal array OA(v, r, s) having v rows, r columns, and s symbols in each column, such that the rows of any two columns produce the s^2 ordered pairs of symbols μ times each; necessarily $v = \mu s^2$. Placing treatment i in block m of replicate q if and only if the m^{th} symbol occurs in row i, column q, produces an affine resolvable design (v, r, k) for $k = v/s$. This process is reversible, i.e., strength two orthogonal arrays and affine resolvable designs are equivalent combinatorial objects (see Shrikhande and Bhagwandas (1969) and Morgan (1996)). Now λ_{ij} is the number of columns in the orthogonal array for which rows i and j share the same symbol. These numbers are the basis for the *power moments* of a fractional factorial design as defined by Xu (2003). Good factorial designs are found by sequentially *minimizing* the power moments (e.g., Theorem 2 of Xu (2003)); in a broad sense this says to make the λ_{ij} *small*. Thus the orthogonal arrays sought here are quite different from those pursued in the fractional factorial literature.

Rep #1

S_1	S_{s+1}		S_{s^2-s+1}
S_2	S_{s+2}	$\cdots$	S_{s^2-s+2}
$\vdots$	$\vdots$		$\vdots$
S_s	S_{2s}		S_{s^2}

Rep #2

S_1	S_2		S_s
S_{s+1}	S_{s+2}	$\cdots$	S_{2s}
$\vdots$	$\vdots$		$\vdots$
S_{s^2-s+1}	S_{s^2-s+2}		S_{s^2}

Figure 1. First two replicates of an arbitrary affine resolvable design.

Rep #1

S_1	S_3
S_2	S_4

Rep #2

S_1	S_2
S_3	S_4

Rep #3

S_{11}	S_{12}
S_{21}	S_{22}
S_{31}	S_{32}
S_{41}	S_{42}

Rep #4

S_{111}, S_{121}	S_{112}, S_{122}
S_{211}, S_{221}	S_{212}, S_{222}
S_{311}, S_{321}	S_{312}, S_{322}
S_{411}, S_{421}	S_{412}, S_{422}

Rep #5

$S_{1111}, S_{1211}, S_{1121}, S_{1221}$	$S_{1112}, S_{1212}, S_{1122}, S_{1222}$
$S_{2111}, S_{2211}, S_{2121}, S_{2221}$	$S_{2112}, S_{2212}, S_{2122}, S_{2222}$
$S_{3111}, S_{3211}, S_{3121}, S_{3221}$	$S_{3112}, S_{3212}, S_{3122}, S_{3222}$
$S_{4111}, S_{4211}, S_{4121}, S_{4221}$	$S_{4112}, S_{4212}, S_{4122}, S_{4222}$

Figure 2. Affine resolvable design for $s = 2$ with 5 replicates.

The second description, here called the *standard description*, takes direct advantage of the block intersection property. Fix any ordering of the replicates, then the first two replicates produce a partition of the treatments into sets $S_1, S_2, \ldots, S_{s^2}$, each set of size μ (see Figure 1). Replicate $x > 2$ may then be described in terms of subsets of sets of treatments appearing in replicate $x-1$, as follows: for $e = 1, \ldots, s^2$ and $x = 3, \ldots, r$, the set $S_{e\,m_1m_2\cdots m_{x-2}}$ to be the subset of $S_{e\,m_1m_2\cdots m_{x-3}}$ that appears in block m_{x-2} of replicate x. This is displayed for five replicates with $s = 2$ in Figure 2 where, for example, S_{11} is the subset of S_1 appearing in the first block of replicate three, S_{112} is the subset of S_{11} appearing in the second block of replicate four, and S_{1121} is the subset of S_{112} in the first block of replicate five. Denote the number of treatments in $S_{e\,m_1m_2\cdots m_x}$ by $v_{e\,m_1m_2\cdots m_x} \geq 0$.

The two descriptions provide two paths for attacking the PV-aberration problem. The standard description is employed for the remainder of this section and throughout Section 3, providing a common framework for all of the results obtained. Some of these, though not all, can also be derived with roughly equivalent effort working with the OA formulation and OA identities. The OA description is taken up again in Section 4, allowing best designs to be plucked from existing OA enumerations.

The standard description admits useful formulae for the η_{du}. Write $m = (m_1, \ldots, m_{r-2})$ where each $m_i \in \{1, \ldots, s\}$. Starting with $s = 2$ as an example, if m and m' differ in every coordinate, then members of S_{1m} have never occurred with members of $S_{4m'}$, and members of S_{2m} have never occurred with members of $S_{3m'}$. Observe that η_{d0} simply counts the treatment pairs formed by each member of S_{1m} with each member of $S_{4m'}$, and each member of S_{2m} with each member of $S_{3m'}$. That is, $\eta_{d0} = \sum\sum(v_{1m}v_{4m'} + v_{2m}v_{3m'})$, the sums being over all m and m' such that the Hamming distance between m and m' is $h(m, m') = r - 2$. Extending this perspective, for any subscript e, let $B(e)$ be the collection of subscripts for the sets among $S_1, \ldots, S_{s^2}$ that are contained in a small block with S_e in either of the first two replicates (other than e itself). For instance, $B(1) = \{2, \ldots, s\} \cup \{s + 1, 2s + 1, (s - 1)s + 1\}$ (see Figure 1). Let $A(e)$ be all other subscripts (other than e itself). Following the same reasoning for general s demonstrated for $s = 2$ above gives

$$\eta_{d0} = \frac{1}{2}\sum_{e}\sum_{e' \,\in\, A(e)}\sum_{\substack{m,m' \ni: \\ h(m,m')=r-2}}\sum v_{em}v_{e'm'}, \tag{2.2}$$

which is a special case of this more general expression for $u = 0, 1, \ldots, r - 1$:

$$\eta_{du} = \frac{1}{2}\Bigg[\sum_{e}\sum_{e' \,\in\, A(e)}\sum_{\substack{m,m' \ni: \\ h(m,m')=r-2-u}}\sum v_{em}v_{e'm'} + \sum_{e}\sum_{e' \,\in\, B(e)}\sum_{\substack{m,m' \ni: \\ h(m,m')=r-1-u}}\sum v_{em}v_{e'm'}$$
$$+ \sum_{e}\sum_{\substack{m,m' \ni: \\ h(m,m')=r-u}}\sum v_{em}v_{em'}\Bigg]. \tag{2.3}$$

The number of treatment pairs in a block in every replicate is $\eta_{dr} = \sum_e\sum_m v_{em}$ $(v_{em} - 1)/2$.

