Optimal Experimentation in Two Blocks

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Summary

Faced with cost, time, or other pressures to keep an experiment small, blocking can be an effective tool for increasing precision of treatment comparisons. The simplest implementation of blocking is a division of experimental units into two equi-sized subsets, allocating one degree of freedom to explain unit heterogeneity. Small experiments will have block size k smaller than the number of treatments v being compared. This paper solves the problem of optimal allocation of treatments to two small, equi-sized blocks. The solution depends on the optimality criterion employed as well as the ratio $\frac{k}{v}$.

Some key words and phrases: Binary Design, incomplete block design, A-optimality, D-optimality, E-optimality.

1 Introduction

Scarcity of resources not infrequently plays a significant role in designing an experiment. In a study examining factors affecting vehicle traction, engineers asked us for a plan incorporating three speeds, five loads, and five sand types (thus $3 \times 5 \times 5$ treatment combinations) to be executed over two days of experimentation. Strong interactions were expected. Speed/load combinations were to be run through sand pits in which lines of sensors were buried. Each day would begin with working the sand in each pit to a roughly uniform consistency and burying the sensors (which could not be left out overnight). This and obvious environmental variation made blocking by day a prudent choice. Allocating five minutes per run, with set-up, break-down and transport time it was not possible to run every treatment each day. An incomplete block design with two blocks and 75 treatments was needed.

Design theory offers a number of strategies to help the statistician get around some of the constraints in situations like this one. One possibility is to posit adequacy of a low-order polynomial model in the quantitative factors, allowing one to ask that the number of levels of some factors, and thus the number of treatments, be reduced. Another, for non-quantitative factors, is to discount interaction terms and employ a blocked fractional factorial design. Should treatments not possess an underlying factorial structure, yet another option is simply to ask experimenters to curtail their goals. What design theory does not offer is a direct answer to the experimenter's initial question: for the selected treatments of interest, what design will maximize precision of all possible treatment comparisons when having only two small blocks of material with which to work? Even a decision to reduce the scope of the experiment, should it be made, will be on firmer footing once the answer to this question is known, so that what is gained and what is lost is fully understood.

Following the standard formulation of the block design problem, let $\mathcal{D}(v, b, k)$ denote the class of all connected block designs having v treatments arranged in b blocks of equal size $k \leq v$. For $b = 2$ there are $2k$ experimental units in total. If $2k = 2v$ the universally optimal design (Kiefer, 1975) is to allocate each treatment to one unit in each block: the well-known randomized complete block design. If $2k < v$ then not every treatment can be used, and if $2k = v$ then any design is disconnected (i.e. not every contrast can be estimated). The problem requiring study is for settings with $k < v < 2k$, where there can be many incomplete block designs with varying efficiencies from which to choose.

Block designs are judged by measures of variance defined as functions of the treatment effects information matrix, commonly denoted by C_d, the subscript d making explicit the dependence on design $d \in \mathcal{D}$. This matrix is known (eg, Shah and Sinha,

1989) to be

$$C_d = Diag(r_{d1}, r_{d2}, \ldots, r_{dv}) - k^{-1} N_d N_d' \qquad (1)$$

where r_{di} is the number of units allocated treatment i by d and $N_d = (n_{dij})$ with n_{dij} signifying the number of units in block j allocated treatment i. C_d is nonnegative definite, has non-positive off-diagonal elements and has rows sums zero for all $d \in \mathcal{D}(v, b, k)$. Connected designs have C_d of rank $v - 1$.

A design d is *equireplicate* if $r_{d1} = r_{d2} = \ldots = r_{dv}$. Treatment i of d is *binary* if it is allocated to r_{di} distinct blocks, that is, if n_{dij} is 0 or 1 for all j. Design d is binary if all its treatments are binary. While some other work has been done, design theory has concentrated on settings where bk is a multiple of v so that equireplication is possible. Optimality arguments then usually lead to binary, equireplicate designs. The problem here does not allow equireplication, and it will be seen that the optimality of binary assignment depends on the criterion employed.

Commonly used and statistically sensible optimality criteria are defined in terms of the eigenvalues of C_d. Let these be $0 = z_{d0} < z_{d1} \leq \ldots \leq z_{d,v-1}$. Design $d^* \in D$ is E-optimal if $\frac{1}{z_{d^*1}} \leq \frac{1}{z_{d1}}$ (equivalently $z_{d^*1} \geq z_{d1}$); is A-optimal if $\sum_{i=1}^{i=v-1} \frac{1}{z_{d^*i}} \leq \sum_{i=1}^{i=v-1} \frac{1}{z_{di}}$; and is D-optimal if $\prod_{i=1}^{i=v-1} \frac{1}{z_{d^*i}} \leq \prod_{i=1}^{i=v-1} \frac{1}{z_{di}}$ (equivalently $\prod_{i=1}^{i=v-1} z_{d^*i} \geq \prod_{i=1}^{i=v-1} z_{di}$); each inequality holding for all $d \in \mathcal{D}$. The statistical meaning of these criteria is discussed by, among others, Shah and Sinha (1989). Each is a natural measure of variance of treatment contrasts, so that smaller values correspond to better designs.

This paper determines A-, D-, and E-optimal designs in $\mathcal{D}(v, 2, k)$ for each k satisfying $k < v < 2k$. These problems are solved in sections 3, 4, and 5, respectively. The surprising result is that E-optimal designs can be highly nonbinary. Section 2 lays out an optimality tool needed for the derivations. Section 6 provides further discussion, including a comparison of optimal designs. Some of the derivations in this paper are best followed with an algebraic manipulator, such as Maple or Mathematica, in hand.

2 Matrix Averaging

A key tool required in later proofs is *matrix averaging*, explained here. An optimality criterion $\Phi : C_d \to \Re$ is matrix convex if for any C_{d_1} and C_{d_2} and all $0 \leq \theta \leq 1$, $\Phi(\theta C_{d_1} + (1-\theta)C_{d_2}) \leq \theta\Phi(C_{d_1}) + (1-\theta)\Phi(C_{d_2})$. The A, D, and E criteria are all matrix convex (Kiefer, 1975). The importance of this is that bounds for a criterion's value can be found by "averaging" an information matrix as follows.

Definition Let $P_1, \ldots, P_t$ be t permutation matrices of order v. An *averaging* of the information matrix C_d is $\overline{C}_d = \frac{1}{t}\sum_{i=1}^{t} P_i C_d P_i'$. $\overline{C}_d$ is called an *average matrix* of C_d.

Theorem 2.1 *Suppose $\overline{C}_d$ is an average matrix of C_d. Then*

(i) $\overline{C}_d$ is nonnegative definite with zero row sums and the same trace as C_d, and

(ii) $\Phi(\overline{C}_d) \leq \Phi(C_d)$ for any matrix convex Φ.

Averaging as a tool for bounding optimality values first appeared in Constantine (1981).

To show that a design d^* is better than any member of a class of competing designs it is enough to show that $\Phi(\overline{C}_d) \geq \Phi(C_{d^*})$ for some averaged version of C_d for members of that class. The question is in choice of the averaging. Let Π_i for $i = 1, \ldots, l$ be a partition of the treatments, $|\Pi_i| = v_i$ ($\sum_i v_i = v$). Then there is a collection of $v_i!$ permutation matrices corresponding to all permutations of the treatments in Π_i. Applying these $\sum_i v_i!$ permutations to an information matrix C_d, the averaged version is generalized block diagonal.

