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OPTIMALITY OF CERTAIN ASYMMETRICAL EXPERIMENTAL DESIGNS

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The problem of finding an optimal design for the elimination of one-way heterogeneity when a balanced block design does not exist is studied. A general result on the optimality of certain asymmetrical designs is proved and applied to the block design setting. It follows that if there is a group divisible partially balanced block design (GD PBBD) with 2 groups and $\lambda_2 = \lambda_1 + 1$, then it is optimal w.r.t. a very general class of criteria including all the commonly used ones. On the other hand, if there is a GD PBBD with 2 groups and $\lambda_1 = \lambda_2 + 1$, then it is optimal w.r.t. another class of criteria. Uniqueness of optimal designs and some other miscellaneous results are also obtained.

1. Introduction. In the usual one-way heterogeneity setting, for specified positive integers b (number of blocks), v (number of varieties), and k (block size), a *design* is a $k \times b$ array of the variety labels $1, 2, \cdots, v$, with blocks as columns. The usual additive model specifies the expectation of an observation on variety i in block j to be $\alpha_i + \beta_j$ (variety effect + block effect), and assumes that the kb observations are uncorrelated with common variance σ^2. Then for a design d, the vector of the kb observation expectations can be written in the following form:

$$X_d\theta = [\, X_d^{(1)} \,\vdots\, X_d^{(2)} \,]\binom{\alpha}{\beta}, \tag{1.1}$$

where α is the v-vector of variety effects, and β is the b-vector of block effects. This is the setup of the linear model.

Usually, for a specified design d, we denote the number of replications of variety i by r_{di}, and the variety-block incidence matrix by $N_d = (n_{dij})_{v\times b}$, where n_{dij} is the number of appearances of variety i in block j.

If we are interested in the estimation of linear combinations of variety effects only, then it is well known that the coefficient matrix of the reduced normal equation for variety effects is:

$$C_d = \text{diag}(r_{d1}, \cdots, r_{dv}) - k^{-1}N_dN_d', \tag{1.2}$$

where $\text{diag}(r_{d1}, \cdots, r_{dv})$ is the diagonal matrix with diagonal elements $r_{d1}, \cdots, r_{dv}$. We denote the (i, j)th entry of N_dN_d' by λ_{dij}. Then $c_{dij} = r_{di}\delta_{ij} - k^{-1}\lambda_{dij}$, where δ_{ij} is the Kronecker symbol.

This matrix C_d, called the *C-matrix* of the design d, is symmetric, nonnegative definite, and has zero row sums. Therefore, the only possible estimable linear combinations of the variety effects are the contrasts (i.e., the linear combinations

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$\Sigma_{i=1}^{v} c_i \alpha_i$ with $\Sigma_{i=1}^{v} c_i = 0$). If we want to estimate all variety contrasts, then we are led to consider connected designs only, i.e., those for which rank $(C_d) = v - 1$.

The theory of optimal experimental designs is concerned with the problem of selecting a design which minimizes some functional ψ of C_d over all possible designs. ψ is called an *optimality criterion.*

The commonly used criteria are:

(1) D-optimality: $\psi(C_d) = \Pi_{i=1}^{v-1} \mu_{di}^{-1}$ (or, equivalently, $\psi^*(C_d) = -\Sigma_{i=1}^{v-1} \log \mu_{di}$),

(2) A-optimality: $\psi(C_d) = \Sigma_{i=1}^{v-1} \mu_{di}^{-1}$,

(3) E-optimality: $\psi(C_d) = \max_{1 \leqslant i \leqslant v-1} \mu_{di}^{-1}$, where $\mu_{d1}, \cdots, \mu_{d,v-1}$ are the eigenvalues of C_d excluding one multiplicity of zero.

For a discussion of the statistical meanings of these criteria, see Kiefer (1958, 1959).

In Kiefer (1974), the following family of criteria was also introduced:

(4) Φ_p-criterion: $\psi(C_d) = \Sigma_{i=1}^{v-1} \mu_{di}^{-p}$, $0 < p < \infty$.

Kiefer (1958) generalized the notion of balanced incomplete block designs (BIBD) to balanced block designs (BBD), and proved that for fixed k, b, and v, if a BBD exists, then it is D-, A-, and E-optimal over all block designs with the same parameters. Later, in Kiefer (1975), a striking result on universal optimality of BBD's was established.

