ON OPTIMALITY PROPERTIES OF SIMPLE BLOCK DESIGNS IN THE APPROXIMATE DESIGN THEORY

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Abstract: Optimality properties of approximate block designs are studied under variations of (1) the class of competing designs, (2) the optimality criterion, (3) the parametric function of interest, and (4) the statistical model. The designs which are optimal turn out to be the product of their treatment and block marginals, and uniform designs when the support is specified in advance. Optimality here means uniform, universal, and simultaneous j_p -optimality. The classical balanced incomplete block designs are embedded into this approach, and shown to be simultaneously j_p -optimal for a maximal system of identifiable parameters. A geometric account of universal optimality is given which applies beyond the context of block designs.

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1. Introduction

It is common practice to divide the theory of experimental design into two parts: the approximate theory deals with optimality characterizations of approximate designs, and the exact theory investigates construction and properties of exact designs. In the present paper we shall be less orthodox and apply the approximate theory to simple block designs, which usually are viewed as a prime domain of the exact design theory. A similar approach has been chosen in recent independent work by Giovagnoli & Wynn (1981).

Given v varieties, or treatments, i = 1, ..., v, and b blocks j = 1, ..., b, an exact block design of size n is a set of integers $n_{ij} \in \{0, ..., n\}$ which sum to n, directing the experimenter to observe n_{ij} times the i-th treatment in the j-th block. In this paper we shall discuss approximate block designs instead, i.e. sets of weights $w_{ij} \in [0, 1]$ which sum to 1, indicating that a proportion w_{ij} of all observations is to be taken with the i-th treatment in the j-th block.

The approximate theory will provide the tools to discuss optimality properties of

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block designs (1) under variation of the class of competing designs (all designs, all designs with given treatment marginals, or given block marginals, or both, or given support), (2) under variation of the optimality criterion (uniform optimality, universal optimality, j_p -optimality), (3) under variation of the parametric function to be investigated (treatment contrasts, block contrasts, maximal systems of identifiable parameters), and (4) under variation of the statistical model (interaction effects, additive effects).

Perhaps our final Theorem 7 is the result which surprises most. The classical balanced incomplete block designs (BIBDs) have always been studied with the set of treatment contrasts being the parameters under investigation. While I was unable to establish any distinguished optimality properties of BIBDs, for the treatment contrasts, Theorem 7 does prove a unique optimality property of BIBDs, for a maximal system of identifiable parameters.

Section 2 sets out with a review and some extensions of optimality characterizations developed in Pukelsheim (1980). Section 3 offers a geometric account of universal optimality, and generalizes Kiefer's (1975) original concept for balanced designs and Cheng's (1978) version for asymmetrical designs, both of which were presented in the context of block designs only.

In Section 4 we discuss block designs with the statistical model including the interaction effects of all possible treatment block combinations. In contrast, Sections 5 and 6 assume additive treatment and block effects, in Section 5 every weight w_{ij} may be positive. The approximate theory suggests a generalization of BIBDs in the sense that the support of feasible designs is restricted to be contained in a preassigned set S of treatment block combinations; the concluding Section 6 is devoted to such 'incompletely supported' block designs.

2. Uniform optimality and j_p -optimality

For convenience of reference we briefly recall those optimality characterizations of Pukelsheim (1980) which we shall need in the sequel, including some minor amendments. As usual, the regression function f on the design space \mathfrak{X} is an \mathbb{R}^k -valued function with compact image $f(\mathfrak{X})$, Ξ is the set of all design measures ξ on \mathfrak{X} , and the information matrix of ξ is $M(\xi) = \int_{\mathfrak{X}} f(x)f(x)' \, d\xi$, a prime denoting transposition. Further, K is a fixed $k \times t$ matrix of rank s, and $\mathfrak{A}(K)$ is the convex cone of all non-negative definite $k \times k$ matrices whose range contains the range of K. We shall say that $K'\beta$ is identifiable under ξ if $M(\xi)$ lies in $\mathfrak{A}(K)$. The matrix $J(M(\xi)) = (K'M(\xi)^-K)^+$ will be called the information matrix of ξ for $K'\beta$ provided $K'\beta$ is identifiable under ξ , otherwise we set $J(M(\xi)) = 0$.

In the following statements Π is a subset of Ξ such that $\mathfrak{M} = M(\Pi)$ is a closed convex subset of $M(\Xi)$ and $K'\beta$ is identifiable under at least one design measure in Π , ξ is a fixed member of Π under which $K'\beta$ is identifiable, M is the information matrix of ξ , and C is its information matrix for $K'\beta$.

If M has maximal rank in \mathfrak{M} , then ξ is uniformly optimal for $K'\beta$ in Π if and only if

$$K'M^{-}AM^{-}K \le K'M^{-}K$$
, for all $A \in \mathfrak{M}$; (1)

and then any other design $\eta \in \Pi$ with information matrix A is also uniformly optimal for $K'\beta$ in Π if and only if

$$AM^{-}K = K. (2)$$

In (1) maximality of the rank of M is convenient to work with but not necessary, see Theorem 4(a). Next consider the information functionals j_p , $p \in]-\infty, +1]$, i.e. the generalized means of order $p > -\infty$ of the positive eigenvalues of the information matrices for $K'\beta$. The design ξ has Π -maximal j_p -information for $K'\beta$ if and only if there exists a g-inverse G of M with

trace
$$K'GAG'KC(K'M^-K)^{1-p}C \le \operatorname{trace} C(K'M^-K)^{1-p}$$
, for all $A \in \mathfrak{M}$;
(3)

and in case p < 1 then any other design $\eta \in \Pi$ with information matrix A also has Π -maximal j_p -information for $K'\beta$ if and only if

$$AG'K = K. (4)$$

Finally we turn to $j_{-\infty}$ -, i.e. E-optimality. Define S to be the set of all $t \times t$ matrices of the form zz' such that z is a normalized eigenvector of $K'M^-K$ corresponding to $\lambda_{\max}(K'M^-K)$. The design ξ has Π -maximal $j_{-\infty}$ -information for $K'\beta$ if and only if there exist a g-inverse G of M and a matrix $E \in \text{conv } S$ such that

trace
$$K'GAG'KE \le \lambda_{\max}(K'M^{-}K)$$
, for all $A \in \mathfrak{M}$; (5)

and then any other design $\eta \in \Pi$ with information matrix A which also has Π -maximal $j_{-\infty}$ -information for $K'\beta$ necessarily satisfies

$$AG'KE = KE. (6)$$

These characterizations follow from Corollaries 5.2, 5.3, 8.2 and a remark after Corollary 8.1 in Pukelsheim (1980).