With these expressions in hand, methods for constructing minimum PV-aberration designs can be obtained. A general method based on sets of mutually orthogonal Latin squares (MOLS) is given next.

Let $L_1, \ldots, L_{r-2}$ be a set of $r - 2$ MOLS of order s, and let L_0 be the $s \times s$ array whose entries are the s^2 sets of size μ exactly as displayed in the first replicate of Figure 1. The first two replicates of an affine resolvable design are as displayed in Figure 1. For each $y = 1, \ldots, r-2$, block m of replicate $y+2$ contains the sets of L_0 that are in the same cells as the m^{th} symbol of L_y. It is easy to see that this produces an affine resolvable design with r replicates, since any two blocks from different replicates intersect in exactly one of the sets $S_1, \ldots, S_{s^2}$.

Not obvious, but proven next, is that this design, call it d^*, has minimum PV-aberration. Examples of d^* are given in the first paragraph of Section 3 and by Example 1 of Section 5.

Theorem 1. *The affine resolvable design d^* has minimum PV-aberration.*

Proof. It will be shown that only designs of the form d^* minimize η_{d0}, and that η_{d^*} is the same vector regardless of the choice of orthogonal Latin squares. As always the first two replicates of any affine resolvable design are as displayed in Figure 1. To begin, consider $r = 3$. Then m in S_{em} is a singleton and η_{d0} is

$$\begin{aligned}
\eta_{d0} &= \frac{1}{2}\sum_e \sum_{e'\in A(e)} \sum_m \sum_{m'\neq m} v_{em}v_{e'm'} = \frac{1}{2}\sum_e \sum_{e'\in A(e)} \sum_m v_{em}(v_{e'} - v_{e'm}) \\
&= \frac{1}{2}\sum_e \sum_{e'\in A(e)} \sum_m v_{em}(\mu - v_{e'm}) = \frac{s^2(s-1)^2}{2}\mu^2 - \frac{1}{2}\sum_e\sum_m v_{em}\Bigg(\sum_{e'\in A(e)} v_{e'm}\Bigg) \\
&= \frac{s^2(s-1)^2}{2}\mu^2 - \frac{1}{2}\sum_e\sum_m v_{em}\Bigg((s-1)\mu - \frac{1}{2}\sum_{e'\in B(e)} v_{e'm}\Bigg) \\
&\qquad \text{(by affineness of reps 1 and 3)} \\
&= \frac{(s-1)(s-2)}{2}\mu v + \frac{1}{4}\sum_m\sum_e\sum_{e'\in B(e)} v_{em}v_{e'm}. \qquad (2.4)
\end{aligned}$$

From (2.4), η_{d0} attains its minimum value if and only if $v_{em}v_{e'm} = 0$ for every $m \in \{1,\ldots,s\}$, $e \in \{1,\ldots,s^2\}$, and $e' \in B(e)$. That is, η_{d0} is minimized if and only if any two treatments from distinct sets and in the same block in replicates one or two, are in different blocks in replicate three. Now if the treatments in any set S_e are not all in the same block in replicate three, then the minimum cannot be attained, for there are then at most $s-2$ blocks into which treatments from the other $s-1$ sets occurring with S_e in replicate one can be placed. Thus each block in replicate three must consist of s of the sets $S_1,\ldots,S_{s^2}$, and $e' \in B(e) \Rightarrow S_e$ and $S_{e'}$ are in different blocks in replicate three. This says precisely that the minimum for η_{d0} is uniquely attained when the blocks of replicate three are disjoint transversals of L_0, that is, when they are formed as in d^*.

For a design with two replicates the number of treatment pairs that have not occurred in a block is $\eta_{d0} = (s-1)^2\mu v/2$, and for three replicates the minimum PV-aberration design has $\eta_{d0} = (s-1)(s-2)\mu v/2$, a decrease of $(s-1)\mu v/2$ due to the third replicate. It is easy to see that any choice of L_1 to build d^* gives the same vector η_{d^*}, which is $((s-1)(s-2)\mu v/2, 3(s-1)\mu v/2, 0, s^2\mu(\mu-1)/2)$. Thus for three replicates, only designs of form d^* have minimum PV-aberration.

Moreover, it is now clear that for $r \geq 3$, the absolute minimum of η_{d0} is achieved if and only if, relative to the first two replicates, each of replicates

$3, \ldots, r$ independently decreases η_{d0} by the maximal amount of $(s-1)\mu v/2$. This happens if and only if (i) for each of these replicates the blocks are disjoint transversals of L_0, and (ii) no two of the sets $S_1, \ldots, S_{s^2}$ occur together in more than one small block. Property (i) says that the replicates correspond to $r-2$ Latin squares as in the construction for d^*, and property (ii) says those Latin squares are orthogonal. Thus minimization of η_{d0} requires a design of form d^*. Regardless of the MOLS $L_1, \ldots, L_{r-2}$ employed to build d^*,

$$\eta_{d^*} = \left(\frac{(s-1)(s-r+1)}{2}\mu v, \frac{(s-1)r}{2}\mu v, 0, \ldots, 0, \frac{1}{2}(\mu-1)v \right).$$

This is because any two treatments in the same set S_e occur together in one small block in every replicate, and any other two treatments, from sets S_e and $S_{e'}$ say, occur together in no or one small block as S_e and $S_{e'}$ do the same. This completes the proof.