Balanced block designs exist only for some restricted class of parameter values v, b, and k. When $k < v$, and a BIBD does not exist, Bose and Nair (1939) suggested the use of partially balanced incomplete block designs (PBIBD) which we now generalize to partially balanced block designs (PBBD) as follows:

Given v symbols $1, 2, \cdots, v$, a relation satisfying the following conditions is said to be an *association scheme with m classes*:

1. Any two symbols are either 1st, 2nd, . . . or mth associates. The relation of association is symmetric, that is, if the symbol α is an sth associate of the symbol β, then β is also an sth associate of α.
2. Each symbol α has n_s sth associates. The number n_s is independent of α.
3. If any two symbols α and β are sth associates, then the number of symbols that are tth associates of α and uth associates of β is independent of the pair of sth associates α and β (i.e., it depends only on s, t, and u).

If we are given an association scheme with m classes ($m > 1$) for the v varieties, then a *PBBD* is a design such that:

1. $v \nmid k$, and each variety occurs in each block $\text{int}(k/v)$ or $\text{int}(k/v) + 1$ times, where $\text{int}(x) \equiv$ the largest integer $\leqslant x$.
2. All the r_{di}'s are equal.
3. If varieties i and j are sth associates, then the quantity λ_{dij} depends only on s. We denote it by λ_s.
4. There are at least two distinct λ_s's.

Note that when $k < v$, this is a little bit different from the conventional definition, in that we have found it convenient to exclude BBD's from PBBD's.

A PBBD with 2 associate classes is called *group divisible* (GD) if the varieties can be divided into several groups, each containing the same number of varieties, such that two varieties are first associates if and only if they are in the same group.

If d is a group divisible PBBD with 2 groups and $\lambda_2 = \lambda_1 + 1$, then d is called a *most-balanced group divisible* PBBD (MB GD PBBD) *of type* 1; and if $\lambda_1 = \lambda_2 + 1 > 1$, then d is called a *most-balanced group divisible* PBBD *of type* 2. (Again, we use PBIBD if $k < v$.)

Takeuchi (1961, 1963) was the first one to investigate the optimality of group divisible PBBD's. By a delicate computation, he showed that if a BIBD does not exist, but there is an MB GD PBIBD of type 1, then it is E-optimal. (Actually, he proved more. The same result holds for any GD PBIBD with $\lambda_2 = \lambda_1 + 1$.) Later, Conniffe and Stone (1974, 1975) proved that in the same situation, any MB GD PBIBD of type 1 is A-optimal over those designs in which each variety has the same number of replications and appears in each block at most once. Conniffe and Stone's result seems weaker in the sense that they did not prove optimality over all designs, but it is their method that allows us to explore further.

Later, we shall remove the restriction in Conniffe and Stone's paper mentioned above, and prove that the same design actually is optimal with respect to a large class of optimality criteria that include A-, E-, D-, all Φ_p-criteria, $0 < p < \infty$, and more. At the same time, we will also investigate the optimality of an MB GD PBBD of type 2. It turns out that this kind of design is optimal with respect to another class of optimality criteria. For convenience of later reference, we now divide the optimality criteria which we shall consider into two classes:

Let $\bar{c}_{\mathfrak{D}} = \max_{d \in \mathfrak{D}} \operatorname{tr} C_d$, where $\mathfrak{D}$ is the class of designs under consideration.

(a) *Optimality criteria of type 1*: $\psi_f(C_d) = \sum_{i=1}^{v-1} f(\mu_{di})$, where f is a real-valued function defined on $[0, \bar{c}_{\mathfrak{D}}]$ such that

(1) f is continuous, strictly convex, and strictly decreasing on $[0, \bar{c}_{\mathfrak{D}}]$. We include here the possibility that $f(0) = \lim_{x \to 0^+} f(x) = +\infty$.

(2) f is continuously differentiable on $(0, \bar{c}_{\mathfrak{D}})$, and f' is strictly concave on $(0, \bar{c}_{\mathfrak{D}})$, i.e., $f' < 0$, $f'' > 0$, and $f''' < 0$ on $(0, \bar{c}_{\mathfrak{D}})$.

(b) *Optimality criteria of type 2*: Same as (a) except that the strict concavity of f' is replaced by strict convexity, i.e., $f''' > 0$ on $(0, \bar{c}_{\mathfrak{D}})$.

We also define a *generalized optimality criterion of type i* ($i = 1, 2$) to be the pointwise limit of a sequence of type i criteria.