There is only one choice of a g-inverse of M if M is non-singular. There is only one choice for the matrix E in (5) and (6) provided the eigenvalue $\lambda_{\max}(K'M^-K)$ is simple. If M has maximal rank in $\mathfrak M$ then G may be replaced by an arbitrary g-inverse M^- of M throughout. In particular, (3) becomes independent of the choice of G, and the apparent discontinuity between (3) and (5) vanishes, as follows.

Proposition 1. Let $\xi \in \Pi$ be a design measure whose information matrix M has maximal rank in \mathfrak{M} . If ξ has Π -maximal j_p -information for $K'\beta$, for all $p \in]-\infty, 0[$, then ξ also has Π -maximal $j_{-\infty}$ and j_0 -information for $K'\beta$.

Proof. By continuity in p, (3) extends to p=0. Let $\lambda_1 > \cdots > \lambda_r > 0$ be the distinct

positive eigenvalues of $K'M^-K$, with associated pairwise orthogonal projection matrices $E_1, ..., E_r$. Multiply (3) by λ_1^{p+1} to obtain

trace
$$K'M^-AM^-K\left\{E_1+\sum_{i=2}^r (\lambda_i/\lambda_1)^{-p-1}E_i\right\} \leq \lambda_1\operatorname{trace}\left\{E_1+\sum_{i=2}^r (\lambda_i/\lambda_1)^{-p}E_i\right\}$$
.

As p tends to $-\infty$ this tends to (5), with $E = E_1/\text{trace } E_1$. \square

Obviously (6) coincides with (4) and is sufficient, besides being necessary, provided E can be chosen to be a multiple of K^+K . This is possible whenever the design ξ is balanced for $K'\beta$, i.e. when its information matrix for $K'\beta$ equals ϱK^+K , for some $\varrho>0$. Moreover, if the design ξ is balanced for $K'\beta$ and has Π -maximal j_{p_0} -information for $K'\beta$, for some $p_0>-\infty$, then ξ has Π -maximal j_p -information for $K'\beta$, for all $p\in [-\infty,+1]$, see Corollary 8.3 in Pukelsheim (1980). For a design to be simultaneously optimal with respect to all j_p -criteria it is not necessary to be balanced for $K'\beta$, see Theorems 5 and 7.

We conclude Section 2 by some general remarks on Kronecker product designs, those designs being closely related to the results of Section 4. Suppose an information functional j on NND(s) has two Kronecker factors j_1 on NND(s_1) and j_2 on NND(s_2); by definition, this means that $s = s_1 s_2$, j_1 and j_2 are information functionals on NND(s_1) and NND(s_2), respectively, and the information functionals j, j_1, j_2 and their polar functions j^0, j_1^0, j_2^0 satisfy $j(C_1 \otimes C_2) = j_1(C_1)j_2(C_2)$ and $j^0(D_1 \otimes D_2) = j_1^0(D_1)j_2^0(D_2)$ whenever C_i , $D_i \in \text{NND}(s_i)$, i = 1, 2. Given $k_i \times s_i$ matrices K_i of rank s_i , i = 1, 2, define $K = K_1 \otimes K_2$ and $k = k_1 k_2$. Let \mathfrak{M}_i be compact convex subsets of NND(k_i) which intersect $\mathfrak{A}(K_i)$, i = 1, 2, and introduce \mathfrak{M} as the convex hull of all products of the form $A_1 \otimes A_2$ with $A_1 \in \mathfrak{M}_1$, $A_2 \in \mathfrak{M}_2$. Then \mathfrak{M} is a compact convex subset of NND(k) which intersects $\mathfrak{A}(K)$, and Theorem 5 of Pukelsheim (1980) permits the following generalization of a result due to Hoel (1965, p. 1099), cf. Krafft (1978, p. 286):

Proposition 2. If $M_i \in \mathfrak{M}_i$ has \mathfrak{M}_i -maximal j_i -information for $K_i'\beta_i$, i = 1, 2, then $M_1 \otimes M_2$ has \mathfrak{M} -maximal j-information for $K'(\beta_1 \otimes \beta_2)$. If $M_i \in \mathfrak{M}_i$ has maximal rank in \mathfrak{M}_i and is uniformly optimal for $K_i'\beta_i$ in \mathfrak{M}_i , i = 1, 2, then $M_1 \otimes M_2$ is uniformly optimal for $K'(\beta_1 \otimes \beta_2)$ in \mathfrak{M} . \square

Every j_p functional on NND(s) factorizes into the corresponding j_p functions on NND(s_i), provided $s = s_1 s_2$. A special situation arises when the design space \mathfrak{X} is a Cartesian product $\mathfrak{X}_1 \times \mathfrak{X}_2$, and the regression function f on \mathfrak{X} is the Kronecker product of two regression functions f_i on \mathfrak{X}_i . Then the set of all design measures on \mathfrak{X} is the convex hull of all products of the form $\xi_1 \otimes \xi_2$, where ξ_i is a design measure on \mathfrak{X}_i , and the associated sets of information matrices behave similarly. An extension to more than two Kronecker factors is immediate.

3. Universal optimality

In this section Π will be an arbitrary subset of Ξ such that $K'\beta$ is identifiable under at least one $\xi \in \Pi$. As before, $\mathfrak{M} = M(\Pi)$ is the set of information matrices associated with Π , but \mathfrak{M} need neither be closed nor convex; by $J(\mathfrak{M})$ we denote the corresponding set of information matrices for $K'\beta$. Kiefer (1975) introduced universal optimality in the situation of simple block designs; without reference to this particular setting, his Proposition 1 takes the following more general form, with an almost instant proof.

Theorem 1 (Line projection). Let $\xi \in \Pi$ be a design measure under which $K'\beta$ is identifiable, and let C be its information matrix for $K'\beta$. If ξ is balanced for $K'\beta$, and if C maximizes trace D over $D \in J(\mathfrak{M})$, then ξ has Π -maximal j-information for $K'\beta$, for all functions $j : NND(t) \to \mathbb{R}$ such that

- (a) $j(D) \le j(\{\text{trace } D/s\}K^+K)$, for all $D \in J(\mathfrak{M})$, and
- (b) $j(bK^+K)$ is isotone $b \ge 0$.