3. Minimum PV-Aberration with Two Blocks per Replicate

Affine resolvable designs with two blocks per replicate are shown for up to five replicates, in the standard representation, in Figure 2. The block intersection number is $\mu = v/4$, and so v must be a multiple of 4. This section will determine the minimum PV-aberration designs for $s = 2$ and $r \leq 5$.

For $r = 2$ the best (and only) affine design is the first two replicates in Figure 2. To this add the replicate

$$\text{Rep \#3} \quad \boxed{\boxed{\begin{array}{c} S_2 \\ S_3 \end{array}} \quad \boxed{\begin{array}{c} S_1 \\ S_4 \end{array}}} \tag{3.1}$$

to get the unique minimum-PV aberration design in three replicates, having $\eta_{d0} = 0$. In terms of the third replicate in Figure 2, this choice results from selecting set sizes $v_{11} = v_{41} = 0$ and $v_{21} = v_{31} = \mu$. This is an example of design d^* of Theorem 1.

Affine resolvability places a number of restrictions on the set sizes v_{em}. These restrictions may be written as a collection of linear equations, any solution to which specifies an affine resolvable design, so long as that solution consists entirely of nonnegative integers. For instance, there are eight set sizes for the third replicate in Figure 2, but in fact only one is linearly independent: all designs are specified by all values of $v_{11} \in \{0, \ldots, \mu/2\}$. While the numbers of sets, and consequently the number of independent set sizes, grow with r, they are still manageable for $r \leq 5$. Minimum PV-aberration designs can be determined for these cases by solving the equations with the additional restriction that η_{d0} be minimized. When there are multiple solutions, these are compared on η_{d1}, then η_{d2}, and so on. Details of this approach are presented in the subsections below covering four and five replicates.

3.1. Four replicates with two blocks per replicate

For four replicates there are 24 set sizes $v_{11}, v_{21}, \ldots, v_{42}$ and $v_{111}, v_{121}, \ldots,$ v_{422} (cf. Figure 2). Linear restrictions on these quantities arise from the basic properties of any affine resolvable design for $s = 2$: each replicate contains all v treatments, each block contains $v/2$ treatments, and any two blocks from different replicates intersect in $v/4$ treatments. Let B_{fg} be the g^{th} block in replicate f. As previously mentioned, v_{11} determines all of the v_{em} for the third replicate, since

$$\begin{array}{ll} \frac{v}{4} = |B_{11} \cap B_{31}| = v_{11} + v_{21} \;\Rightarrow & v_{21} = \frac{v}{4} - v_{11} \\ \frac{v}{4} = |B_{21} \cap B_{31}| = v_{11} + v_{31} \;\Rightarrow & v_{31} = \frac{v}{4} - v_{11} \\ \frac{v}{2} = |B_{31}| = \sum_e v_{e1} = v_{11} + \left(\frac{v}{4} - v_{11}\right) + \left(\frac{v}{4} - v_{11}\right) + \; v_{41} \Rightarrow & v_{41} = v_{11}, \end{array} \tag{3.2}$$

and $v_{e1} + v_{e2} = v/4$ for $e = 1, \ldots, 4$. For the fourth replicate, in addition to $v_{em2} = v_{em} - v_{em1}$ for $e = 1, \ldots, 4$ and $m = 1, 2$, there are four independent restrictions specified by $v/4 = |B_{11} \cap B_{41}| = |B_{21} \cap B_{41}| = |B_{31} \cap B_{41}| = |B_{32} \cap B_{41}|$. These yield

$$\begin{aligned} v_{221} &= \tfrac{v}{4} - v_{111} - v_{121} - v_{211} \\ v_{321} &= \tfrac{v}{4} - v_{111} - v_{121} - v_{311} \\ v_{411} &= \tfrac{v}{4} - v_{111} - v_{211} - v_{311} \\ v_{421} &= 2v_{111} + v_{121} + v_{211} + v_{311} - \tfrac{v}{4}. \end{aligned} \tag{3.3}$$

There are thus five free variables $v_{11}, v_{111}, v_{121}, v_{211}, v_{311}$. The determined variables above satisfy $0 \leq v_{221} \leq v_{22} = v_{11}$, $0 \leq v_{321} \leq v_{32} = v_{11}$, $0 \leq v_{411} \leq v_{41} = v_{11}$, and $0 \leq v_{421} \leq v_{42} = v/4 - v_{11}$. Thus the free variables, in addition to being nonnegative integers, must satisfy

$$\begin{array}{ccccc} \frac{v}{4} - v_{11} - v_{111} \leq & v_{121} + v_{211} & \leq & \frac{v}{4} - v_{111} \\ \frac{v}{4} - v_{11} - v_{111} \leq & v_{121} + v_{311} & \leq & \frac{v}{4} - v_{111} \\ \frac{v}{4} - v_{11} - v_{111} \leq & v_{211} + v_{311} & \leq & \frac{v}{4} - v_{111} \\ \frac{v}{4} - 2v_{111} & \leq v_{121} + v_{211} + v_{311} \leq & \frac{v}{2} - v_{11} - 2v_{111} \\ 0 & \leq & v_{111} & \leq & \frac{v_{11}}{2}, \end{array} \tag{3.4}$$

the last line with no loss of generality, and likewise $v_{11} \leq v/8$.

The initial problem is to satisfy the constraints (3.4) while minimizing $\eta_{d0} = v_{111}v_{422} + v_{121}v_{412} + \cdots + v_{222}v_{311}$. The best designs will be among those having $\eta_{d0} = 0$, whenever that value is achievable. The possibilities for $\eta_{d0} = 0$ are explored in the following two cases.