Note that the A-, D-, and Φ_p-criteria are of type 1, and the E-criterion is a generalized criterion of type 1 (being the limit of Φ_p-criteria, as $p \to \infty$). There do exist functions satisfying the requirements for a type 2 criterion. For example, let $f(x) = \varepsilon x^3 - ax$ over the interval $[0, \bar{c}_{\mathfrak{D}}]$ of interest, where $\varepsilon > 0$, $a > 0$, and ε, compared with a, is small.

Actually, we will prove the optimality of a more general class of designs containing MB GD PBBD's. John and Mitchell (1977) defined regular graph designs (RGD) for the case $k < v$. Generally (whether or not $k < v$), a block design d with parameters b, v, k will be called a *regular graph design* if

(1) Each variety occurs in each block $\operatorname{int}(k/v)$ or $\operatorname{int}(k/v) + 1$ times, and all r_{di}'s are equal.

(2) For $i \neq j$, and $i' \neq j'$, $|\lambda_{dij} - \lambda_{di'j'}| = 0$ or 1.

A regular graph design d will be called an *extreme* RGD *of type* 1 if C_d has two distinct nonzero eigenvalues $\mu > \mu'$, and the multiplicity of μ' equals $v - 2$. On the other hand, if the multiplicity of μ equals $v - 2$, then d is called an *extreme* RGD *of type* 2. It is clear that for given parameters, if there is a BBD, then there is no extreme RGD of either type, and vice versa.

In Section 2, partial generalizations of Kiefer's (1975) result on the universal optimality of completely symmetric designs to some special asymmetrical cases are given. These results are then used in Section 3 to establish the optimality of most of the extreme RGD's including MB GD PBBD's (of both types). In Section 4, we state Takeuchi's uniqueness result on E-optimality in a more general form and prove a dual result. Based on these generalizations, the uniqueness of optimal designs when an MB GD PBBD exists is established. Section 5 contains some simple result about the existence and nonexistence of MB GD PBBD's. Finally, in Section 6, we briefly discuss the situation where both BBD's and extreme RGD's do not exist. Two possible candidates for optimal designs are compared, and one of them is seen to be better for $v > 4$.

In what follows, we always assume $v > 2$.

2. Some general results. Kiefer (1975) proved a theorem on universal optimality.

THEOREM 2.1 (Kiefer). *Let $\mathcal{B}_{v,0}$ consist of the $v \times v$ symmetric nonnegative definite matrices with zero row sums. Suppose a class $\mathcal{C} = \{C_d : d \in \mathfrak{D}\}$ of matrices in $\mathcal{B}_{v,0}$ contains a C_{d^*} such that*

(a) *C_{d^*} is completely symmetric*, i.e., *C_{d^*} is of the form $aI_v + bJ_v$, where I_v is the $v \times v$ identity matrix, and J_v is the $v \times v$ matrix consisting of* 1*'s.*

(b) $\operatorname{tr} C_{d^*} = \max_{d \in \mathfrak{D}} \operatorname{tr} C_d$.

Then C_{d^*} minimizes $\Phi(C_d)$ over $d \in \mathfrak{D}$ for all $\Phi : \mathcal{B}_{v,0} \to (-\infty, +\infty]$ satisfying

(i) *Φ is convex,*

(ii) *$\Phi(bC)$ is nonincreasing in the scalar $b \geq 0$,*

(iii) *Φ is invariant under each permutation of rows and (the same on) columns.*

This is an important tool for proving the optimality of symmetric designs. It can be generalized partially to some special asymmetrical cases as follows:

THEOREM 2.2. *Let $\mathcal{C} = \{C_d : d \in \mathfrak{D}\}$ be a class of matrices in $\mathcal{B}_{v,0}$ and $v > 2$.*

(a) *Suppose $C_{d^*} \in \mathcal{C}$ has two distinct nonzero eigenvalues $\mu > \mu'$, the multiplicity* *of* μ *being* 1, *and*

(2.1) $$C_{d^*} \text{ maximizes tr } C_d \text{ over } d \in \mathfrak{D},$$

(2.2) $$\text{tr } C_{d^*}^2 < (\text{tr } C_{d^*})^2/(v-2),$$

(2.3) $$C_{d^*} \text{ maximizes tr } C_d - [(v-1)/(v-2)]^{\frac{1}{2}} \times \left[\text{tr } C_d^2 - (\text{tr } C_d)^2/(v-1)\right]^{\frac{1}{2}} \text{ over all } d \in \mathfrak{D}.$$

Then C_{d^*} *is optimal* w.r.t. *all generalized criteria of type* 1 *over all* $d \in \mathfrak{D}$.