Proof. Taking traces in $C = \varrho K^+ K$ gives $\varrho = \text{trace } C/s$. For $D \in J(\mathfrak{M})$ then $j(D) \leq j(\{\text{trace } D/s\}K^+K) \leq j(\{\text{trace } C/s\}K^+K) = j(C)$.

By $\mathfrak{J}(K^+K)$ we shall denote the class of functions j which satisfy (a) and (b); of course, not all these functions admit an interpretation as an information functional. But $\mathfrak{J}(K^+K)$ does comprise all j_p -criteria. This follows from $j_p(D) \leq j_1(D) = j_1(D) \cdot j_p(K^+K) = j_p(j_1(D)K^+K)$, and $j_1(D) = \text{trace } D/s$. If a design fulfills the hypotheses of Theorem 1 it will be said to have Π -maximal \mathfrak{J} -information for $K'\beta$. Since $\mathfrak{J}(K^+K)$ includes also j_0 , again (4) describes which multiplicities are possible.

Theorem 1 also covers the block design setting in Kiefer (1975). There $K'\beta$ is a maximal set of treatment contrasts and $K^+K=K_v$, where K_v is the completely symmetric $v\times v$ matrix with on-diagonal entries 1-1/v and off-diagonal entries -1/v. Let P(D) be the average $(v!)^{-1}\sum \Gamma_\tau'D\Gamma_\tau$, where the summation extends over all permutations τ of $(1,\ldots,v)$, and Γ_τ is the permutation matrix determined by τ . It is implicit in Kiefer's proof of his Proposition 1 that $P(D)=\{\text{trace }D/(v-1)\}K_v$. Hence if j is concave and permutationally invariant then j is in the class $\Im(K_v)$, since

$$j(D) = (v!)^{-1} \sum j(\Gamma_{\tau}' D \Gamma_{\tau}) \le j(P(D)) = j(\{\text{trace } D/(v-1)\}K_v).$$

Bounds for trace D/s can be derived using the dual problem (D) of Pukelsheim (1980). Namely, when the variable N of (D) is taken to be of the form K'^+K^+/ν , with $\nu>0$, and when the set \mathfrak{M} of information matrices is closed and convex, then Theorem 3 $(op.\ cit.)$ yields

$$\sup_{D \in J(\mathfrak{M})} \operatorname{trace} D/s \le \max_{x \in \mathfrak{X}} \|K^+ f(x)\|^2 / s.$$

Here equality always holds if $K = I_k$, equality also holds in the situations of Theorems 3(b) and 4(b); equality does not hold in Theorem 6, even when the better bound $\max_{M \in \mathfrak{M}} \operatorname{trace} K^+ M K^{+} / s$ is used. The present argument is based on the observation that $\operatorname{trace} D / s$ equals $j_1(D)$.

However, the trace function makes its appearance in Theorem 1, not as an optimality criterion, but due to the fact that $\langle C, D \rangle = \operatorname{trace} C'D$ is the Euclidean matrix inner product on the space of all $t \times t$ matrices. Namely, if $D \in J(\mathfrak{M})$ then

$$j_1(D) = \operatorname{trace} D/s = \langle D, K^+K \rangle / \langle K^+K, K^+K \rangle,$$

or in other words, $\{\text{trace }D/s\}K^+K$ is the Euclidean projection of D onto the line spanned by K^+K . Therefore, next to projecting directly into the optimal solution and this trivially being equivalent to the original problem formulation, Theorem 1 proposes the second simplest projection method: first project onto the line spanned by the optimal solution and then solve a 1-dimensional maximization problem along this line. The next step, then, is obvious: first project onto a plane appropriately determined by an optimal solution and then solve a 2-dimensional maximization problem in this plane. Theorem 2.2 of Cheng (1978, p. 1242) is of this type.

Indeed, suppose that optimality is achieved with C being of the form $\mu P + \nu Q$, with μ , ν being scalars and P, Q being matrices. Assume that R is a mapping defined on $J(\mathfrak{M})$ which takes its values in the (P,Q)-plane. Cheng's argument may be understood so as to compare, not C and D in matrix space, but $\mu P + \nu Q$ and R(D) in the (P,Q)-plane.

The following notation allows to present a general result in this spirit, separated from the block design context in Cheng (1978). Define $\mathfrak{P}(s)$ to be the convex cone formed by all matrices of the form K^+KAK^+K , with $A \in PD(t)$. For $D \in \mathfrak{P}(s)$ let $\lambda(D)$ be the R^s -vector of its positive eigenvalues, respecting multiplicities and decreasingly ordered, $\lambda_1(D) \ge \cdots \ge \lambda_s(D)$. On $\mathfrak{P}(s)$ every orthogonally invariant function j(D) decomposes into $\phi(\lambda(D))$, with $\phi: R^s_+ \to R$ being symmetric in its arguments. Recall that the ordering in which points become smaller through averaging is majorization, and that real functions which are order-reversing with respect to majorization are called Schur-concave, see Marshall & Olkin (1979).

Theorem 2 (Plane projection). Let $\xi \in \Pi$ be a design measure under which $K'\beta$ is identifiable, and let C be its information matrix for $K'\beta$. Suppose C has two positive eigenvalues $\mu > \nu$, with multiplicities r and s - r, respectively, and let P and $Q = K^+K - P$ be the associated projection matrices. Assume that R is a function which maps $\mathfrak{P}(s)$ into the non-negative quadrant of the (P,Q)-plane and which leaves C = R(C) fixed.

If C maximizes both trace R(D) and g(R(D)) over $D \in J(\mathfrak{M})$, where the function g is given by

$$g(R) = \operatorname{trace} R - \{ sr/(s-r) \}^{1/2} \{ \operatorname{trace} R^2 - (\operatorname{trace} R)^2/s \}^{1/2},$$
 (7)

then ξ has Π -maximal j-information for $K'\beta$, for all orthogonally invariant functions $j: \mathfrak{P}(s) \to \mathbb{R}$, $j(D) = \phi(\lambda(D))$, say, such that

- (a) $j(D) \le j(R(D))$, for all $D \in J(\mathfrak{M})$,
- (b) j is isotone, and
- (c) ϕ is Schur-concave.