Case 1: $v_{11} = 0$. This says that the third replicate is the one displayed in (3.1). The inequalities (3.4) give $v_{111} = 0$ and $v_{121} = v_{211} = v_{311} = v/8$. Thus the fourth replicate is

$$\begin{array}{c}\text{Rep \#4}\\ \boxed{\begin{array}{cc} \boxed{\begin{array}{c} S_{121}\\ S_{211}\\ S_{311}\\ S_{421}\end{array}} & \boxed{\begin{array}{c} S_{112}\\ S_{222}\\ S_{322}\\ S_{412}\end{array}} \end{array}}\end{array} \tag{3.5}$$

with each set displayed in (3.5) being of size $v/8$.

Case 2: $v_{11} > 0$. Then (3.2) and $v_{11} \le v/8$ say that all the sets S_{e1} and S_{e2} are nonempty. If $\eta_{d0} = 0$, then each of the pairs (S_{11}, S_{42}), (S_{21}, S_{32}), (S_{22}, S_{31}), and (S_{12}, S_{41}) must occur in the same block of replicate four. For the first three of these pairs this says that $(v_{111}, v_{421}) = (0,0)$ or (v_{11}, v_{42}), $(v_{211}, v_{321}) = (0,0)$ or (v_{21}, v_{32}), and $(v_{221}, v_{311}) = (0,0)$ or (v_{22}, v_{31}). But $v_{111} = v_{11}$ contradicts the last inequality in (3.4), so $v_{111} = v_{421} = 0$. This leaves four combinations to explore, each of which leads to a contradiction (e.g., there is no design with $v_{111} = v_{421} = v_{211} = v_{321} = v_{221} = v_{311} = 0$), or to a design that is isomorphic to that found in Case 1. To illustrate the latter, if $(v_{211}, v_{321}) = (0,0)$ and $(v_{221}, v_{311}) = (v_{22}, v_{31})$ then replicate four must be

$$\begin{array}{c}\text{Rep \#4}\\ \boxed{\begin{array}{cc} \boxed{\begin{array}{c} S_{12}\\ S_{22}\\ S_{31}\\ S_{41}\end{array}} & \boxed{\begin{array}{c} S_{11}\\ S_{21}\\ S_{32}\\ S_{42}\end{array}} \end{array}}\end{array} \tag{3.6}$$

and $v/4 = |B_{21} \cap B_{41}| = v_{12} + v_{31} = 2(v/4 - v_{11}) \Rightarrow v_{11} = v/8$, and so all sets in (3.6) have size $v/8$. Now make new sets $S^*_{11} = S_{12}$, $S^*_{12} = S_{22}$, $S^*_{21} = S_{31}$, $S^*_{22} = S_{41}$, $S^*_{31} = S_{32}$, $S^*_{32} = S_{42}$, $S^*_{41} = S_{11}$, and $S^*_{42} = S_{21}$. Then among the blocks found here are $B_{11} = (S_{11}, S_{12}, S_{21}, S_{22}) = (S^*_{41}, S^*_{11}, S^*_{42}, S^*_{12}) = (S^*_1, S^*_4)$, $B_{31} = (S_{11}, S_{21}, S_{31}, S_{41}) = (S^*_{41}, S^*_{42}, S^*_{21}, S^*_{22}) = (S^*_2, S^*_4)$, and $B_{41} = (S_{12}, S_{22}, S_{31}, S_{41}) = (S^*_{11}, S^*_{12}, S^*_{21}, S^*_{22}) = (S^*_1, S^*_2)$, showing that replicates one, three, and four found here are identical to the first three replicates in Case 1, as claimed.

Table 1. Minimum PV-aberration designs for four replicates, two blocks per replicate.

v	$(v_{11}, v_{111}, v_{121}, v_{211}, v_{311})$	$\eta_d = (\eta_{d0}, \eta_{d1}, \eta_{d2}, \eta_{d3}, \eta_{d4})$
$v \equiv 0 \pmod 8$	$\left(0, 0, \frac{v}{8}, \frac{v}{8}, \frac{v}{8}\right)$	$\left(0, \frac{3v^2}{16}, \frac{3v^2}{16}, \frac{v^2}{16}, \frac{v(v-8)}{16}\right)$
$v \equiv 4 \pmod 8$	$\left(\frac{v-4}{8}, 0, 1, \frac{v-4}{8}, \frac{v+4}{8}\right)$	$\left(\frac{v-6}{2}, \frac{3v^2}{16}-(v-5), \frac{3v^2}{16}+3, \frac{v^2}{16}+(v-9), \frac{v(v-8)}{16}-\frac{(v-8)}{2}\right)$

Design variables not shown are determined by (3.2) and (3.3).

Cases 1 and 2 show that $\eta_{d0} = 0$ is uniquely achieved in four replicates, but only for v a multiple of 8. This solves the minimum PV-aberration problem for $v \equiv 0 \pmod 8$, but $v \equiv 4 \pmod 8$ requires further work leaning more heavily on the relations (3.2)$-$(3.4). Writing (2.2) in terms of the five free variables gives

$$\eta_{d0} = \frac{3v^2}{16} - 4x_0^2 - z(v - 4x_0) - (v - 4z)\theta + 2\left(\theta^2 - \sum_{i=1}^{3} x_i^2\right) \tag{3.7}$$

where, for notational simplicity, $z{=}v_{11}$, $x_0 = v_{111}$, $x_1 = v_{121}$, $x_2 = v_{211}$, $x_3 = v_{311}$ and $\theta = x_1 + x_2 + x_3$. The problem is to minimize (3.7) subject to (3.4). The details are left to Appendix A, where again η_{d0} is found to be uniquely (up to isomorphism) minimized. In terms of the free variables, the best designs for four replicates are specified in Table 1, along with their η-distributions.