(b) *Suppose* $C_{d^*} \in \mathcal{C}$ *has two distinct nonzero eigenvalues* $\mu > \mu'$, *the multiplicity of* μ *being* $v - 2$ *and*

(2.4) $$C_{d^*} \text{ maximizes tr } C_d \text{ over } d \in \mathfrak{D}$$

(2.5) $$C_{d^*} \text{ maximizes tr } C_d - \left[(v-1)(v-2)\left(\text{tr } C_d^2 - (\text{tr } C_d)^2/(v-1)\right)\right]^{\frac{1}{2}} \text{ over } d \in \mathfrak{D}.$$

Then C_{d^*} *is optimal* w.r.t. *all generalized criteria of type* 2 *over all* $d \in \mathfrak{D}$.

The proof of Theorem 2.2 is very lengthy. This is due to some technical difficulties. For this reason, the whole proof is presented at the back of the paper as an appendix. To help the readers grasp the idea, we now give a heuristic argument for the case of type 1 criteria ψ_f with $\lim_{x\to 0^+} f(x) = f(0) = \infty$.

With any positive numbers A and B such that $A^2 \geqslant B \geqslant A^2/(v-1)$, we associate the number $P = [B - (v-1)^{-1}A^2]^{\frac{1}{2}}$. It is easily seen that $A^2 \geqslant B \geqslant A^2/(v-1)$ is the necessary and sufficient condition for the existence of $v - 1$ nonnegative numbers $\mu_1, \cdots, \mu_{v-1}$ s.t. $A = \Sigma_{i=1}^{v-1}\mu_i$ and $B = \Sigma_{i=1}^{v-1}\mu_i^2$.

Suppose C is a matrix in $\mathfrak{B}_{v,0}$ s.t. tr $C = A$ and tr $C^2 = B$. Let $\mu_1, \cdots, \mu_{v-1}$ be the eigenvalues of C excluding one multiplicity of zero, and μ^* be the nonzero eigenvalue of the completely symmetric matrix C^* with tr $C^* = A$. Then P is the Euclidean distance between $(\mu_1, \cdots, \mu_{v-1})$ and $(\mu^*, \cdots, \mu^*)$.

Let $S(A, B) = \{(\mu_1, \cdots, \mu_{v-1}) : \mu_i \geqslant 0, \Sigma\mu_i = A, \Sigma\mu_i^2 = B\}$. Firstly, we consider the problem of minimizing ψ_f over $S(A, B)$ for fixed A and B. Since $\lim_{x\to 0^+} f(x) = f(0) = \infty$, the minimum should occur at an interior point of $S(A, B)$ and hence the method of Lagrange's multipliers is applicable. It turns out that all the stationary points have at most two distinct coordinates. This is a consequence of the strict concavity of f' (Lemma A6 of the appendix). The concavity of f' again implies that among these stationary points, ψ_f is an increasing function of the multiplicity of the bigger coordinate (Lemma A3 (iii)). Thus the minimum of ψ_f on $S(A, B)$ is attained at a point which has constant coordinates or has two distinct coordinates such that the bigger one has multiplicity 1.

Solving the equations

$$\mu_1 + (v-2)\mu_2 = A$$
$$\mu_1^2 + (v-2)\mu_2^2 = B$$
$$\mu_1 \geqslant \mu_2,$$

we get

$$\mu_1 = \left(A + [(v-1)(v-2)]^{\frac{1}{2}}P\right)/(v-1)$$

and

$$\mu_2 = \left(A - [(v-1)/(v-2)]^{\frac{1}{2}}P\right)/(v-1).$$

So if $M_f(A, B)$ is the minimum of ψ_f on $S(A, B)$, then

$$M_f(A,B) = f\left(\left(A + [(v-1)(v-2)]^{\frac{1}{2}}P\right)/(v-1)\right) + (v-2)f\left(\left(A - [(v-1)/(v-2)]^{\frac{1}{2}}P\right)/(v-1)\right). \tag{2.6}$$