Proof. Fix $D \in J(\mathfrak{M})$ and define R = R(D), then $j(D) \leq j(R)$, by (a). One has $R = \mu(R)P + \nu(R)Q$, with $\mu(R) = \langle R, P \rangle / \text{trace } P$, and $\nu(R) = \langle R, Q \rangle / \text{trace } Q$. If $\mu(R) > \mu$ introduce a = trace C / trace R. Then $a \geq 1$, since C = R(C) maximizes trace R(D). It follows that $\lambda(aR)$ majorizes $\lambda(C)$, whence (b) and (c) yield $j(R) \leq j(aR) \leq j(C)$.

Otherwise $\mu(R) \le \mu$. We shall show that always $\nu(R) \le \nu$, whence (b) alone implies $j(R) \le j(C)$. The point is to identify the quantity g(R) geometrically. Let $H = \{ \operatorname{trace} R/s \} K^+ K$ be the Euclidean projection of R onto the $K^+ K$ -axis. The length of H, and the distance d between H and R are $||H|| = s^{-1/2} \operatorname{trace} R$ and $d = ||R - H|| = \{ \operatorname{trace} R^2 - (\operatorname{trace} R)^2/s \}^{1/2}$. Define G to be the (non-orthogonal) projection of R onto the $K^+ K$ -axis along the direction of P. Since $\langle P, Q \rangle = 0$, the angle γ between G - R and H - R coincides with the angle between Q and $K^+ K$, i.e.

$$\cos \gamma = \langle Q / || Q ||, K^+ K / || K^+ K || \rangle = \{ (s - r) / s \}^{1/2}$$

and

tan
$$\gamma = \{r/(s-r)\}^{1/2}$$
.

The distance between G and H then is $(\tan \gamma)d$, whence the length of G turns out to be $\|G\| = \|H\| - (\tan \gamma)d = s^{-1/2}g(R)$. Since C maximizes g(R(D)), the point R must lie above or on the line $L = \{C + \alpha P \mid \alpha \in R\}$, i.e. $\nu(R) \le \nu$. Thus the proof is complete. \square

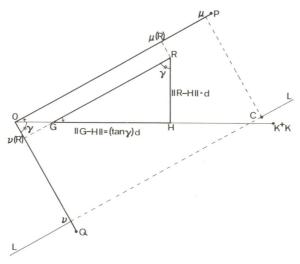


Fig. 1. The proof of Theorem 2 is based on a geometric identification of the quantity g(R) in (7) through $||G|| = ||H|| - ||G - H|| = s^{-1/2}g(R)$.

Applicability of Theorem 2 obviously depends on the choice of the mapping R. Cheng (1978) works with $R(D) = \mu(D)P + \nu(D)Q$ so that D and R(D) have the same projection onto the K^+K -axis, the same length, and $\mu(D) \ge \nu(D)$. Then g in (7) is easier to handle since R simply can be replaced by D. Interpreted in terms of a maximization problem, all of Cheng's criteria satisfy properties (b) and (c), see Marshall & Olkin (1979, p. 64). Hence the additional argument needed to derive Cheng's results from our Theorem 2 is that property (a) holds for his type-1 criteria whenever r=1, and for his type-2 criteria whenever r=1. We shall not pursue this subject here further.

4. Block designs in the interaction model

We now take up the discussion of simple block designs, and first introduce some necessary notation. The equiangular line in \mathbb{R}^v is $1_v = (1, \dots, 1)'$. Setting $J_v = 1_v 1_v'$, the orthodiagonal projection matrix is $K_v = I_v - J_v/v$. The *i*-th Euclidean basis vector in \mathbb{R}^v is e_i , with *i*-th entry 1 and zeroes elsewhere; similarly d_j is the *j*-th basis vector in \mathbb{R}^b . A stochastic vector r, i.e. $r_i \ge 0$ and $\sum r_i = 1$, is called positive if all r_i are positive; examples are $\overline{1_v} = 1_v/v$ and $\overline{1_b} = 1_b/b$. The diagonal matrix with the vector r on the diagonal is denoted by Δ_r ; the notation $[K_v:0]$ indicates blockmatrices.

The design space is $\mathfrak{X} = \{1,\dots,v\} \times \{1,\dots,b\}$. An approximate block design, or simply a *design*, is a probability distribution ξ on \mathfrak{X} ; ξ is taken to be a \mathbb{R}^{vb} -vector, with entries $\xi(i,j)$ in lexicographic order. Any design ξ induces a $v \times b$ weight matrix W, with entries $w_{ij} = \xi(i,j)$. Then $r = W1_b$ and $s = W'1_v$ are the vectors of *treatment marginals* and *block marginals*, respectively. A design of the form $r \otimes s$ is called a *product design*, here the measure theoretic product and the Kronecker product of r and s coincide. In case of uniform marginals $r = \overline{1_v}$ and $s = \overline{1_b}$ a design is called *equi-replicated* and *equi-blocksized*, respectively. The design $\overline{1_v} \otimes \overline{1_b}$ is the *uniform design on* \mathfrak{X} . By \mathfrak{Z} , $\mathfrak{Z}(r,\cdot)$, $\mathfrak{Z}(\cdot,s)$, and $\mathfrak{Z}(r,s)$ we denote the sets of all designs, of all designs with treatment marginals r, of all designs with block marginals s, and of all designs with both treatment marginals r and block marginals s, respectively.

In this section the underlying model is assumed to be $Y_{ijk} = \beta_{ij} + \varepsilon_{ijk}$, the vb parameters β_{ij} being interpreted as interaction effects of the i-th treatment and the j-th block. The regression function $f: \mathfrak{X} \to \mathbb{R}^{vb}$ then is given by $f(i,j) = e_i \otimes d_j$, and a design ξ has information matrix $M(\xi) = \Delta_{\xi}$. We shall only consider the system of treatment effects $(I_v \otimes \overline{I_b})'\beta = (\overline{\beta_1}, \dots, \overline{\beta_v}, \overline$

Theorem 3. (a) The product design $r_0 \otimes \overline{1_b}$ is the only uniformly optimal design for $(I_v \otimes \overline{1_b})'\beta$ in $\Xi(r_0, \cdot)$, its information matrix for $(I_v \otimes \overline{1_b})'\beta$ is Δ_{r_0} .