Definition A symmetric matrix X is *generalized block-diagonal* if it can be partitioned as

$$\begin{pmatrix} A_{n_1\times n_1} & c_{12}J_{n_1\times n_2} & \cdots & c_{1p}J_{n_1\times n_p} \\ c_{21}J_{n_2\times n_1} & A_{n_2\times n_2} & \cdots & c_{2p}J_{n_2\times n_p} \\ \vdots & \vdots & \ddots & \vdots \\ c_{p1}J_{n_p\times n_1} & c_{p2}J_{n_p\times n_2} & \cdots & A_{n_p\times n_p} \end{pmatrix} \qquad (2)$$

where the matrices $A_{n_i\times n_i} = x_iI + y_iJ$ are completely symmetric.

It is evident that $\sum_{i=1}^{p}(n_i-1)$ eigenvalues of (2) are n_i-1 copies of x_i for $i=1,\ldots,p$. Following Morgan and Parvu (2007), the remaining eigenvalues are those of a $p\times p$ matrix.

Lemma 2.2 *Let X be a generalized block-diagonal matrix as given in (2). Also let matrices $A_{n_i\times n_i}$ have eigenvalues x_i with multiplicity n_i-1 and $a_i=x_i+n_iy_i$ with multiplicity 1. Then the eigenvalues of X are x_i with multiplicity n_i-1, and the eigenvalues of the (not necessarily symmetric) matrix:*

$$\widetilde{X}=\begin{pmatrix} a_1 & c_{12}\cdot n_2 & \cdots & c_{1p}\cdot n_p \\ c_{21}\cdot n_1 & a_2 & \cdots & c_{2p}\cdot n_p \\ \vdots & \vdots & \ddots & \vdots \\ c_{p1}\cdot n_1 & c_{p2}\cdot n_2 & \cdots & a_p \end{pmatrix}$$

Extracting functions of eigenvalues is sometimes eased by the following lemma.

Lemma 2.3 *(Vieta's Formulas) If $\lambda_1,\lambda_2,\ldots,\lambda_n$ are the n roots for an n^{th} order equation $P(\lambda)=0$ where $P(\lambda)=a_n\lambda^n+a_{n-1}\lambda^{n-1}+\ldots+a_1\lambda+a_0$, then*

$$\begin{aligned} \lambda_1+\lambda_2+\ldots+\lambda_n &= (-1)\tfrac{a_{n-1}}{a_n} \\ \lambda_1\lambda_2+\lambda_1\lambda_3+\ldots+\lambda_{n-1}\lambda_n &= (-1)^2\tfrac{a_{n-2}}{a_n} \\ &\vdots \\ \lambda_1\lambda_2\ldots\lambda_n &= (-1)^n\tfrac{a_0}{a_n}. \end{aligned} \tag{3}$$

The Intermediate Value Theorem will also be useful so is stated here for convenience.

Lemma 2.4 *Consider $P(\lambda)$ in lemma 2.3 and real numbers a and b. If $P(a)P(b)<0$, then $P(\lambda)$ has at least one root in (a,b).*

3 A-optimal Designs

Write $bk=vr+p$ where p is a non-negative integer no larger than $v-1$. Then p is the number of plots available for use in a block design over and above that needed to replicate each treatment r times. For $b=2$ and $\frac{v}{2}<k<v$ these numbers are $r=1$ and

Block 1:	1	2	$\cdots$	p	p+1	p+2	$\cdots$	k
Block 2:	1	2	$\cdots$	p	k+1	k+2	$\cdots$	2k-p

Figure 1: Binary design d_0

$p = 2k - v$. Up to treatment labeling there is only one binary design d_0 (see Figure 1) in this situation, having exactly p treatments replicated twice, and $v - p$ replicated once.

From (1), the information matrix C_{d_0} for the binary design is

$$C_{d_0} = \begin{pmatrix} 2I_p - \frac{2}{k}J_p & -\frac{1}{k}J_{p,k-p} & -\frac{1}{k}J_{p,k-p} \\ -\frac{1}{k}J_{k-p,p} & I_{k-p} - \frac{1}{k}J_{k-p} & 0_{k-p} \\ -\frac{1}{k}J_{k-p,p} & 0_{k-p} & I_{k-p} - \frac{1}{k}J_{k-p} \end{pmatrix} \tag{4}$$

This matrix has positive eigenvalues 1 with frequency $2(k-p-1)$, 2 with frequency $(p-1)$, $\frac{p}{k}$, and $\frac{v}{k}$. Its A-value is thus

$$A_{d_0} = \sum_{i=1}^{v-1} \frac{1}{z_{d_0 i}} = 2(k-p-1) + \frac{p-1}{2} + \frac{k}{p} + \frac{k}{v}. \tag{5}$$

It will be shown that any non-binary design in $\mathcal{D}(v, 2, k)$ is A-inferior to d_0, and consequently that d_0 is A-optimal. This will be done employing the average matrix technique of section 2 using a partition of the treatments into three subsets.

With p units in excess of that needed for a single replication of all treatments, at least $v - p = 2(k-p)$ treatments must be replicated exactly once. So let $2(k-p) + m$ treatments have just one replicate where $0 \leq m \leq p-1$. If $k - p - s$ is the number of treatments with one replicate in block one, then $k - p + s + m$ of the treatments have one replicate in block two, where $-\frac{m}{2} \leq s \leq k - p$. Connectedness further requires $0 \leq s + m \leq p - 1$. A partition of the treatments into three subsets of sizes $k - p - s$, $k - p + s + m$, and $p - m$ has now been defined. The binary design d_0 has $m = s = 0$.

The symbols s and m just defined will be used throughout:

m = the total excess in treatments with one replicate relative to d_0,

s = the shortfall in treatments in block one with one replicate relative to d_0.

A negative shortfall ($s < 0$) is actually an excess. The sign of s is not a consideration in the A- and D-optimality problems, and it will be seen (lemma 5.2) that $s < 0$ need not be considered for the E-optimality problem.

LEMMA 3.1 *Let d be any design in $\mathcal{D}(v, 2, k)$. The information matrix $\overline{C}_d \equiv C_{\overline{d}}$ obtained by averaging over the partition defined above is, for some values of ζ and η,*

$$C_{\overline{d}} = \begin{pmatrix} I_{k-p-s} - \frac{1}{k}J_{k-p-s} & 0_{k-p-s,k-p+s+m} & -\frac{p+s}{k(p-m)}J_{k-p-s,p-m} \\ 0_{k-p+s+m,k-p-s} & I_{k-p+s+m} - \frac{1}{k}J_{k-p+s+m} & -\frac{p-s-m}{k(p-m)}J_{k-p+s+m,p-m} \\ -\frac{p+s}{k(p-m)}J_{p-m,k-p-s} & -\frac{p-s-m}{k(p-m)}J_{p-m,k-p+s+m} & \zeta I_{p-m} + \eta J_{p-m} \end{pmatrix} \quad (6)$$

and the value ζ satisfies

$$\zeta \;\leq\; \frac{2p - m}{p - m}. \quad (7)$$

PROOF If $s = k - p$ the matrix (6) simplifies from 3×3 block-diagonal to 2×2; this case will not be separately handled. It is simple to verify that the average matrix has this form:

$$\begin{pmatrix} I_{k-p-s} - \frac{1}{k}J_{k-p-s} & 0_{k-p-s,k-p+s+m} & \gamma_1 J_{k-p-s,p-m} \\ 0_{k-p+s+m,k-p-s} & I_{k-p+s+m} - \frac{1}{k}J_{k-p+s+m} & \gamma_2 J_{k-p+s+m,p-m} \\ \gamma_1 J_{p-m,k-p-s} & \gamma_2 J_{p-m,k-p+s+m} & \zeta I_{p-m} + \eta J_{p-m} \end{pmatrix}$$