It follows from the decreasing monotonicity and convexity of f that $M_f(A, B)$ is a decreasing function of A for fixed P and an increasing function of P for fixed A (Lemma A3 (i), (ii)). Accordingly, given two pairs (A, B) and (A', B') such that

$$A \geqslant A' \tag{2.7}$$

and

$$A - [(v-1)/(v-2)]^{\frac{1}{2}}P \geqslant A' - [(v-1)/(v-2)]^{\frac{1}{2}}P', \tag{2.8}$$

(a) if $P \leqslant P'$, then obviously $M_f(A, B) \leqslant M_f(A', B')$;

(b) if $P > P'$, then $A + [(v-1)(v-2)]^{\frac{1}{2}}P > A' + [(v-1)(v-2)]^{\frac{1}{2}}P'$, and hence by (2.6), (2.8) and the decreasing monotonicity of f, $M_f(A, B) \leqslant M_f(A', B')$.

Thus, if d^* is a design satisfying the conditions in part (a) of Theorem 2.2, then d^* is optimal w.r.t. any type 1 criterion ψ_f with $\lim_{x\to 0^+} f(x) = f(0) = +\infty$.

The difficulty with the proof of Theorem 2.2 is that without the assumption $\lim_{x\to 0^+} f(x) = f(0) = \infty$, there is no guarantee that the minimum of ψ_f on $S(A, B)$ will not occur at a point with some coordinate equal to zero, in which event ψ_f may have no minimum over the interior of $S(A, B)$. Thus, with the condition $\lim_{x\to 0^+} f(x) = f(0) = \infty$, the proof is significantly simplified. As a matter of fact, we even do not need condition (2.2). In summary, we conclude:

THEOREM 2.3. *Let $\mathcal{C} = \{C_d : d \in \mathfrak{D}\}$ be a class of matrices in $\mathfrak{B}_{v,0}$, and $v > 2$. Suppose $\mathcal{C}$ contains a matrix C_{d^*} which maximizes* tr C_d *and* tr $C_d - [(v-1)/(v-2)]^{\frac{1}{2}} \times [\text{tr}\, C_d^2 - (\text{tr}\, C_d)^2/(v-1)]^{\frac{1}{2}}$ *over all $d \in \mathfrak{D}$* s.t. *rank $C_d = v - 1$. Also, suppose C_{d^*} has two distinct nonzero eigenvalues $\mu > \mu'$, the multiplicity of μ being* 1, *then C_{d^*} is optimal with respect to any type* 1 *criterion ψ_f such that* $\lim_{x\to 0^+} f(x) = f(0) = +\infty$.

Not only is the proof significantly simplified, but the conditions put on d^* here are also simpler than those in Theorem 2.2. All A-, D-, and Φ_p-criteria are of the type considered in Theorem 2.3.

Note that there is no type 2 analogue of Theorem 2.3. Actually, there is no function f satisfying $f' < 0$, $f'' > 0$, $f''' > 0$ on $(0, c)$ for some $c > 0$, and with

$\lim_{x\to 0^+} f(x) = +\infty$. For, supposing such a function f exists, then $\lim_{x\to 0^+} f'(x) = -\infty$, and $\lim_{x\to 0^+} f''(x) < +\infty$. These two conditions are contradictory to each other.

From the proof of Theorem 2.2, we can easily see that the following corollary holds:

COROLLARY 2.2.1. *Under the same hypothesis as Theorem 2.2, if some $C_d \in \mathcal{C}$ is optimal with respect to a particular criterion (not a generalized one) ψ_f, then C_d has the same eigenvalues with the same multiplicities as C_{d^*}.*

The following lemma gives a sufficient condition for a matrix in $\mathcal{B}_{v,0}$ to have two nonzero eigenvalues with the desired extreme multiplicities.

LEMMA 2.1. *Let $C \in \mathcal{B}_{v,0}$ be a matrix of the form*

$$\begin{bmatrix} (a-c)I_{n_1} + cJ_{n_1} & eJ_{n_1,n_2} \\ eJ_{n_2,n_1} & (b-d)I_{n_2} + dJ_{n_2} \end{bmatrix}$$

with $a - c = b - d \neq 0$ and $e \neq 0$, where J_{n_1,n_2} is the $n_1 \times n_2$ matrix with all entries equal to 1. If C is not completely symmetric, then $c \neq e$, and C has two distinct nonzero eigenvalues: $a - c$ with multiplicity $v - 2$ and $(n_1 - 1)c + (n_2 - 1)d + a + b$ with multiplicity 1. Moreover,