(b) The uniform design on $\mathfrak X$ is the only design which has Ξ -maximal $\mathfrak J$ -information for $(I_v \otimes \overline{I_b})'\beta$, its information matrix for $(I_v \otimes \overline{I_b})'\beta$ is ϱI_v , with $\varrho = 1/v$.

Proof. (a) Define $K = I_{\nu} \otimes \overline{1_b}$ and $M = \Delta_{r_0} \otimes I_b / b$. If $\xi \in \Xi(r_0, \cdot)$ then $K'M^{-1}\Delta_{\xi}M^{-1}K = \Delta_{r_0}^{-1} = K'M^{-1}K$, and (1) gives U-optimality. Uniqueness follows from (2).

(b) The uniform design on \mathfrak{X} is balanced for $K'\beta$. If a competing design η has treatment marginals r, then $J(M(\eta)) \leq \Delta_r$, by (a). Hence

$$j_1 \circ J(M(\eta)) \leq j_1(\Delta_r) = 1/v = j_1 \circ J(M(\overline{1_v} \otimes \overline{1_b})),$$

and Theorem 1 yields the assertion. \Box

The proof again demonstrates that j_1 is a particularly insensitive optimality criterion: *every* equi-blocksized product design is j_1 -optimal for the treatment effects. In particular, (4) is not necessary for uniqueness of j_1 -optimality. Also notice that essentially only uniform optimality and j_0 -optimality remain unaffected by the choice of $(I_v \otimes \overline{I_b})'\beta$ as a maximal system of treatment effects; this is a consequence of Theorem 1 in Pukelsheim (1980) and the order-invariance of j_0 under the general linear group, see Gaffke (1981, Theorem 1). It is straightforward to verify that the uniform design on $\mathfrak X$ also has $\mathcal Z$ -maximal $\mathfrak Y$ -information for the full parameter β , its information matrix for β being ϱI_{vb} , with $\varrho = 1/(vb)$.

While designs with an incomplete support play no role in the model with all interaction effects, unrestricted vs. incomplete supports do make a difference when the effects are additive.

5. Complete block designs in the additive model

The additive model assumes observations $Y_{ijk} = \alpha_i + \gamma_j + \varepsilon_{ijk}$, with treatment effects $\alpha = (\alpha_1, \dots, \alpha_v)' \in \mathbb{R}^v$, and block effects $\gamma = (\gamma_1, \dots, \gamma_b)' \in \mathbb{R}^b$. Thus the full parameter vector for the mean is $\beta = \begin{bmatrix} \alpha \\ \gamma \end{bmatrix} \in \mathbb{R}^{v+b}$, and the regression function f is given by $f(i, j) = \begin{bmatrix} e_i \\ d_j \end{bmatrix}$. For a design ξ with weight matrix W, treatment marginals r and block marginals s, its information matrix is

$$M(\xi) = \begin{bmatrix} \Delta_r & W \\ W' & \Delta_s \end{bmatrix},$$

and its *C-matrix* is, by definition, $C(\xi) = \Delta_r - W \Delta_s^+ W'$. In particular, a product design $r \otimes s$ has weight matrix rs', and *C*-matrix $\Delta_r - rr'$. As usual, the maximal system of treatment contrasts to be considered is $[K_v:0]\beta = (\alpha_1 - \overline{\alpha}, \dots, \alpha_v - \overline{\alpha})'$. It is well known that $[K_v:0]\beta$ is identifiable under ξ if and only if $C(\xi)$ has rank v-1, and then $C(\xi)$ is the information matrix of ξ for $[K_v:0]\beta$. All this is in accor-

dance with the exact theory, see Raghavarao (1971, Section 4.3), or Krafft (1978, §14).

If $[K_v:0]\beta$ is identifiable under ξ then ξ has positive treatment marginals; the converse is also true provided ξ is a product design. For a product design with positive marginals r and s its information matrix M, a g-inverse G of M, and the projection matrix MG are, in turn,

$$M = \begin{bmatrix} \Delta_r & rs' \\ sr' & \Delta_s \end{bmatrix}, \qquad G = \begin{bmatrix} \Delta_r^{-1} - J_v & 0 \\ 0 & \Delta_s^{-1} \end{bmatrix},$$

$$MG = \begin{bmatrix} I_v - r1'_v & r1'_b \\ 0 & I_b \end{bmatrix} = K(r), \quad \text{say}.$$
(8)

Since rank $M = \operatorname{trace} K(r) = v + b - 1$, any such information matrix has maximal rank in the set $M(\Xi)$. Notice that the *g*-inverse *G* is symmetric, and reflexive, i.e. GMG = G. In the remainder of this section, let $r_0 \in \mathbb{R}^v$ and $s_0 \in \mathbb{R}^b$ be fixed positive stochastic vectors.

Theorem 4. (a) The product designs with treatment marginals r_0 are the only uniformly optimal designs for $[K_v:0]\beta$ in $\Xi(r_0,\cdot)$, their common C-matrix is $\Delta_{r_0}-r_0r_0'$.

(b) The equi-replicated product designs are the only designs which have Ξ -maximal \Im -information for $[K_v:0]\beta$, their common C-matrix is ϱK_v , with $\varrho=1/v$.

Proof. (a) Define $K' = [K_v : 0]$, and for the design $r_0 \otimes s_0$ take M and G as in (8). If $\eta \in \Xi(r_0, \cdot)$ then $K'GM(\eta)GK = K'\Delta_{r_0}^{-1}K = K'GK$, and (1) gives U-optimality. Uniqueness follows from (2), since $M(\eta)GK = K$ implies rank $W(\eta) = 1$, and $W(\eta) = r_0 s'$.