That the row sums of $C_{\overline{d}}$ are zero gives the values of γ_1 and γ_2 as seen in (6), and also that $\zeta + (p - m)\eta = -\gamma_1(k - p - s) - \gamma_2(k - p + s + m)$, which simplifies to

$$\zeta + (p - m)\eta = \frac{-(p + s)^2 - (p - m - s)^2 + k(2p - m)}{k(p - m)}. \quad (8)$$

Denote by Ω the set of treatments with more than one replicate in d, $|\Omega| = p - m$. Since C_d and $C_{\overline{d}}$ have the same trace it must hold that

$$(p - m)(\zeta + \eta) = \sum_{i\in\Omega} r_{di} - \frac{1}{k}\sum_{i\in\Omega}\sum_{j=1}^{2} n_{dij}^2 = 2p - m - \frac{1}{k}\sum_{i\in\Omega}\sum_{j=1}^{2} n_{dij}^2. \quad (9)$$

Combining (8) and (9) gives

$$\begin{aligned} \sum_{i\in\Omega}\sum_{j=1}^{2} n_{dij}^2 &= k[(2p - m) - (p - m)(\zeta + \eta)] = k[(2p - m) - (p - m - 1)\zeta - (\zeta + (p - m)\eta)] \\ &= k[(2p - m) - (p - m - 1)\zeta + \frac{(p + s)^2 + (p - m - s)^2 - k(2p - m)}{k(p - m)}]. \quad (10) \end{aligned}$$

If $\zeta > \frac{2p-m}{p-m}$ then (10) gives

$$\begin{aligned}\sum_{i\in\Omega}\sum_{j=1}^{2} n_{dij}^2 &< k[(2p-m)-(p-m-1)\frac{2p-m}{p-m}+\frac{(p+s)^2+(p-m-s)^2-k(2p-m)}{k(p-m)}] \\ &= p-m+\frac{2s(m+s)+p^2}{p-m}. \qquad (11)\end{aligned}$$

On the other hand, since $\sum_{i\in\Omega} n_{di1} = p+s$ and $\sum_{i\in\Omega} n_{di2} = p-m-s$,

$$\begin{aligned}\sum_{i\in\Omega}\sum_{j=1}^{2} n_{dij}^2 &= \sum_{i\in\Omega} n_{di1}^2 + \sum_{i\in\Omega} n_{di2}^2 \\ &\geq \frac{(\sum_{i\in\Omega} n_{di1})^2}{p-m} + \frac{(\sum_{i\in\Omega} n_{di2})^2}{p-m} = p-m+\frac{2s(m+s)+p^2}{p-m},\end{aligned}$$

contradicting (11). □

By lemma 2.2, the nonzero eigenvalues of $C_{\overline{d}}$ in (6) are 1 with frequency $2(k-p)+m-2$, ζ with frequency $p-m-1$, and the two nonzero eigenvalues of the following 3×3 matrix :

$$\widetilde{C}_{\overline{d}} = \begin{pmatrix} \frac{p+s}{k} & 0 & -\frac{p+s}{k} \\ 0 & \frac{p-m-s}{k} & -\frac{p-m-s}{k} \\ -\frac{(p+s)(k-p-s)}{k(p-m)} & -\frac{(p-s-m)(k-p+s+m)}{k(p-m)} & \zeta+\eta(p-m) \end{pmatrix} \qquad (12)$$

where (8) specifies the value of $\zeta+\eta(p-m)$.

Now the main result of this section can be stated and proved.

THEOREM 3.2 *The binary design d_0 is uniquely A-optimal in $\mathcal{D}(v,2,k)$.*

PROOF The two nonzero eigenvalues λ_1 and λ_2 of (12) are the roots of the equation $|\widetilde{C}_{\overline{d}} - \lambda I_3| = 0$, which simplifies to

$$k^2(m-p)\lambda^2 - k(km-2kp+mp+2ms+2s^2)\lambda + (2k-p)(m-p+s)(p+s) = 0 \quad (13)$$

Invoking lemma 2.3 gives the sum of their inverses:

$$\frac{1}{\lambda_1}+\frac{1}{\lambda_2} = \frac{\lambda_1+\lambda_2}{\lambda_1\lambda_2} = \frac{k(km-2kp+mp+2ms+2s^2)}{(2k-p)(m-p+s)(p+s)}$$

and so $A_{\bar{d}} = \sum_{i=1}^{v-1} \frac{1}{z_{\bar{d}i}}$ is

$$\begin{aligned} A_{\bar{d}} &= 2(k-p)+m-2+\frac{(p-m-1)}{\zeta}+\frac{k(km-2kp+mp+2ms+2s^2)}{(2k-p)(m-p+s)(p+s)} \\ &\overset{(7)}{\geq} 2(k-p)+m-2+\frac{(p-m-1)(p-m)}{2p-m}+\frac{k(km-2kp+mp+2ms+2s^2)}{(2k-p)(m-p+s)(p+s)} \end{aligned} \quad (14)$$

Taking the difference $A_{\bar{d}} - A_{d_0}$ from (14) and (5) and after some simplification

$$\sum_{i=1}^{v-1} \frac{1}{z_{\bar{d}i}} - \sum_{i=1}^{v-1} \frac{1}{z_{d_0 i}} \geq \frac{m(p+1)}{4p-2m} + \frac{k(k-p)(2(s+\frac{m}{2})^2 + m(p-\frac{m}{2}))}{(2k-p)p(p-m-s)(p+s)}. \quad (15)$$

It is easy to see that right side of (15) is always greater than zero as long as s and m are not zero simultaneously. □

4 D-optimal Designs

The main result of this section is:

Theorem 4.1 *The binary design d_0 is uniquely D-optimal in $\mathcal{D}(v,2,k)$.*

Proof Minimizing D-value is equivalent to maximizing the product of nonzero eigenvalues of C_d, which for the binary design d_0 is

$$\prod_{i=1}^{v-1} z_{d_0 i} = 2^{p-1}\frac{p(2k-p)}{k^2}. \quad (16)$$

The product of eigenvalues for an arbitrary design d can be bounded by that of the average matrix (6) in lemma 3.1. Lemma 2.3 applied to (13) shows that $\lambda_1\lambda_2 = (2k-p)(p-m-s)(p+s)/(k^2(p-m))$. Using also (7) and the sentence preceding (12),

$$\prod_{i=1}^{v-1} z_{\bar{d}i} \leq \frac{(2k-p)(\frac{2p-m}{p-m})^{p-m}(p-m-s)(p+s)}{k^2(2p-m)}. \quad (17)$$

A bound for the D-efficiency of $\bar{d}$ relative to d_0, $\mathrm{D}(\bar{d}, d_0) = (\prod_{i=1}^{v-1} z_{\bar{d}i})/(\prod_{i=1}^{v-1} z_{d_0 i})$, is given by the ratio of (17) to (16). After some simplification this is

$$\mathrm{D}(\bar{d}, d_0) \leq \frac{(\frac{2p-m}{p-m})^{p-m}}{2^p} \times \frac{2(p-m-s)(p+s)}{(2p-m)p}. \quad (18)$$