3.2. Five replicates with two blocks per replicate

As seen in Figure 2, the fifth replicate is represented by 32 additional variables. Given the variables from replicate four, all those in the second block are determined by those in the first block via $v_{em2} = v_{em} - v_{em1}$ (in this subsection $m = (m_1, m_2)$ and each $m_i \in \{1, 2\}$). The sixteen first-block variables are subject to the five linearly independent constraints $v/4 = |B_{11} \cap B_{51}| = |B_{21} \cap B_{51}| = |B_{31} \cap B_{51}| = |B_{41} \cap B_{51}| = |B_{42} \cap B_{51}|$. These resolve to

$$\begin{aligned}
v_{2221} &= \frac{v}{4} - v_{1111} - v_{1121} - v_{1211} - v_{1221} - v_{2111} - v_{2121} - v_{2211}\\
v_{3221} &= \frac{v}{4} - v_{1111} - v_{1121} - v_{1211} - v_{1221} - v_{3111} - v_{3121} - v_{3211}\\
v_{4121} &= \frac{v}{4} - v_{1111} - v_{1121} - v_{2111} - v_{2121} - v_{3111} - v_{3121} - v_{4111}\\
v_{4211} &= \frac{v}{4} - v_{1111} - v_{1211} - v_{2111} - v_{2211} - v_{3111} - v_{3211} - v_{4111}\\
v_{4221} &= 3v_{1111} + 2v_{1121} + 2v_{1211} + v_{1221} + 2v_{2111} + v_{2121} + v_{2211} + 2v_{3111}\\
&\quad + v_{3121} + v_{3211} + v_{4111} - \frac{v}{2}.
\end{aligned} \tag{3.8}$$

Thus there are 11 free variables for replicate five, making a total of 16 free variables in the standard representation of the five replicate design. While an analytic solution in the fashion of Section 3.1 would appear to be unwieldy (to say the least), judicious use of software makes a full solution feasible, as will be seen.

The key insight is that very small values of η_{d0} give an abundance of information about the variables in replicate five. Write $e' = A(e)$, which here is a singleton (e.g., $A(1) = 4$), and $m_i' = 3 - m_i$. Consider $\eta_{d0} = 0$. The expression for η_{d0} in (2.2) is the sum of eight products $v_{1m_1m_2m_3}v_{4m_1'm_2'm_3'}$ and eight products $v_{2m_1m_2m_3}v_{3m_1'm_2'm_3'}$, which collectively contain each of the 32 variables once. If $\eta_{d0} = 0$ then every one of these products is zero, implying that at least 16 of the replicate five variables are zero. If v_{em1} (say) is zero, then either $v_{em} = 0$ (determining a replicate four parameter) or $v_{em2} = v_{em}$ (determining a replicate five parameter in terms of a nonzero replicate four parameter). The former case also forces $v_{em2} = 0$, while $v_{e'm'1}$ and $v_{e'm'2}$ may take any values subject only to $v_{e'm'1} + v_{e'm'2} = v_{e'm'}$. The latter case forces $v_{e'm'2} = v_{e'm'}$ and consequently $v_{e'm'1} = 0$.

Here then is a route for determining all designs having $\eta_{d0} = 0$:

1. Specify a subset of the 16 replicate four variables to be set to zero, all others taken to be positive.
2. Given the selection in step 1, specify the corresponding information about the replicate five variables (as given in the preceding paragraph). For each pair $(v_{em}, v_{e'm'})$ neither of which is set to zero in step 1, this entails a selection of which of the two pairs $(v_{em1}, v_{e'm'1})$ and $(v_{em2}, v_{e'm'2})$ is set to $(0, 0)$, and which is set to $(v_{em}, v_{e'm'})$.
3. Solve the system of equations comprised of the five constraints (3.8) and the specifications in steps 1 and 2. Discard solutions violating nonnegative integer requirements.
4. Repeat for each distinct selection of variables in step 1 and for each selection of pairs set to $(0, 0)$ in step 2.

This algorithm assumes $0 < v_{11} < v/4$ so that all third replicate variables are positive. For $v_{11} = 0$ (for which any design is isomorphic to a design with $v_{11} = v/4$), the third replicate is that shown in (3.1) and $\eta_{d0} = 0$ has been achieved if there is any five replicate solution including (3.1). Section 3.1 established that there was exactly one four replicate design including (3.1), making this a simple case to handle separately. This, in fact, produces the five replicate solution for $v \equiv 0 \pmod 8$ shown in Table 2.

While any one iteration of this algorithm would be a straightforward task with pen and paper, there are far too many iterations to complete manually.

Table 2. Minimum PV-aberration designs for five replicates, two blocks per replicate.