(b) Equi-replicated product designs are balanced for $K'\beta$. If a competing design η has treatment marginals r, then $C(\eta) \leq \Delta_r - rr'$, by (a). The Cauchy Inequality yields

trace
$$(\Delta_r - rr') = 1 - r'r \le 1 - 1/v$$
,

with equality only for $r = \overline{1}_p$. Hence

$$j_1 \circ C(\eta) \le (1 - 1/v)/(v - 1) = 1/v = j_1 \circ C(\overline{1_v} \otimes s),$$

and Theorem 1 yields the assertion. \Box

For block contrasts part (a) reads: The product designs with block marginals s_0 are the only uniformly optimal designs for $[0:K_b]\beta$ in $\Xi(\cdot,s_0)$. This immediately yields Kurotschka's result (1971, p. 227) that $r_0 \otimes s_0$ is the only uniformly optimal design for $[K_v:0]\beta$, as well as for $[0:K_b]\beta$, in $\Xi(r_0,s_0)$. For j_0 -optimality the exact analogue of part (b) is given in Krafft (1978, p. 343). Of course, for block contrasts the designs in part (b) must be equi-blocksized. The only product design which is

both equi-replicated and equi-blocksized is the uniform design on \mathfrak{X} . Therefore, this design is \mathfrak{F} -optimal for $[K_v:0]\beta$, as well as for $[0:K_b]\beta$. Moreover, it is also optimal for $K(r)'\beta$, i.e. for a maximal linearly independent system of identifiable linear forms of β . The following hierarchy complements the results of Kurotschka (1971, pp. 227, 231).

Theorem 5. For all $p \in [-\infty, +1]$ one has:

- (a) $r_0 \otimes s_0$ has $\Xi(r_0, s_0)$ -maximal j_p -information for $K(r_0)'\beta$.
- (b) $r_0 \otimes \overline{1_b}$ has $\Xi(r_0, \cdot)$ -maximal j_p -information for $K(r_0)'\beta$.
- (c) $1_{\nu} \otimes s_0$ has $\Xi(\cdot, s_0)$ -maximal j_p -information for $K(\overline{1_{\nu}})'\beta$.
- (d) $\overline{1}_v \otimes \overline{1}_b$ has Ξ -maximal j_p -information for $K(\overline{1}_p)'\beta$.

Moreover, if $p \neq -\infty$, +1, then these designs are the only designs with the stated properties.

Proof. With M, G, and K(r) as in (8), define $K = MG = K(r_0)$. Then $K'M^-K = G$, and $C = G^+$. Fix some competing information matrix

$$M(\eta) = A = \begin{bmatrix} \Delta_r & W \\ W \in \Delta_s \end{bmatrix}.$$

For $p>-\infty$ optimality will follow from (3). In fact, trace G^+G^{1-p} equals trace G^{-p} or trace $(G^+)^p$, according as p<0 or p>0. Furthermore,

$$G'KC(K'M^{-}K)^{1-p}CK'G = G^{1-p},$$

so that we must evaluate trace AG^{1-p} , i.e.

trace
$$\Delta_r (\Delta_{r_0}^{-1} - J_v)^{1-p} + \operatorname{trace} \Delta_s \Delta_{s_0}^{p-1}$$
. (9)

Define $G_{11} = \Delta_{r_0}^{-1} - J_v$, and fix p < 0. When $r = r_0$ then the first term in (9) is trace $G_{11}^{-p} - 1_v' G_{11}^{-p} r_0 = \text{trace } G_{11}^{-p}$, since r_0 is a nullvector of G_{11} and hence also of G_{11}^{-p} . It is now easily verified that (9) equals trace G^{-p} for either part (a), (b), (c), and (d). If p > 0 then $G^{1-p} = G(G^+)^p$, and trace $AG^{1-p} = \text{trace } (G^+)^p$, by a similar argument. Proposition 1 extends optimality to $p = -\infty$, 0. Uniqueness follows from (4), solving $AG = K(r_0)$ for W. \square

The system $K(r_0)'\beta$ does depend on the choice of the *g*-inverse G, see the definition in (8). Part (d) admists a stronger version in the symmetrical case v=b: the design $\overline{1_v}\otimes\overline{1_v}$ has Ξ -maximal \mathfrak{F} -information for $K(\overline{1_v})'\beta$, is information matrix for $K(\overline{1_v})'\beta$ being

$$Q\begin{bmatrix} K_v & 0 \\ 0 & I_v \end{bmatrix}$$

with $\varrho = 1/v$.

The uniform design on \mathfrak{X} is the unique approximate analogue of an exact balanced block design (BBD), and of an exact balanced incomplete block design (BIBD), in

as far as these designs aim to have "all n_{ij} 's as nearly equal as possible", required by Kiefer (1975, p. 333). However, a BIBD may also be understood as a design for situations when not all treatment block combinations are feasible, or in other words, when the support of feasible designs must satisfy certain restrictions.

6. Incomplete block designs in the additive model

With the same model assumptions as in Section 5, we now study the class $\Xi(S)$ of designs whose support is contained in a fixed subset S of \mathfrak{X} . Define $\Xi(S;\cdot,s_0)=\Xi(S)\cap\Xi(\cdot,s_0)$, and notice that the induced set of information matrices is closed and convex. Associate with the support set S the $v\times b$ indicator matrix N, with entries $n_{ij}=1$ if $(i,j)\in S$, and $n_{ij}=0$ otherwise. Thus $n=1'_vN1_b$ is the number of points in S, interest concentrates on n< vb. By definition, the uniform design on S has weight matrix $\overline{N}=N/n$, this is the approximate analogue of a binary design in the exact theory. The treatment contrasts $[K_v:0]\beta$ are identifiable under the uniform design on S if and only if the indicator matrix N of S is connected; this follows from the exact theory, see Raghavarao (1971, p. 49), or Krafft (1978, p. 195).

Theorem 6. Let ξ be the uniform design on a set $S \subset \mathfrak{X}$.

- (a) If ξ has positive block marginals s_0 and S has a connected indicator matrix, then ξ has $\Xi(S; \cdot, s_0)$ -maximal j_1 -information for $[K_v : 0]\beta$.
- (b) If ξ is equi-blocksized and S has a connected indicator matrix, then ξ has $\Xi(S)$ -maximal j_1 -information for $[K_n:0]\beta$.
- (c) If ξ has positive block marginals s_0 and is balanced for $[K_v:0]\beta$, then ξ is the only design which has $\Xi(S;\cdot,s_0)$ -maximal \Im -information for $[K_v:0]\beta$.
- (d) If ξ is equi-blocksized and balanced for $[K_v:0]\beta$, then ξ has $\Xi(S)$ -maximal \Im -information for $[K_v:0]\beta$, with C-matrix ϱK_v , $\varrho = (1-b/n)/(v-1)$.