Block 1:	1	2	$\cdots$	2p-k	2p-k+1	2p-k+1	2p-k+2	2p-k+2	$\cdots$	2p-k+(k-p)=p	p
Block 2:	1	2	$\cdots$	2p-k	p+1	p+2	p+3	p+4	$\cdots$	2k-p-1	2k-p

Figure 2: Non-binary design d^*

The second factor of (18) is $\frac{2(p-m-s)(p+s)}{p(2p-m)} = \frac{p(2p-m)-(m+s)^2-s^2-m(p-m)}{p(2p-m)} \leq 1$, with strict inequality unless $m = s = 0$ (which is d_0). The proof is complete if also $W(m) = \frac{(\frac{2p-m}{p-m})^{p-m}}{2^p} \leq 1$. Writing $x = \frac{p-m}{2p-m} < 1$,

$$\frac{d}{dm}\log(W(m)) = 1 - x + \log(x) = \sum_{j=2}^{\infty} \frac{(-1)^{j-1}}{j}(x-1)^j < 0$$

so that $W(m) \leq W(0) = 1$. $\square$

5 E-optimal Designs

The E-optimality problem for $\mathcal{D}(v, 2, k)$ turns out to be considerably more complicated than those for A and D. To begin, partition $\mathcal{D}$ into two subclasses, $\mathcal{D}_1$ consisting of designs having all $r_{di} \in \{1, 2\}$, and $\mathcal{D}_2 = \mathcal{D}/\mathcal{D}_1$ having those designs for which some treatment has more than two replicates.

Lemma 5.1 *In the class $\mathcal{D}_1$, binary design d_0 is the unique E-optimal design if $\frac{v}{2} < k < \frac{5v}{6}$; non-binary design d^* (see Figure 2) is the unique E-optimal design if $\frac{5v}{6} < k < v$; and both d^* and d_0, and only these two designs, are E-optimal if $k = \frac{5v}{6}$.*

Concrete examples for d^* and d_0 are found at the end of this section.

Proof For the binary design the smallest nonzero eigenvalue, found following (4), is $z_{d_0 1} = \frac{p}{k} = \alpha$ (say). Noting that existence of d^* requires $p > \frac{k}{2}$ ($\Leftrightarrow k > \frac{2v}{3}$), that for d^* is found from its information matrix:

$$C_{d^*} = \begin{pmatrix} 2I_{2p-k} - \frac{2}{k}J_{2p-k} & -\frac{1}{k}J_{2p-k,2(k-p)} & -\frac{2}{k}J_{2p-k,k-p} \\ -\frac{1}{k}J_{2(k-p),2p-k} & I_{2(k-p)} - \frac{1}{k}J_{2(k-p)} & 0_{2(k-p),k-p} \\ -\frac{1}{k}J_{k-p,2p-k} & 0_{k-p,2(k-p)} & 2I_{k-p} - \frac{4}{k}J_{k-p} \end{pmatrix} \quad (19)$$

Applying lemma 2.2, the positive eigenvalues of C_{d^*} are: 1 with frequency $2(k-p)-1$, 2 with frequency $p-2$, and the nonzero eigenvalues of the matrix

$$\widetilde{C}_{d^*} = \begin{pmatrix} \frac{4(k-p)}{k} & -\frac{2(k-p)}{k} & -\frac{2(k-p)}{k} \\ -\frac{2p-k}{k} & \frac{2p-k}{k} & 0 \\ -\frac{2(2p-k)}{k} & 0 & \frac{2(2p-k)}{k} \end{pmatrix} \tag{20}$$

The eigenvalue equation $|\widetilde{C}_{d^*} - \lambda I_3| = 0$ reduces to

$$F(\lambda) = k^2\lambda^2 - (k^2 + 2kp)\lambda - 4k^2 + 10kp - 4p^2 = 0. \tag{21}$$

It is now easy to check that

$$\begin{aligned} F(0) &= 2(2p-k)(2k-p) > 0 & \qquad F(\tfrac{p}{k}) &= (k-p)(5p-4k) \\ F(1) &= -4(k-p)^2 < 0 & \qquad F(2) &= 2(2p-k)(k-p) > 0 \end{aligned}$$

So by lemma 2.4 one root, z_{d^*1}, is in the interval $(0,1)$, and the other is in $(1,2)$. If $\alpha = \frac{p}{k} < \frac{4}{5}$ then $F(\alpha) < 0$ and lemma 2.4 says $z_{d^*1} < \alpha$, that is, d^* is E-inferior to d_0. Similarly, if $\alpha > \frac{4}{5}$ then $z_{d^*1} > \alpha$ and d^* is E-better than d_0. Obviously these two designs are E-equal when $\alpha = \frac{4}{5}$. Note that $\alpha = \frac{4}{5}$ is equivalent to $k = \frac{5v}{6}$.

For $\alpha > \frac{4}{5}$, z_{d^*1} is found by solving (21):

$$\begin{aligned} z_{d^*1} &= \frac{k + 2p - \sqrt{17k^2 - 36kp + 20p^2}}{2k} && (22) \\ &= \frac{1}{2} + \alpha - \frac{1}{2}\sqrt{17 - 36\alpha + 20\alpha^2}. && (23) \end{aligned}$$

Now the task is to eliminate other members of $\mathcal{D}_1$ relative to d_0 and d^*. Every design $d \in \mathcal{D}_1$ has the same numbers $2(k-p)$ and p of treatments with one and two replicates respectively. So the combinatorial structure of any such d can be described as follows. Found only in block one are $k-p-s$ treatments replicated once, where $0 \le s \le k-p$, and $s+y$ treatments replicated twice, where $y \ge 0$. Found only in block two are $k-p+s$ treatments with one replicate and y treatments with two replicates. The two blocks have in common $p-s-2y$ treatments with two replicates (see Figure 3).

Block 1:	(k-p-s) 1-rep trts	s non-binary 2-rep trts	y non-binary 2-rep trts	(p-s-2y) binary 2-rep trts
Block 2:	(k-p+s) 1-rep trts		y non-binary 2-rep trts	(p-s-2y) binary 2-rep trts

Figure 3: General Design Structure in $\mathcal{D}_1(v, 2, k)$

Connectedness requires that $s + 2y < p$. If $s = y = 0$ the design is d_0 while d^* is found by setting $s = k - p$ and $y = 0$. The information matrix C_d is:

$$\begin{pmatrix} I_{k-p+s} - \frac{1}{k}J_{k-p+s} & 0_{k-p+s,k-p-s} & 0_{k-p+s,s+y} & -\frac{2}{k}J_{k-p+s,y} & -\frac{1}{k}J_{k-p+s,p-s-2y} \\ 0_{k-p-s,k-p+s} & I_{k-p-s} - \frac{1}{k}J_{k-p-s} & -\frac{2}{k}J_{k-p-s,s+y} & 0_{k-p-s,y} & -\frac{1}{k}J_{k-p-s,p-s-2y} \\ 0_{s+y,k-p+s} & -\frac{2}{k}J_{s+y,k-p-s} & 2I_{s+y} - \frac{4}{k}J_{s+y} & 0_{s+y,y} & -\frac{2}{k}J_{s+y,p-s-2y} \\ -\frac{2}{k}J_{y,k-p+s} & 0_{y,k-p-s} & 0_{y,s+y} & 2I_y - \frac{4}{k}J_y & -\frac{2}{k}J_{y,p-s-2y} \\ -\frac{1}{k}J_{p-s-2y,k-p+s} & -\frac{1}{k}J_{p-s-2y,k-p-s} & -\frac{2}{k}J_{p-s-2y,s+y} & -\frac{2}{k}J_{p-s-2y,y} & 2I_{p-s-2y} - \frac{2}{k}J_{p-s-2y} \end{pmatrix} \tag{24}$$

If $y = 0$ or $s = k - p$ the information matrix collapses to fewer partitioned components.