v	$(v_{11}, v_{111}, v_{121}, v_{211}, v_{311}, v_{1111}, v_{1121}, v_{1211}, v_{1221}, v_{2111}, v_{2121}, v_{2211}, v_{3111}, v_{3121}, v_{3211}, v_{4111})$ $\eta_d = (\eta_{d0}, \eta_{d1}, \eta_{d2}, \eta_{d3}, \eta_{d4}, \eta_{d5})$
$v \equiv 0 \pmod 8$	$(0, 0, \frac{v}{8}, \frac{v}{8}, \frac{v}{8}, 0, 0, \frac{v}{8}, 0, 0, \frac{v}{8}, 0, 0, \frac{v}{8}, 0, 0)$ $(0, \frac{v^2}{16}, \frac{v^2}{4}, \frac{v^2}{8}, 0, \frac{v(v-8)}{16})$
$v \equiv 0 \pmod{36}$	$(\frac{v}{12}, 0, \frac{v}{6}, \frac{v}{12}, \frac{v}{12}, 0, 0, \frac{v}{18}, 0, \frac{v}{12}, \frac{v}{36}, 0, \frac{v}{12}, \frac{v}{36}, 0, \frac{v}{36})$ $(0, \frac{119v^2}{1296}, \frac{61v^2}{324}, \frac{29v^2}{216}, \frac{4v^2}{81}, \frac{47v^2}{1296} - \frac{v}{2})$
$v \equiv 0 \pmod{28}$	$(\frac{v}{14}, 0, \frac{3v}{28}, \frac{v}{14}, \frac{3v}{28}, 0, \frac{v}{14}, \frac{v}{28}, \frac{v}{14}, \frac{v}{14}, 0, 0, \frac{v}{28}, 0, 0, \frac{v}{14})$ $(0, \frac{75v^2}{784}, \frac{5v^2}{28}, \frac{55v^2}{392}, \frac{5v^2}{98}, \frac{27v^2}{784} - \frac{v}{2})$
$v \equiv 0 \pmod{12}$	$(\frac{v}{12}, 0, \frac{v}{6}, \frac{v}{12}, \frac{v}{12}, 0, 0, \frac{v}{6}, 0, 0, \frac{v}{12}, 0, 0, \frac{v}{12}, 0, \frac{v}{12})$ $(0, \frac{5v^2}{48}, \frac{5v^2}{36}, \frac{5v^2}{24}, 0, \frac{7v^2}{144} - \frac{v}{2})$
$v \equiv 4 \pmod 8$	$(\frac{v+4}{8}, 1, \frac{v-4}{8}, \frac{v-12}{8}, \frac{v-12}{8}, 1, 0, 0, 0, \frac{v-12}{8}, 1, 0, \frac{v-12}{8}, 0, 1, 1)$ $(1, \frac{v^2}{16} + v - 11, \frac{v^2}{4} - 2v + 18, \frac{v^2}{8} + 2, 2v - 19, \frac{v^2}{16} - \frac{3v}{2} + 9)$

Best design for given v is in first applicable row. For example, for $v = 36$ use second row (not fourth or fifth), for $v = 72$ use first row (not second or fourth). Design variables not shown are determined by (3.2), (3.3), and (3.8).

This is a task for a computer; symbolic software for linear algebra can perform the iterations quickly and in full generality. It is a simple matter to write code to generate the selections and feed each to a symbolic equations solver (this author used Maple). Even with machine processing, the task would be too lengthy were it not possible to significantly reduce the number of iterations relative to "all." Reductions are achieved by application of the basic, design-preserving symmetries apparent in Figure 2:

- The blocks within replicate three can be reversed, as can those within replicate four and those within replicate five.
- Sets S_1 and S_4 can be interchanged, as can sets S_2 and S_3.
- The pair of sets (S_1, S_4) can be interchanged with the pair (S_2, S_3).

These symmetries can be used in combination with other considerations to great effect. For example, at most eight of the sixteen variables from replicate four can be set to zero, for with $v_{11} > 0$, at most one of v_{em1}, v_{em2} can be zero. Of the four v_{em} with the same e, at most two can be zero, and there are only two ways in which two can be set to zero (otherwise the design becomes isomorphic to one having $v_{11} = 0$). Applying the symmetries above, additional restrictions are: (i) $\#\{m : v_{1m} = 0\} + \#\{m : v_{4m} = 0\} \geq \#\{m : v_{2m} = 0\} + \#\{m : v_{3m} = 0\}$ (otherwise interchange (S_1, S_4) with (S_2, S_3)), (ii) $\#\{m : v_{1m} = 0\} \geq \#\{m : v_{4m} = 0\}$ (otherwise interchange S_1 and S_4), (iii) $\#\{m : v_{2m} = 0\} \geq \#\{m : v_{3m} = 0\}$ (otherwise interchange S_2 and S_3), (iv) $v_{111} = 0$ (otherwise reverse blocks within replicate three and/or replicate four).

Implementing this algorithm shows that, unlike for four replicates in Section 3.1, there is not a unique solution to $\eta_{d0} = 0$. Here solutions for the same v are found having different η_d vectors, from which the best is selected in accord with Definition 1. Results appear in Table 2.

Like for four replicates in Section 3.1, η_{d0} cannot achieve zero for every v. Setting $\eta_{d0} = 1$, now exactly one of the products $v_{em1}v_{e'm'2}$ is nonzero, which can be taken (using suitable symmetries) to be $v_{1111}v_{4222} = 1$. Since then $v_{1112}v_{4221} = 0$, this implies either $v_{111} = 1$ or $v_{422} = 1$, so (again using suitable symmetries) take $v_{111} = v_{1111} = v_{4222} = 1$. With this change, the ideas above for solving $\eta_{d0} = 0$ are easily transferred, so the details will not be repeated. Results appear in Table 2, completing the minimum PV-aberration problem for five replicates.

4. A Catalog of Minimum PV-Aberration Designs

The methods of Sections 2 and 3 provide best affine resolvable designs for the ranges of r shown in Table 3. The values of s displayed are sufficient to cover all numbers of treatments up to $v = 200$.

A further result based on deletion of replicates is easily added. Whenever an affine resolvable design is a BIBD, all of its λ_{ij} are identical so it trivially has minimum PV-aberration. Removing any one replicate decreases some λ_{ij} by one, leaving the rest unchanged; this too is a minimum PV-aberration design. Now an affine resolvable design is a BIBD whenever $r = (\mu s^2 - 1)/(s - 1) = r_{max}$. Recalling from Section 2 that each replicate in an affine resolvable design corresponds to a column of an orthogonal array, further deletions can be used with small s in accord with the following result.

Theorem 2. (Shrikhande and Bhagwandas (1969), and Vijayan (1976)) *$OA(v, r_{max} - w, s)$ can be extended to $OA(v, r_{max}, s)$ if (i) $s = 2$, $w \leq 4$, or (ii) $s = 3$, $w \leq 2$.*

Thus deletion of any two replicates from an affine resolvable BIBD with $s = 2$ or $s = 3$ produces a minimum PV-aberration design. For $s = 2$, the same result holds for deletion of three replicates provided that the deleted replicates, when considered as an affine resolvable design d, minimize aberration of the vector $(\eta_{d3}, \eta_{d2}, \eta_{d1}, \eta_{d0})$. Likewise deletion of a four-replicate subdesign d requires minimizing aberration of $(\eta_{d4}, \eta_{d3}, \eta_{d2}, \eta_{d1}, \eta_{d0})$ over all 4-replicate affine resolvable designs.