(a) *If $c > e$, then $a - c < (n_1 - 1)c + (n_2 - 1)d + a + b$.*
(b) *If $c < e$, then $a - c > (n_1 - 1)c + (n_2 - 1)d + a + b$.*

PROOF. If $\alpha \neq \beta$, then we have

$$(2.9)\qquad [(\alpha-\beta)I_n + \beta J_n]^{-1} = \{(\alpha-\beta)[(n-1)\beta+\alpha]\}^{-1}\{[(n-1)\beta+\alpha]I_n - \beta J_n\}.$$

Using the formula $\det\begin{bmatrix} A & B \\ C & D \end{bmatrix} = (\det A)\det(D - CA^{-1}B)$ and (2.9), we have

$$(2.10)\qquad \det\begin{bmatrix} (a-c)I_{n_1} + cJ_{n_1} & eJ_{n_1,n_2} \\ eJ_{n_2,n_1} & (b-d)I_{n_2} + dJ_{n_2} \end{bmatrix}$$
$$= (a-c)^{n_1-1}(b-d)^{n_2-1}\{(n_2-1)[(n_1-1)cd + ad] - n_1 n_2 e^2 + [(n_1-1)c + a]b\}$$
$$= 0.$$

The characteristic polynomial of

$$\begin{bmatrix} (a-c)I_{n_1} + cJ_{n_1} & eJ_{n_1,n_2} \\ eJ_{n_2,n_1} & (b-d)I_{n_2} + dJ_{n_2} \end{bmatrix}$$

is $(a - \lambda - c)^{n_1 - 1}(b - \lambda - d)^{n_2 - 1}\{(n_2 - 1)[(n_1 - 1)cd + (a - \lambda)d] - n_1 n_2 e^2 + [(n_1 - 1)c + a - \lambda](b - \lambda)\}$. Also, (2.10) implies that the nonzero eigenvalues are $a - c$, with multiplicity $v - 2$, and the nonzero solution of $\lambda^2 - \lambda[(n_1 - 1)c + a] - b\lambda - (n_2 - 1)\,d\lambda$, i.e., $a + b + (n_1 - 1)c + (n_2 - 1)d$, with multiplicity 1. Thus

$$\begin{aligned} &(n_1 - 1)c + (n_2 - 1)d + a + b - (a - c) \\ &= (n_1 - 1)c + (n_2 - 1)d + a + b - (a - c) - (b + (n_2 - 1)d + n_1 e) \\ &= n_1 c - n_1 e, \end{aligned}$$

which is > 0 if and only if $c > e$. □

This lemma together with Theorem 2.2 will be used in the next section to establish the optimality of MB GD PBBD's.

3. Optimality of extreme RGD. Firstly, we state without proof the following trivial lemma:

LEMMA 3.1. *For given positive integers s and t, the minimum of $\Sigma_{i=1}^{s} n_i^2$ subject to $\Sigma_{i=1}^{s} n_i = t$, where the n_i's are nonnegative integers, is obtained when $t - s\,\mathrm{int}(t/s)$ of the n_i's are equal to $\mathrm{int}(t/s) + 1$, and the others are equal to $\mathrm{int}(t/s)$.*

Let d' be an RGD. Then d' is $(M \cdot S)$-optimal in the sense of Eccleston and Hedayat (1974), i.e., d' maximizes $\mathrm{tr}\, C_d$ over all designs and minimizes $\mathrm{tr}\, C_d^2$ over the set $\{d : \mathrm{tr}\, C_d = \mathrm{tr}\, C_{d'}\}$. For, kC_d has integral entries $\forall d \in \mathfrak{D}$, and by Lemma 3.1, $\mathrm{tr}\, C_d^2 = \Sigma_i c_{dii}^2 + \Sigma_{i \neq j} c_{dij}^2$ is minimized by a design d' such that all the diagonal elements of $C_{d'}$ are equal, and for $i \neq j$, the numbers $kc_{d'ij}$ are as nearly equal as possible, that is, d' is an RGD.