From lemma 2.2 the nonzero eigenvalues of C_d in (24) are: 1 with frequency $2(k - p) - 2$, 2 with frequency $p - 3$, and the four nonzero eigenvalues of the following matrix:

$$\begin{pmatrix} \frac{p-s}{k} & 0 & 0 & -\frac{2y}{k} & -\frac{p-s-2y}{k} \\ 0 & \frac{p+s}{k} & -\frac{2(s+y)}{k} & 0 & -\frac{p-s-2y}{k} \\ 0 & -\frac{2(k-p-s)}{k} & 2 - \frac{4(s+y)}{k} & 0 & -\frac{2(p-s-2y)}{k} \\ -\frac{2(k-p+s)}{k} & 0 & 0 & \frac{2(k-2y)}{k} & -\frac{2(p-s-2y)}{k} \\ -\frac{k-p+s}{k} & -\frac{k-p-s}{k} & -\frac{2(s+y)}{k} & -\frac{2y}{k} & \frac{2(k-p+s+2y)}{k} \end{pmatrix} \tag{25}$$

The eigenvalues of (25) are 2 and the roots of

$$\begin{aligned} F_d(\lambda) &= k^2\lambda^3 - 2k(2k - s - 2y)\lambda^2 + (4k^2 + 2kp - p^2 \\ &\quad -6ks + 2ps - s^2 - 12ky + 4py)\lambda - 2(2k - p)(p - s - 2y) = 0 \end{aligned} \tag{26}$$

Corresponding to the collapsing of partitions in (24), function F_d in (26) is still the characteristic polynomial for $y = 0$ but not $s = k - p$. There are thus two cases to consider: $s < k - p$ with $s > 0$ if $y = 0$, and $s = k - p$. In interest of space and because the manipulations are similar, only the former is shown here.

First F_d is evaluated at a few easily simplified points:

$$F_d(0) = -2(p - s - 2y)(2k - p) < 0$$

$$
\begin{aligned}
F_d(\alpha) &= \frac{4(k-p)^2(s+2y)-ps^2}{k} \\
F_d(1) &= (k-p-s)(k-p+s) > 0
\end{aligned}
$$

So z_{d1} is in $(0,1)$, and lemma 2.4 says that $z_{d1} < x$ for any x such that $F_d(x) > 0$.

If $\frac{p}{k} \leq \frac{4}{5}$ then $F_d(\frac{p}{k}) = \frac{[4(k-p)^2-ps]s+8(k-p)^2y}{k} > \frac{(4[k-p)^2-p(k-p)]s+8(k-p)^2y}{k} > 0 \Rightarrow$ $z_{d1} < \frac{p}{k}$, that is, d is E-inferior to d_0.

For $\frac{p}{k} > \frac{4}{5}$ write $\gamma = k-p-s$ for some $0 < \gamma \leq k-p$. Using $F(\lambda)$ in (21) (which has z_{d^*1} as a root), a bit of algebra shows that F_d can be re-expressed as

$$
\begin{aligned}
F_d(\lambda) &= (\lambda - 1 - \frac{2\gamma}{k})F(\lambda) \\
&\quad + \gamma(6k-8p-\gamma)\lambda - (12k-22p+\frac{8p^2}{k})\gamma + 4y[(2-\lambda)k-p](1-\lambda)
\end{aligned}
$$

Since $z_{d^*1} < 1$, the trailing term $4y[(2-\lambda)k-p](1-\lambda)$ is nonnegative (positive unless $y=0$) at $\lambda = z_{d^*1}$ and so

$$
F_d(z_{d^*1}) \geq \gamma(6k-8p-\gamma)z_{d^*1} - (12k-22p+\frac{8p^2}{k})\gamma \tag{27}
$$

Using $p = \alpha k$ and z_{d^*1} from (23), after dropping the factor $\frac{-\gamma k}{2}$ the RHS of (27) can be rewritten as

$$
\Theta = \frac{\gamma}{k}(1+2\alpha-\sqrt{17-36\alpha+20\alpha^2}) - 2(-3+4\alpha)(3-4\alpha+\sqrt{17-36\alpha+20\alpha^2})
$$

If $\Theta < 0$ the proof is complete. Since $\frac{\gamma}{k} < (1-\alpha)$ and also $1+2\alpha-\sqrt{17-36\alpha+20\alpha^2} > 0$ for $\frac{4}{5} < \alpha < 1$,

$$
\begin{aligned}
\Theta &< (1-\alpha)(1+2\alpha-\sqrt{17-36\alpha+20\alpha^2}) - 2(-3+4\alpha)(3-4\alpha+\sqrt{17-36\alpha+20\alpha^2}) \\
&= 19+30\alpha^2-47\alpha-(7\alpha-5)\sqrt{17-36\alpha+20\alpha^2}
\end{aligned}
$$

But $(7\alpha-5)\sqrt{17-36\alpha+20\alpha^2} > 0$ for $\alpha > \frac{4}{5}$, so $\Theta < 0$ is implied by $T(\alpha) < 0$ where

$$
\begin{aligned}
T(\alpha) &= (19+30\alpha^2-47\alpha)^2 - [(7\alpha-5)\sqrt{17-36\alpha+20\alpha^2}]^2 \\
&= -8(\alpha-2)(\alpha-1)(2\alpha-1)(5\alpha-4)
\end{aligned}
$$

Obviously $T(\alpha) < 0$ for every $\alpha \in (\frac{4}{5}, 1)$. $\square$

Lemma 5.1 reduces the class of possible E-optimal designs to d_0, d^*, and designs with at least one treatment replicated three times or more. The next two lemmas further restrict the potential competitors.

LEMMA 5.2 *Any design in $\mathcal{D}(v, 2, k)$ with both blocks containing at least $k - p + 1$ treatments with one replicate is E-inferior to the binary design d_0.*

PROOF For any normalized vector l and any d, an upper bound for z_{d1} is $\frac{v}{v-x^2} l' C_d l$ where $x = l'1$ (Morgan, 2007, lemma 2). Here define a group of treatments as any $k - p + 1$ treatments having replication one and appearing in the first block. Similarly define a second group of singly-replicated treatments appearing in the second block. Let l be the normalized contrast vector comparing these two groups. Then $x = 0$ and $l' C_d l = \frac{p-1}{k} < \frac{p}{k}$. □

LEMMA 5.3 *Any design in $\mathcal{D}(v, 2, k)$ with more than $k - \frac{p}{2}$ singly-replicated treatments appearing in the same block is E-inferior to the binary design d_0.*

PROOF Suppose WLOG treatments $1, 2, \ldots, k - t$ are singly-replicated and appear in the same block. Let l be the v-vector with 1's in positions $1, \ldots, k - t$ and 0 otherwise. Then normalizing l and applying the result cited in the proof of lemma 5.2,

$$z_{d1} \leq \frac{v}{(k-t)(v-k+t)} \sum_{i,i'=1}^{k-t} (C_d)_{ii'} = \frac{vt}{(v-k+t)k} = \frac{(2k-p)t}{(k-p+t)k}$$

which is less than $z_{d_0 1} = \frac{p}{k}$ if and only if $t < \frac{p}{2}$. □

Recalling the definition of m from section 3, if a design is to be E-optimal, then lemma 5.3 says it must satisfy $m + s \leq \frac{p}{2}$ (note that $p = 2k - v$). Lemma 5.2 further implies $s \geq 0$. These restrictions set the stage for lemma 5.4.