Table 3. Solutions found for $s \leq 14$.

s	2	3	4	5	6	7	8	9	10	11	12	13	14
$r \leq$	5	4	5	6	3	8	9	10	4	12	7	14	5

So that they may be easily accessed for application, all of these designs (for up to 200 treatments and 23 replicates) have been compiled in an online catalog at *designtheory.org*, a website devoted to free storage and access to block designs and many of their properties. The designs are stored there as xml files, in *external representation format* (see Bailey, Cameron, Dobcsanyi, Morgan and Soicher (2006)), along with lists of canonical efficiency factors, pairwise variances, and much more. Mutually orthogonal Latin squares, needed for the construction of d^* in Theorem 1, can be found in Abel, Colbourn and Dinitz (2007).

Taking further advantage of the orthogonal array representation of an affine resolvable design, best designs can be found whenever all nonisomorphic orthogonal arrays OA(v, r, s) for s symbols in v rows and r columns have been enumerated. OA enumeration has been pursued with some vigor of late, with the following cases now completed: OA$(12, r, 2)$ for $r \leq 11$, OA$(16, r, 2)$ for $r \leq 15$, and OA$(20, r, 2)$ for $r \leq 19$, all in Sun, Li and Ye (2008); OA$(24, r, 2)$ for $r \leq 7$, OA$(28, r, 2)$ for $r \leq 6$, and OA$(32, r, 2)$ for $r \leq 6$, all in Angelopoulos, Evangelaras, Koukouvinos and Lappas (2007); and OA$(18, r, 3)$ for $r \leq 7$ in Evangelaras, Koukouvinos and Lappas (2007). All of these lists have been searched to determine a minimum PV-aberration design, and these designs have all been added to the online catalog.

At this writing the catalog contains 522 designs, including all parameter combinations with $v \leq 20$ for which an affine resolvable design can exist. Because all of these designs are affine, they are excellent resolvable designs. Being additionally optimized for estimation of pairwise contrasts will make them the preferred choice in most applications.

5. Examples and Discussion

Two detailed examples are shown next, covering Theorem 1 and the methods of Section 3. While both example designs can be downloaded from the web catalog, numbers outside the catalog's range require the techniques they illustrate. Those interested in the analysis of data from affine resolvable designs are referred to the thorough coverage of this topic in Caliński, Czajka and Pilarczyk (2009). That paper includes examples of, and data from, applications of these designs in agricultural trials.

Example 1. A four replicate, affine resolvable design with minimal PV-aberration, for $v = 18$ treatments in blocks of size $k = 6$, can be found with

Rep #1			Rep #2			Rep #3			Rep #4		
1	7	13	1	3	5	1	5	3	1	5	3
2	8	14	2	4	6	2	6	4	2	6	4
3	9	15	7	9	11	9	7	11	11	9	7
4	10	16	8	10	12	10	8	12	12	10	8
5	11	17	13	15	17	17	15	13	15	13	17
6	12	18	14	16	18	18	16	14	16	14	18

Figure 3. A minimal PV-aberration design for 18 treatments in blocks of size 6.

the construction underlying Theorem 1. First write $v = \mu s^2 = 2(3)^2$. The 18 treatments are partitioned into $s^2 = 9$ sets of $\mu = 2$ treatments each: $S_1 = \{1,2\}, S_2 = \{3,4\}, \ldots, S_9 = \{17,18\}$. Placing the S_i's into blocks as displayed in general form in Figure 1 gives the first two replicates of the design (Figure 3).

Finding the remaining two replicates requires $4-2 = 2$ mutually orthogonal Latin squares of order $s = 3$. They are:

1	2	3
3	1	2
2	3	1

1	3	2
3	2	1
2	1	3

Superimpose the first of these squares on the first 3×3 square in Figure 1; sets S_i coincident with number j in this Latin square are placed in block j of the third replicate. Thus the first block of the third replicate contains S_1, S_5, S_9, the second contains S_3, S_4, S_8, and the third S_2, S_6, S_7. Superimpose the second Latin square on the first 3×3 square in Figure 1 to similarly get the fourth replicate in Figure 3.

Example 2. A five replicate, affine resolvable design with minimal PV-aberration, for $v = 16$ treatments in blocks of size $k = 8$, results from the calculations in Section 3. The design can be built from the information in Table 2; the values there tell the sizes of the subsets in the third through fifth replicates shown in general form in Figure 2. The sets comprising the first two replicates are $S_1 = \{1,2,3,4\}$, $S_2 = \{5,6,7,8\}$, $S_3 = \{9,10,11,12\}$, and $S_4 = \{13,14,15,16\}$. Reading from the first row of Table 2, the relevant information for the third replicate is $v_{11} = 0$. This says no part of S_1 is in the first block of replicate three so that $S_{11} = \varnothing$ and $S_{12} = S_1$. The remainder of replicate three follows from affineness with respect to the first two replicates; see Figure 4.

For the fourth replicate, Table 2 says $v_{121} = v_{211} = v_{311} = 2$. So any two treatments from each of $S_{12} = S_1$, $S_{21} = S_2$, and $S_{31} = S_3$ are placed in the first

Rep #1		Rep #2		Rep #3		Rep #4		Rep #5	
1	9	1	5	5	1	1	3	1	3
2	10	2	6	6	2	2	4	2	4
3	11	3	7	7	3	5	7	7	5
4	12	4	8	8	4	6	8	8	6
5	13	9	13	9	13	9	11	11	9
6	14	10	14	10	14	10	12	12	10
7	15	11	15	11	15	13	15	13	15
8	16	12	16	12	16	14	16	14	16

Figure 4. A minimal PV-aberration design for 16 treatments in blocks of size 8.

block of replicate four. It follows that $v_{421} = 2$ and that block, and consequently the fourth replicate, is completed by any two treatments from $S_{42} = S_4$.