Let the two distinct values of $\lambda_{d'ij}$ for $i \neq j$ be $\lambda_1'(d')$ and $\lambda_2'(d')$ with $\lambda_2'(d') = \lambda_1'(d') + 1$. For each variety i_0, let $n_{i_0}(d') = \#\{j : j \neq i_0, \text{ and } \lambda_{d'i_0 j} = \lambda_1'(d')\}$. Then $n_{i_0}(d')$ is independent of i_0. So we may drop the subscript i_0. Then we have

THEOREM 3.1. *For fixed v, b, k, let d^* be an extreme* RGD *of type* 1 *such that either $\lambda_1'(d^*) > 0$, or $\lambda_1'(d^*) = 0$ and $n(d^*) < v/2$. Then d^* is optimal over all designs with respect to any generalized criterion of type* 1. *If an extreme* RGD *of type* 1 *described above exists and if d is a design which is optimal with respect to some particular type* 1 *criterion ψ_f, then d must be an extreme* RGD *of type* 1.

PROOF. By Theorem 2.2, d^* is optimal over $\mathfrak{D}$ with respect to all type 1 criteria if (2.2) and (2.3) hold. We now verify these conditions.

For convenience, we write n, λ_1' and λ_2' instead of $n(d^*)$, $\lambda_1'(d^*)$ and $\lambda_2'(d^*)$, respectively. Also, for any design d, we write $A_d = \mathrm{tr}\, C_d$, $B_d = \mathrm{tr}\, C_d^2$, and $P_d = [B_d - A_d^2/(v-1)]^{\frac{1}{2}}$. Then it is easily seen that $c_{d^*ii} = A_{d^*}/v$, $\forall i$, and for $i \neq j$, there are vn of the c_{d^*ij}'s $= -[v^{-1}(v-1)^{-1}A_{d^*} - k^{-1}(v-1)^{-1}(v-1-n)]$, and $v(v-1-n)$ of the c_{d^*ij}'s $= -[v^{-1}(v-1)^{-1}A_{d^*} - k^{-1}(v-1)^{-1}(v-1-n) + k^{-1}] = -[v^{-1}(v-1)^{-1}A_{d^*} + k^{-1}(v-1)^{-1}n]$. In this case, we have

$$v^{-1}(v-1)^{-1}A_{d^*} - k^{-1}(v-1)^{-1}(v-1-n) = k^{-1}\,\mathrm{int}\big(v^{-1}(v-1)^{-1}kA_{d^*}\big). \tag{3.1}$$

By a straightforward computation,

$$P_{d^*}^2 = k^{-2}(v-1)^{-1}vn(v-1-n). \tag{3.2}$$

Also, (2.2) is equivalent to

$$A_{d^*}^2 > (v-1)(v-2)P_{d^*}^2. \tag{3.3}$$

We have

$$\begin{aligned} kA_{d^*}/v &= n\lambda_1' + (v-1-n)(\lambda_1'+1) \\ &= (v-1)\lambda_1' + v - 1 - n. \end{aligned} \tag{3.4}$$

If $\lambda_1' > 0$, then $kA_{d^*}/v > v-1$, which clearly implies (3.3). If $\lambda_1' = 0$, then $A_{d^*} = k^{-1}v(v-1-n)$. In this case, (3.3) is a consequence of the assumption that $v > 2n$.

Now, we shall verify (2.3), i.e., for any $d \in \mathfrak{D}$,

$$A_{d^*} - A_d \geqslant [(v-1)/(v-2)]^{\frac{1}{2}}(P_{d^*} - P_d). \tag{3.5}$$

From (3.2), we have

$$[(v-1)/(v-2)]^{\frac{1}{2}}P_{d^*} = k^{-1}[vn(v-1-n)/(v-2)]^{\frac{1}{2}}. \tag{3.6}$$

Therefore, $A_{d^*} - A_d \geqslant k^{-1}[vn(v-1-n)/(v-2)]^{\frac{1}{2}} \Rightarrow (3.5)$.

Thus, supposing (3.5) does not hold for some d, we have

$$A_{d^*} - A_d < k^{-1}[vn(v-1-n)/(v-2)]^{\frac{1}{2}}. \tag{3.7}$$

We may also assume $A_{d^*} > A_d$, since d^* is $(M \cdot S)$-optimal $\Rightarrow$ (3.5) is satisfied if $A_d = A_{d^*}$.