LEMMA 5.4 *Any design in which some treatment has more than two replicates cannot be E-optimal in $\mathcal{D}(v, 2, k)$. That is, no design in $\mathcal{D}_2$ is E-optimal.*

Block 1:	(k-p-s) 1-rep trts	t_3 binary 2-rep trts	t_1 non-binary 2-rep trts	m trts
Block 2:	(k-p+s+m) 1-rep trts	t_3 binary 2-rep trts	t_2 non-binary 2-rep trts	m trts

Figure 4: Averaging Structure in $\mathcal{D}(v, 2, k)$

Proof Designs in $\mathcal{D}_2$ are exactly those for which $m \geq 1$. The proof proceeds by averaging over a partition for an arbitrary member of $\mathcal{D}_2$, one subset of which consists of m appropriately chosen treatments.

As discussed in section 3, there are $2(k-p)+m$ singly-replicated treatments, of which $k-p-s$ appear in block 1 and $k-p+s+m$ appear in block 2. For any selected $d \in \mathcal{D}_2$, at least $p-2m$ treatments have exactly two replicates. Let the number of treatments having exactly two replicates and occurring only in block i of d be t_i, $i = 1, 2$. Then the number of treatments with two replicates and occurring in both blocks is at least $t_3 = p - 2m - t_1 - t_2$. Identify such a set of t_3 treatments, thereby also identifying exactly m treatments other than the $p - 2m = t_1 + t_2 + t_3$ so far identified as having exactly two replicates, and the $2(k-p)+m$ treatments having exactly one replicate. Then a partition of the treatments into six subsets of sizes $k-p-s$, $k-p+s+m$, t_1, t_2, t_3 and m (see Figure 4) has been defined.

The average matrix corresponding to this partition is

$$\begin{pmatrix} \omega I_m + \psi J_m & \xi_1 J & \xi_2 J & \xi_3 J & \xi_4 J & \xi_5 J \\ \xi_1 J & 2I_{t_3} - \frac{2}{k} J_{t_3} & -\frac{2}{k} J & -\frac{2}{k} J & -\frac{1}{k} J & -\frac{1}{k} J \\ \xi_2 J & -\frac{2}{k} J & 2I_{t_1} - \frac{4}{k} J_{t_1} & 0 & -\frac{2}{k} J & 0 \\ \xi_3 J & -\frac{2}{k} J & 0 & 2I_{t_2} - \frac{4}{k} J_{t_2} & 0 & -\frac{2}{k} J \\ \xi_4 J & -\frac{1}{k} J & -\frac{2}{k} J & 0 & I_{k-p-s} - \frac{1}{k} J_{k-p-s} & 0 \\ \xi_5 J & -\frac{1}{k} J & 0 & -\frac{2}{k} J & 0 & I_{k-p+s+m} - \frac{1}{k} J_{k-p+s+m} \end{pmatrix} . \tag{28}$$

where $\xi_1, \ldots, \xi_5$ and $\omega + m\psi$ are determined by all row and column sums of (28) being zero. As will be seen, individual values of ω and ψ are not needed.

The eigenvalues of (28) are, by lemma 2.2, 1 with frequency $2(k-p)+m-2$, 2 with frequency $p-2m-3$, ω with frequency $m-1$, and the eigenvalues of

$$\begin{pmatrix} a & -\frac{3t_3}{k} & -\frac{2t_1w_1}{km} & -\frac{2w_2t_2}{km} & -\frac{w_1(k-p-s)}{km} & -\frac{w_2(k-p+s+m)}{km} \\ -\frac{3m}{k} & \frac{2(k-t_3)}{k} & -\frac{2t_1}{k} & -\frac{2t_2}{k} & -\frac{k-p-s}{k} & -\frac{k-p+s+m}{k} \\ -\frac{2w_1}{k} & -\frac{2t_3}{k} & \frac{2k-4t_1}{k} & 0 & -\frac{2(k-p-s)}{k} & 0 \\ -\frac{2w_2}{k} & -\frac{2t_3}{k} & 0 & \frac{2k-4t_2}{k} & 0 & -\frac{2(k-p+s+m)}{k} \\ -\frac{w_1}{k} & -\frac{t_3}{k} & -\frac{2t_1}{k} & 0 & \frac{p+s}{k} & 0 \\ -\frac{w_2}{k} & -\frac{t_3}{k} & 0 & -\frac{2t_2}{k} & 0 & \frac{p-s-m}{k} \end{pmatrix} \tag{29}$$

where $a = \frac{3km-5m^2-2m(s+t_2-t_1)-2(s+t_2-t_1)^2}{km}$, $w_1 = s+2m+t_2-t_1$ and $w_2 = m-s-t_2+t_1$. The parameters w_1 and w_2 are the numbers of plots taken by the m treatments of the partition in block 1 and 2 respectively. They must be nonnegative and cannot be zero simultaneously. That is,

$$w_1 = s+2m+t_2-t_1 \geq 0, \quad w_2 = m-s-t_2+t_1 \geq 0, \quad w_1+w_2 \neq 0 \tag{30}$$

The average matrix will collapse to smaller dimensions if any of t_1, t_2, t_3, or $k-p-s$ are zero; all designs considered have $m \geq 1$.

Let $G(\lambda)$ be the characteristic polynomial of (29). The approach from here parallels proofs earlier in the paper: first establish $G(0) > 0$ and $G(1) < 0$ (proving $z_{d1} < 1$), then show $G(z_{d_01}) < 0$ for $k \leq \frac{5v}{6}$ and $G(z_{d^*1}) < 0$ for $k > \frac{5v}{6}$. The messy, tedious details are relegated to the appendix. □

Combining lemmas 5.1 and 5.4 gives the main result of this section. Examples of E-optimal designs follow the Theorem.

Theorem 5.5 *In the class $\mathcal{D}(v,2,k)$, the binary design d_0 is the unique E-optimal design if $\frac{v}{2} < k < \frac{5v}{6}$; the non-binary design d^* is the unique E-optimal design if $\frac{5v}{6} < k < v$; and both d^* and d_0, and only these two designs, are E-optimal if $k = \frac{5v}{6}$.*

Example 1 Consider block size $k = v-2$. If $v = 9$ then $k < \frac{5v}{6}$ and the E-optimal design in $\mathcal{D}(9,2,7)$, is:

Block 1:	1	2	$\cdots$	5	6	7
Block 2:	1	2	$\cdots$	5	8	9

However, if $v = 13$ then $k > \frac{5v}{6}$ and the E-optimal design in $\mathcal{D}(13, 2, 11)$, is:

Block 1:	1	2	$\cdots$	7	8	8	9	9
Block 2:	1	2	$\cdots$	7	10	11	12	13

6 Comparisons and Discussion

A general observation from sections 3-5 is that for experiments in two blocks, conventional criteria lead to different design choice. This section further explores the interplay of the A, D, and E criteria.