Proof. Parts (a) and (b) will follow from (3). Define $K' = [K_v : 0]$, $M = M(\xi)$, and $C = C(\xi)$. Then trace C = 1 - b/n. As g-inverse of M choose

$$G = \begin{bmatrix} C^{+} & -C^{+} \bar{N} \Delta_{s_{0}}^{-1} \\ -\Delta_{s_{0}}^{-1} \bar{N}' C^{+} & \Delta_{s_{0}}^{-1} + \Delta_{s_{0}}^{-1} \bar{N}' C^{+} \bar{N} \Delta_{s_{0}}^{-1} \end{bmatrix}, \qquad GK = \begin{bmatrix} I_{v} \\ -\Delta_{s_{0}}^{-1} \bar{N}' \end{bmatrix} C^{+},$$
(10)

cf. Krafft (1978, p. 200). If $\eta \in \Xi(S)$ then

$$A = M(\eta) = \begin{bmatrix} \Delta_r & W \\ W' & \Delta_s \end{bmatrix}$$

satisfies

trace
$$K'GAGKCC$$
 = trace $K_{\upsilon}(\Delta_{r} - W\Delta_{s_{0}}^{-1}\bar{N}' - \bar{N}\Delta_{s_{0}}^{-1}W' + \bar{N}\Delta_{s_{0}}^{-1}\Delta_{s}\Delta_{s_{0}}^{-1}\bar{N}')$
= $1 - n^{-1}\sum_{j} s_{j}/s_{0j}$,

by straightforward calculation. The last expression equals 1 - b/n both if (a) $s = s_0$, or if (b) $s_0 = \overline{1_b}$.

Parts (c) and (d) follow from Theorem 1. In (c) uniqueness is obtained from (4), since here AGK = K implies $W(\eta) = \bar{N}$.

Theorem 6 calls for a series of remarks. In parts (c) and (d) the j_p -information of ξ for $[K_v:0]\beta$ is equal to $\varrho=(1-b/n)/(v-1)$, and thus depends on the cardinality of S, but neither on the particular support points, nor on the particular block marginals, nor on p. Hence we may add to (c): no design with n support points and positive block marginals contains more j_p -information for $[K_v:0]\beta$ than ξ . Similarly for part (d): no design with n support points contains more j_p -information for $[K_v:0]\beta$ than ξ . However, the set of all designs with n (or less) support points does not induce a convex set of information matrices.

Some designs with 12 or less support points are listed in Table 1. Designs ξ_1 and ξ_2 show that positive block marginals are not necessary for optimality. In fact, blocks with weights 0 can always be added without changing the *C*-matrix. The assumption of positive block marginals simply serves to exclude this triviality. In this sense, designs ξ_4 through ξ_7 also apply to 3 treatments in 6 blocks. Notice that

Table 1 Designs to illustrate Theorem 6

ξ ₁	$W_1 = \frac{1}{12} \begin{pmatrix} 1 & 1 & 0 & 1 & 1 & 0 \\ 1 & 0 & 1 & 1 & 0 & 1 \\ 0 & 1 & 1 & 0 & 1 & 1 \end{pmatrix}$	$C_1 = \frac{1}{4}K_3$
ξ_2	$W_2 = \frac{1}{12} \begin{pmatrix} 2 & 2 & 0 & 0 & 0 & 0 \\ 2 & 0 & 2 & 0 & 0 & 0 \\ 0 & 2 & 2 & 0 & 0 & 0 \end{pmatrix}$	$C_2 = \frac{1}{4}K_3$
ξ_3	$W_3 = \frac{1}{12} \begin{pmatrix} 1 & 0 & 0 & 1 & 1 & 1 \\ 0 & 1 & 0 & 1 & 1 & 1 \\ 0 & 0 & 1 & 1 & 1 & 1 \end{pmatrix}$	$C_3 = \frac{1}{4}K_3$
ξ_4	$W_4 = \frac{1}{12} \begin{pmatrix} 0 & 0 & 0 & 4 \\ 0 & 0 & 0 & 4 \\ 0 & 0 & 0 & 4 \end{pmatrix}$	$C_4 = \frac{1}{3}K_3$
ξ_5	$W_5 = \frac{1}{12} \begin{pmatrix} 1 & 0 & 0 & 3 \\ 0 & 1 & 0 & 3 \\ 0 & 0 & 1 & 3 \end{pmatrix}$	$C_5 = \frac{1}{4}K_3$
ξ ₆	$W_6 = \frac{1}{12} \begin{pmatrix} 2 & 0 & 0 & 2 \\ 0 & 2 & 0 & 2 \\ 0 & 0 & 2 & 2 \end{pmatrix}$	$C_6 = \frac{1}{6}K_3$
ξ ₇	$W_7 = \frac{1}{12} \begin{pmatrix} 3 & 0 & 0 & 1 \\ 0 & 3 & 0 & 1 \\ 0 & 0 & 3 & 1 \end{pmatrix}$	$C_7 = \frac{1}{12}K_3$

despite of their different supports the designs ξ_1, ξ_2, ξ_3 , and ξ_5 all share the same C-matrix. In particular, no uniqueness statement holds in Theorem 6(d). Design ξ_4 is an equi-replicated product design and hence better than ξ_5 et al., by Theorem 4(b). On the other hand, ξ_5 is better than ξ_6 , whence in Theorem 6(a) and 6(c) optimality does not extend from $\Xi(S; \cdot, s_0)$ to $\Xi(S)$.

In the exact version, however, optimality in Theorem 6(a) does extend to all exact designs of size n with positive block-marginals, see Kiefer (1958, p. 689) or Krafft (1978, p. 338). Namely, define m to be the minimal positive weight w_{ij} of such an exact design η . Then

trace
$$C(\eta) = 1 - m^2 \sum_{ij} s_j^{-1} (w_{ij}/m)^2 \le 1 - m^2 \sum_{ij} s_j^{-1} w_{ij}/m = 1 - mb$$
,

with equality if and only if all w_{ij} equal either 0 or m. But η is an exact design of size n, whence $m \ge 1/n$, and trace $C(\eta) \le 1 - b/n = \text{trace } C(\xi)$, with equality if and only if η is another uniform design on n support points. (This argument fails for approximate designs: $\eta = \xi_7$ is not as good as ξ_6 , but has minimal weight $\frac{1}{12} < \frac{1}{6} = 1/n$.) A similar extension holds for Theorem 6(c), and here η is also optimal if and only if η is another uniform design on n support points which is balanced for $[K_p:0]\beta$.