With the fourth replicate in place, now use $v_{1211} = v_{2121} = v_{3121} = 2$ and, from (3.8) and the zeros specified in Table 2, $v_{4211} = 2$. So $S_{1211} = S_{121}$, $S_{2121} = S_{212}$, $S_{3121} = S_{312}$, and $S_{4211} = S_{421}$, determining the fifth replicate of Figure 4.

The technique of Section 3, based on the standard representation introduced in Section 2, becomes rapidly more demanding as either r or s grows. This is to be expected, for the equivalent problem of searching all orthogonal arrays, beyond the smallest cases, is notoriously difficult. Pushing on to $r \geq 6$ for $s = 2$, or to $r \geq 5$ for $s = 3$, is likely to require additional knowledge as to how the problem can be reduced, be it through exploiting additional symmetries, mathematical derivation of additional restrictions on the variables v_{em} that are consonant with minimum aberration, or some combination of the two.

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Appendix: Minimizing η_{d0} for $(v, r, 2) = (4 \pmod 8), 4, 2)$

Noting that x_1, x_2, and x_3 are interchangeable (this corresponds in Figure 2 to permutations of blocks within replicates, and of sets within blocks of the first two replicates), there is no loss of generality in taking $x_1 \leq x_2 \leq x_3 \leq v/4 - z$ (the last inequality from (3.2)). Minimizing (3.7) first for fixed z, x_0, and θ, says to maximize $\sum_{i=1}^{3} x_i^2$ for fixed θ. A simple majorization argument shows this is accomplished by sequentially minimizing x_1, and then x_2. Since θ is fixed, minimizing x_1 is equivalent to maximizing x_2+x_3, and by the third line of (3.4), $x_2+x_3 \le v/4-x_0$. Putting $x_1=\theta+x_0-v/4$ and $x_2+x_3=v/4-x_0$ in (3.7) gives

$$\begin{aligned}\eta_{d0} &\geq \frac{3v^2}{16}-4x_0^2-z(v-4x_0)-(v-4z)\Big(x_1-x_0+\frac{v}{4}\Big)\\ &\quad+2\bigg[\Big(x_1-x_0+\frac{v}{4}\Big)^2-x_1^2-x_2^2-\Big(\frac{v}{4}-x_0-x_2\Big)^2\bigg]\\ &=-\frac{v^2}{16}-4x_0^2-4x_2^2+(v-4x_0)x_2+4(z-x_0)x_1+vx_0 \qquad \text{(A.1)}\end{aligned}$$

where, since $x_2+x_3=v/4-x_0$ and $x_1 \le x_2 \le x_3 \le v/4-z$,

$$0 \le x_1 \le x_2 \le \frac{1}{2}\Big(\frac{v}{4}-x_0\Big) \qquad \text{(A.2)}$$

and, from the first and third lines of (3.4),

$$\frac{v}{4}-z-x_0-x_2 \le x_1 \le \frac{v}{4}-x_0-z. \qquad \text{(A.3)}$$

Importantly, the RHS of (A.2) need not be an integer, though x_2 must be; this is why different solutions are found depending on the (mod 8) value of v. The minimization proceeds in two steps.

Step 1 : *minimize with* $x_0=0$. From (A.1) the quantity to be minimized is

$$H(z,x_1,x_2)=-\frac{v^2}{16}-4x_2^2+vx_2+4zx_1 \qquad \text{(A.4)}$$

which, from (A.2) and (A.3), is subject to the constraints $v/4-z-x_2 \le x_1 \le x_2$ for $(v-4z)/8 \le x_2 \le (v-4)/8$. If $z=0$ there are no feasible values for x_2, so $z \ge 1$. Also $z \le v/8 \Rightarrow z \le (v-4)/8$. Since (A.4) is linear in x_1 with positive slope,

$$\begin{aligned}H(z,x_1,x_2) &\geq H\Big(z,\frac{v}{4}-z-x_2,x_2\Big)\\ &=-\frac{v^2}{16}-4x_2^2-4z^2-4zx_2+v(x_2+z)\equiv \widetilde{H}(z,x_2). \qquad \text{(A.5)}\end{aligned}$$

Now $\widetilde{H}(z,x_2)$ is concave in x_2, so is minimized as a function of x_2 at either $x_2=(v-4)/8$ or $x_2=\lfloor(v-4z)/8\rfloor$, the latter value depending on the parity of z. Thus three evaluations of (A.5) are required, each of which produces a concave function of z, and which are then minimized by evaluating at the endpoints for z. This produces the minimum value of $v/2-3$ for η_{d0} when $x_0=0$ at the values $(z,x_0,x_1,x_2,x_3)=(v_{11},v_{111},v_{121},v_{211},v_{311})=((v-4)/8,0,1,(v-4)/8,(v+4)/8)$

and $(1, 0, (v-4)/8, (v-4)/8, (v+4)/8)$. These yield the same η_d vectors; indeed, it may be shown that they are isomorphic solutions.

Step 2 : *minimize with* $x_0 > 0$. Now fix a positive integer value for x_0. The same sequence of evaluations is carried out as in Step 1, with the appropriate endpoints as given by (A.2) and (A.3) (which are now a bit more complicated). For $x_0 > 1$ many of the evaluations do not require attending to the integer nature of the endpoints as done in Step 1; this subcase is easily eliminated as inferior to $x_0 = 0$. Not surprisingly, $x_0 = 1$ requires care in strictly adhering to the exact integer endpoints, but it, too, produces a minimum larger than $v/2 - 3$. Thus the unique minimum PV-aberration design was identified in Step 1, as listed in Table 1.

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