Definition A design is said to be ϕ_η-optimal for fixed $\eta \geq 0$ if among all competing designs d it minimizes $\phi_\eta(C_d) = (\sum_{i=1}^{v-1}(z_{di})^{-\eta})^{\frac{1}{\eta}}$

Introduced by Kiefer (1975), the ϕ_η criteria include A, D, and E as $\eta = 1$, $\eta = 0$, and $\eta \to \infty$, respectively. These criteria provide a useful bridge for assessing the relative strengths of d_0 and d^* beyond what is revealed by A, D, and E alone. This is done by comparing $\phi_\eta(C_{d_0})$ and $\phi_\eta(C_{d^*})$ for all η. Of the many examples we have examined (including all $v \leq 100$), two are shown below, both having $\frac{k}{v} > \frac{5}{6}$.

We have found no example where d^* is ϕ_η-superior to d_0 for any η when $\frac{k}{v} < \frac{5}{6}$. On the other hand, for $\frac{k}{v} > \frac{5}{6}$, we have found d_0 to be ϕ_η-inferior to d^* for all but a relatively small set of η. This small set is of the form $\eta \leq \widetilde{\eta}$, with d^* superior for all $\eta > \widetilde{\eta}$. An obvious implication is that unless overriding weight is placed on the A-criterion, d^* is the better choice for $\frac{k}{v} > \frac{5}{6}$.

Example 2 Table 1 presents the ϕ_η-comparisons of d_0 and d^* for $\mathcal{D}(24, 2, k)$, in which $k/v > 5/6 \Leftrightarrow k \geq 21$.

k	21	22	23
$\widetilde{\eta}$	5.401	4.494	4.459

Table 1: $\widetilde{\eta}$ for $v = 24$ and $21 \leq k \leq 23$

EXAMPLE 3 Table 2 presents the ϕ_η-comparisons of d_0 and d^* for $\mathcal{D}(100, 2, k)$, in which $k/v > 5/6 \Leftrightarrow k \geq 84$.

k	84	85	86	87	88	89	90	91
$\tilde{\eta}$	9.771	7.316	6.253	5.628	5.213	4.923	4.714	4.566
k	92	93	94	95	96	97	98	99
$\tilde{\eta}$	4.465	4.405	4.384	4.405	4.474	4.614	4.872	5.421

Table 2: $\tilde{\eta}$ for $v = 100$ and $84 \leq k \leq 99$

A different comparison can be had through the E_t-criterion, which is $\sum_{i=1}^{t} \frac{1}{z_{di}}$ for fixed $t \in \{1, \ldots, v-1\}$. If d is E_t-optimal then it minimizes the largest average variance over all t-dimensional subspaces of the $(v-1)$-dimensional subspace of all treatment contrasts. E_1-optimality is the E-optimality of section 5, and E_{v-1}-optimality is the A-optimality of section 3. With the eigenvalues for d^* and d_0 in hand, this can be easily shown:

THEOREM 6.1 *For $k > \frac{5v}{6}$, d^* is E_t-better than d_0 for $1 \leq t < 2(v-k)$, and d_0 is E_t-better than d^* for $2(v-k) \leq t \leq v-1$.*

E-optimality is a minimax criteria, and this theorem tells us how deeply d^*'s advantage over d_0 extends in a minimax sense. The depth of that advantage decreases as k grows.

In closing we offer one last observation. There are designs other than d^* which are E-better then d_0, and these designs vary with respect to their A-behavior. Proof of the following can be found in Jin (2004). The parameters s and y are defined in Figure 3.

THEOREM 6.2 *Consider the class $\mathcal{D}_1(v, 2, k)$ with $\frac{k}{v} > \frac{5}{6}$. The following hold:*

(i) A necessary condition for a non-binary design to be E-superior to d_0 is $s \geq \lfloor \frac{4(k-p)^2}{p} \rfloor + 1$. This necessary condition is sufficient when $y = 0$.

(ii) Among all non-binary designs that are E-superior to d_0, the design with $s = \lfloor \frac{4(k-p)^2}{p} \rfloor + 1$ and $y = 0$ is A-best and D-best.

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A Further Details for the Lemma 5.4 Proof

The proof proceeds from the paragraph following (30), using the reduced average matrix (29). The first job is to show there is a positive eigenvalue less than one for (29). The characteristic polynomial for (29), after removing the factors λ and $\lambda - 2$, multiplying by $k^2 m$, and employing the definitions of w_1, w_2, and t_3, is

$$\begin{aligned}
G(\lambda) \;=\; & \lambda^4 k^2 m + \lambda^3[2k(t_1-t_2)^2 - 4kst_1 + 4k(s+m)t_2 + 2ks^2 + 2ksm + 2km^2 - 7k^2 m] \\
& +\lambda^2[(-10k+2p+m)(t_1-t_2)^2 + 2(10ks - km - 2ps + m^2)t_1 \\
& \quad -2(10ks + 11km - 2ps - 2pm - m^2)t_2 \\
& \quad +16k^2 m + 2kpm - 10ksm - 10ks^2 - 8km^2 + 2ps^2 + 2psm - p^2 m - 2sm(s+m)] \\
& +\lambda[(16k - 6p - m)(t_1-t_2)^2 - 2(16ks - 3km - 6ps + pm + m^2)(t_1 - t_2) \\
& \quad +4(11km - 4pm + m^2)t_2 \\
& \quad +16ks^2 + 16ksm - 12k^2 m + 12km^2 - 6ps^2 + 5p^2 m - 2pm^2 + 4sm(s+m)] \\
& -2(2k-p)[2(t_1-t_2)^2 - (4s-m)(t_1-t_2) + 6mt_2 + 2(m^2+ms+s^2) - 3mp]
\end{aligned}$$

The last line in the above expression, which is $G(0)$, can be rearranged as

$$\begin{aligned}
G(0) &= 4(2k-p)(m-s+t_1-t_2)(2m+s-t_1+t_2) + 6(2k-p)m(p-2m-t_1-t_2) \\
&= 4(2k-p)w_1 w_2 + 6(2k-p)mt_3
\end{aligned}$$

Now $t_3 \geq 0$ and from (30) $w_1 w_2 > 0$, so $G(0) > 0$. Direct evaluation gives $G(1) = -2m(k-p-s)(k-p+m+s) < 0$. Thus $z_{d1} \in (0,1)$ for any d inducing the full 6×6 matrix (29), i.e. for any d not having any $t_i = 0$ or $s = k - p$, in which cases the correct version of (29) has smaller dimension. It can be shown that $G(\lambda)$ as given above reduces to the correct polynomial if any $t_i = 0$, so the result for z_{d1} holds in these cases. If $s = k - p$, the characteristic polynomial can be expressed as $Q(\lambda)$ (say) where $G(\lambda)|_{s=k-p} = (1-\lambda)Q(\lambda)$. For any $\lambda < 1$, $(1-\lambda)Q(\lambda)$ and $Q(\lambda)$ have the same sign, so again the result holds.

It remains to show that $G(z_{d_0 1}) < 0$ when $p \leq \frac{4k}{5}$, and $G(z_{d^* 1}) < 0$ when $p > 4k/5$. These are nontrivial tasks, each requiring investigation of several involved subcases.

While the general thrust of the arguments for these two tasks are similar, working with $G(z_{d^*1})$ is relatively more difficult due to z_{d^*1} being irrational. Here only some cases for $G(z_{d^*1})$ are explored. The complete proof can be seen in Jin's (2004) dissertation, where it consumes 29 pages.

The main points of the proof are as follows. $G(z_{d^*1})$ is a quadratic function of t_1 and t_2. This function of (t_1, t_2) is concave and has no solution to the equations $\partial G/\partial t_1 = 0 = \partial G/\partial t_2$. Its maximum value must therefor lie somewhere on the boundaries, i.e., on the lines $t_1 = 0$, $t_2 = 0$, $t_1 + t_2 = p - 2m$, $t_2 - t_1 = m - s$ or $t_1 - t_2 = s + 2m$. The values on the five lines are all smaller than zero, and so $G(z_{d^*1}) < 0$. Some of the fairly extensive technical details for this straightforward line of thought follow.