The question whether for n>vb there exists some n point support S such that as in Theorem 6(d) the uniform design on S is equi-blocksized and balanced for $[K_v:0]\beta$ belongs to the combinatorial part of the theory, the answer is in the affirmative if and only if there exists a BIBD with n/b observations per block. A design which is balanced for $[K_v:0]\beta$ need not be equi-blocksized, see Table 1, nor equireplicated, see John (1964, p. 899), Tyagi (1979, p. 335). This is slightly different with equi-blocksized uniform designs ξ on S: then ξ is balanced for $[K_v:0]\beta$ if and only if the indicator matrix N of S satisfies

$$NN' = (v - \lambda)I_v + \lambda J_v$$
, for some scalars v, λ , (11)

and in this case (1) ξ is equi-replicated, (2) v = n/v and $\lambda = \{n/(vb)\}\{(n-b)/(v-1)\}$ are positive integers, (3) n > v + b - 1, and (4) rank $N = v \le b$. The proof runs as in the exact theory.

As an application we now show that in the symmetrical case v = b uniqueness holds in Theorem 6(d). For

$$A = \begin{bmatrix} \Delta_r & W \\ W' & \Delta_s \end{bmatrix}$$

condition (4) yields $\Delta_r - bW\bar{N}' = \varrho K_v$ and $W = b\bar{N}\Delta_s$. When the support of W is contained in S this entails $r = \overline{1_v}$ and $bN\Delta_sN' = NN'$. Hence W must be equireplicated, and in case v = b also equi-blocksized, proving $W = \bar{N}$.

Any equi-blocksized uniform design ξ on n support points which is balanced for $[K_v:0]\beta$ is an approximate analogue of an exact BIBD of size n, in as far as the support must not consist of more than n points. But the dominating role that BIBDs

play in the exact theory is not supported by Theorem 6. As a matter of fact, ξ_1, ξ_2, ξ_3 , and ξ_5 perform identically for $[K_v:0]\beta$, but only ξ_1 is a BIBD. However, any design ξ as above needs more than v+b-1 support points, and its information matrix M has maximal rank v+b-1. More precisely, the g-inverse G of (10) becomes

$$G = \frac{1}{\varrho} \begin{bmatrix} K_v & -bK_v\bar{N} \\ -b\bar{N}'K_v & \varrho bI_b + b^2\bar{N}'K_v\bar{N} \end{bmatrix}, \quad \varrho = (1 - b/n)/(v - 1), \tag{12}$$

and is symmetric and reflexive, and the projection matrix MG equals $K(\overline{1}_v)$ of (8). Thus Theorem 5 suggests that ξ is j_p -optimal also for the maximal system $K(\overline{1}_v)'\beta$ of linear forms of β and our final theorem will prove this to be true, reflecting yet another and surprising aspect of the property of being 'balanced'. The difficulty lies in the task to handle powers of G without knowing its spectral decomposition, here Seely's (1971) notion and results on quadratic subspaces of symmetric matrices are the main aid.

Theorem 7. If the uniform design ξ on a subset S of \mathfrak{X} is equi-blocksized and balanced for $[K_v:0]\beta$, i.e. for the treatment contrasts, then ξ has $\Xi(S)$ -maximal j_p -information for $K(\overline{1_v})'\beta$, i.e. for a maximal identifiable system, for all $p \in [-\infty, +1]$. Moreover, if $p \neq -\infty; +1$ then ξ is the only design with this property.

Proof. Theorem 5(d) covers the case $S = \mathfrak{X}$. Otherwise define $w = (v - \lambda)/n^2$, so that (11) implies the relations

$$\overline{NN'}K_v = wK_v, \quad w = (vb - n)/\{vbn(v - 1)\}, \quad b/v = b\varrho + b^2w.$$
 (13)

Take $A = M(\eta)$, with $\eta \in \mathfrak{Y}(S)$. For $p \in]-\infty, 0[$ replace -p by t. Then t > 0, and (3) turns into

trace
$$A(\varrho G)^{t+1} \le \varrho$$
 trace $(\varrho G)^t$. (14)

Introduce B as the linear space spanned by the four matrices

$$V_{1} = \begin{bmatrix} K_{v} & 0 \\ 0 & 0 \end{bmatrix}, \qquad V_{2} = \begin{bmatrix} 0 & -K_{v}\bar{N} \\ -\bar{N}'K_{v} & 0 \end{bmatrix},$$
$$V_{3} = \begin{bmatrix} 0 & 0 \\ 0 & I_{b} \end{bmatrix}, \qquad V_{4} = \begin{bmatrix} 0 & 0 \\ 0 & \bar{N}'K_{v}\bar{N} \end{bmatrix}.$$

It is easy to see that $(V_i + V_j)^2 \in \mathfrak{B}$, for all i, j = 1, ..., 4. Hence \mathfrak{B} is a quadratic subspace of symmetric matrices, and as such closed under formation of positive powers, of Moore-Penrose inverses, and of positive powers of Moore-Penrose inverses, see Seely (1971, pp. 711, 712).

This applies to $\varrho G = V_1 + bV_2 + \varrho bV_3 + b^2V_4 \in \mathfrak{B}$: for every t > 0 there exist scalars a_t, b_t, c_t, d_t such that

$$(\varrho G)^t = a_t V_1 + b_t V_2 + c_t V_3 + d_t V_4$$

and

$$a_{t+1} = a_t + b_t b w, b_{t+1} = a_t b + b_t b / v = b_t + c_t b + d_t b w,$$

$$c_{t+1} = \varrho b c_t, d_{t+1} = b_t b + c_t b^2 + d_t b / v.$$
(15)

The recurrence relation (15) compares coefficients in $(\varrho G)^{t+1} = (\varrho G)^t (\varrho G)$. Thus the right-hand side of (14) equals $a_t(1-b/n)+c_{t+1}+d_tw(1-b/n)$, and invoking (15) and (13) some computation shows that the left-hand side takes on the same value. This proves optimality for $p \in]-\infty,0[$, and Proposition 1 extends optimality to $p=-\infty,0$. If $p \in]0,1]$ then a similar argument establishes trace $A(\varrho G)(G^+)^p \leq \varrho$ trace $(G^+)^p$, i.e. (3). Uniqueness follows from (4), since the two bottom blocks in $AG=K(\overline{1}_{\nu})$ imply $W(\eta)=\overline{N}$. \square

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