Recall from (22) that $z_{d^*1} = \frac{k+2p-\sqrt{17k^2-36kp+20p^2}}{2k} = \alpha + \frac{1}{2}(1-\sqrt{17-36\alpha+20\alpha^2}) = \alpha + \frac{1}{2}(1-\delta)$, say, introducing the symbol δ to simplify the expression (which is best left to software so is not shown here) of $G(z_{d*1})$. It can be seen that $0 < \delta < 1$ for $\frac{4}{5} < \frac{p}{k} = \alpha < 1$. Considering $G(z_{d*1})$ as a functon of t_1 and t_2, differentiate to find

$$\frac{\partial^2 G(z_{d*1})}{\partial t_1^2} = \frac{\partial^2 G(z_{d*1})}{\partial t_2^2} = -\frac{\partial^2 G(z_{d*1})}{\partial t_1 \partial t_2} = -\frac{\partial^2 G(z_{d*1})}{\partial t_2 \partial t_1}$$
$$= -\frac{(k-2p+2\delta)[9k^2-18kp+8p^2+2mp+km(1-\delta)+6k\delta(k-p)+k^2\delta^2]}{2k^2} \quad (31)$$

Evaluation of (31) requires showing $k - 2p + k\delta > 0$. This is easily done with a simple plot as follows. Replacing δ by its actual value gives $k - 2p + k\delta = k(1 - 2\alpha + \sqrt{17-36\alpha+20\alpha^2})$. Plotting $1-2\alpha+\sqrt{17-36\alpha+20\alpha^2}$ shows that it is always greater than zero for $\alpha \in (\frac{4}{5}, 1)$. It can be similarly shown that $9k^2 - 18kp + 8p^2 + 6k\delta(k-p) + k^2\delta^2 > 0$ for $p > \frac{4}{5}k$.

As a consequence, the Hessian for $G(z_{d^*1})$ with respect to t_1 and t_2 is non-positive definite, implying $G(z_{d^*1})$ is concave with respect to t_1 and t_2. If there is a solution to the equations $\partial G(z_{d^*1})/\partial t_1 = 0 = \partial G(z_{d^*1})/\partial t_2$ in the feasible (t_1, t_2) range, then that solution maximizes $G(z_{d^*1})$; if no such solution exists, $G(z_{d^*1})$ is maximized on a boundary of the feasible region.

So set $\partial G(z_{d^*1})/\partial t_1 = 0$ and solve for t_1, call the solution $\hat{t}_{11}$. Likewise set $\partial G(z_{d^*1})/\partial t_2 = 0$ and again solve for t_1, call the solution $\hat{t}_{12}$ (again, this is an onerous task if done manually, but easily left to software). Setting $\hat{t}_{11} = \hat{t}_{12}$ and cancelling their common denominator gives

$$[15k^2 - 26kp + 8p^2 + k^2\delta^2 + 2k\delta(4k - 3p)] + [4mp + 2km(1 - \delta)] = 0.$$

The second bracketed term is obviously positive (since $m > 0$). Dividing the first bracketed term by k^2 produces a function of α alone which, when plotted, is positive for $\alpha \in (\frac{4}{5}, 1)$. Thus there is no solution to $\partial G(z_{d^*1})/\partial t_1 = 0 = \partial G(z_{d^*1})/\partial t_2$. The maximum value for $G(z_{d^*1})$ must be on the boundaries identified above.

Now the truly tedious part begins: checking the values of $G(z_{d^*1})$ on the boundary lines. Here the line $t_1 = 0$ will be examined; other cases are in Jin (2004). Writing G_1^* for $-16k^2 G(z_{d^*1})$ evaluated at $t_1 = 0$,

$$\begin{aligned}
G_1^* \;=\; & 4(k - 2p + k\delta)[9k^2 - 18kp + 8p^2 + 2mp + km(1 - \delta) + 6k\delta(k - p) + k^2\delta^2]t_2^2 \\
& +8(k - 2p + k\delta)[(k + 2p - k\delta)m^2 + (3k - 4p + k\delta)(4k - 2p + k\delta)m \\
& \qquad\qquad + s(3k - 4p + k\delta)(3k - 2p + k\delta)]t_2 \\
& +(3k - 2p + k\delta)L
\end{aligned}$$

where

$$\begin{aligned}
L \;=\; & 4[5k^2 - 8kp + 4p^2 - 2s(k + 2p - k\delta) + k\delta(2k - 4p + k\delta)]m^2 \\
& +4s[3k^2 - 10kp + 8p^2 - 2s(k + 2p - k\delta) + k\delta(4k - 6p + k\delta)]m \\
& +4s^2(k - 2p + k\delta)(3k - 4p + k\delta) \\
& +km(1 - \delta)(3k - 4p + k\delta)(5k - 2p + k\delta).
\end{aligned}$$

The goal is to show $G_1^* > 0$. Now $3k - 4p + k\delta > k - 2p + k\delta \geq k - 2p + 2\delta > 0$ for $p > 4k/5$, the last inequality having been established following (31), so the coefficient of t_2 in G_1^* is positive. The coefficient of t_2^2 is positive by comparison with (31). It remains to show that $L > 0$.

The two expressions in L in square brackets are each decreasing in s, so can be bounded by setting $s = k - p$ and simplifying as follows:

$$5k^2 - 8kp + 4p^2 - 2s(k + 2p - k\delta) + k\delta(2k - 4p + k\delta) \geq (k - 2p + k\delta)(3k - 4p + k\delta)$$

and

$$3k^2 - 10kp + 8p^2 - 2s(k + 2p - k\delta) + k\delta(4k - 6p + k\delta) \geq 2(3k - 4p)(3k - 4p + k\delta)$$

But

$$2(3k-4p)(3k-4p+k\delta) = -2(k-2p+k\delta)(3k-4p+k\delta) + 2(4k-6p+k\delta)(3k-4p+k\delta)$$

so

$$\begin{aligned} L \;\geq\; & 4(k - 2p + k\delta)(3k - 4p + k\delta)(m - s)^2 + 8ms(4k - 6p + k\delta)(3k - 4p + k\delta) \\ & + km(1 - \delta)(3k - 4p + k\delta)(5k - 2p + k\delta). \end{aligned} \tag{32}$$

If $4k - 6p + k\delta \geq 0$ then $L > 0$. If $4k - 6p + k\delta < 0$, drop the leading term on the RHS of (32) and set $s = k - p$ to get

$$\begin{aligned} L/m \;&\geq\; 8(k-p)(4k - 6p + k\delta)(3k - 4p + k\delta) + k(1 - \delta)(3k - 4p + k\delta)(5k - 2p + k\delta) \\ &=\; 2(3k - 4p + k\delta)[10k^2 - 23kp + 14p^2 + (2k - 3p)k\delta]. \end{aligned}$$

where the last line is found by replacing $k^2\delta^2$ by $17k^2 - 36kp + 20p^2$. One may verify that $10k^2 - 23kp + 14p^2 + (2k - 3p)k\delta = k^2[10 - 23\alpha + 14\alpha^2 + (2 - 3\alpha)\delta] > 0$ by simply plotting for $\alpha \in (\frac{4}{5}, 1)$. $\square$