Because kC_d has integral entries, $A_d = A_{d^*} - k^{-1}\alpha$ for some positive integer $\alpha < [vn(v-1-n)/(v-2)]^{\frac{1}{2}}$. Thus

$$\begin{aligned} v^{-1}(v-1)^{-1}A_d &= v^{-1}(v-1)^{-1}A_{d^*} - k^{-1}v^{-1}(v-1)^{-1}\alpha \\ &\geqslant v^{-1}(v-1)^{-1}A_{d^*} - k^{-1}(v-1)^{-1}(v-1-n) \\ &= k^{-1}\operatorname{int}\big(v^{-1}(v-1)^{-1}kA_{d^*}\big). \end{aligned}$$

Since $A_{d^*} > A_d$, we conclude that

$$\begin{aligned} &v^{-1}(v-1)^{-1}A_{d^*} - k^{-1}(v-1)^{-1}(v-1-n) \\ &\quad = k^{-1}\operatorname{int}\big(v^{-1}(v-1)^{-1}kA_d\big). \end{aligned} \tag{3.8}$$

Hence by Lemma 3.1, $\operatorname{tr}(C_d^2) \geqslant \operatorname{tr}(C^2)$, where C is a matrix $(c_{ij})_{v\times v}$ such that $c_{ii} = A_d/v$, $\forall_i$, and for $i \neq j$, there are $vn + \alpha$ of the c_{ij}'s $= -[v^{-1}(v-1)^{-1}A_{d^*} - k^{-1}(v-1)^{-1}(v-1-n)]$, and $v(v-1-n) - \alpha$ of the c_{ij}'s $= -[v^{-1}(v-1)^{-1}A_{d^*} - k^{-1}(v-1)^{-1}(v-1-n) + k^{-1}] = -[v^{-1}(v-1)^{-1}A_{d^*} + k^{-1}(v-1)^{-1}n]$.

Hence

$$(3.9)\quad P_d^2 \geqslant \left[v^{-1}(v-1)^{-1}A_{d^*} - k^{-1}(v-1)^{-1}(v-1-n)\right]^2(vn+\alpha)$$
$$+\left[v^{-1}(v-1)^{-1}A_{d^*} + k^{-1}(v-1)^{-1}n\right]^2\left[v(v-1-n)-\alpha\right]$$
$$+\left[\left(A_{d^*}-k^{-1}\alpha\right)/v\right]^2 v - \left(A_{d^*}-k^{-1}\alpha\right)^2/(v-1)$$
$$= k^{-2}(v-1)^{-1}vn(v-1-n) + k^{-2}(v-1)^{-1}\alpha(v-1-2n)$$
$$-k^{-2}v^{-1}(v-1)^{-1}\alpha^2.$$

Now, (3.5) is equivalent to

$$(3.10)\quad k^{-1}\alpha - k^{-1}\left[vn(v-1-n)/(v-2)\right]^{\frac{1}{2}} \geqslant -\left[(v-1)/(v-2)\right]^{\frac{1}{2}}P_d,$$

i.e.,

$$(3.11)\quad \left(k^{-1}\alpha - k^{-1}\left[vn(v-1-n)/(v-2)\right]^{\frac{1}{2}}\right)^2 \leqslant P_d^2(v-1)/(v-2).$$

By (3.9), a sufficient condition for (3.11) is

$$(3.12)\quad \left(k^{-1}\alpha - k^{-1}\left[vn(v-1-n)/(v-2)\right]^{\frac{1}{2}}\right)^2$$
$$\leqslant k^{-2}(v-2)^{-1}vn(v-1-n) + k^{-2}(v-2)^{-1}$$
$$\times\alpha(v-1-2n) - k^{-2}v^{-1}(v-2)^{-1}\alpha^2,$$

or, equivalently,

$$(3.13)\quad \alpha - 2\left[vn(v-1-n)/(v-2)\right]^{\frac{1}{2}} \leqslant (v-2)^{-1}(v-1-2n) - v^{-1}(v-2)^{-1}\alpha.$$

This is the same as

$$(3.14)\quad v^{-1}(v-2)^{-1}\alpha(v-1)^2 \leqslant 2\left[vn(v-1-n)/(v-2)\right]^{\frac{1}{2}} + (v-2)^{-1}(v-1-2n).$$

Now, $v^{-1}(v-2)^{-1}(v-1)^2 \leqslant \frac{4}{3}$ for $v \geqslant 3$. So a sufficient condition for (3.14) is

$$(3.15)\quad \left(\tfrac{2}{3}\right)\left[vn(v-1-n)/(v-2)\right]^{\frac{1}{2}} \geqslant -(v-1-2n)/(v-2).$$

The minimum of the left side of (3.15) is $2v^{\frac{1}{2}}/3$, and the maximum of the right side is $(v-3)/(v-2)$. Therefore, (3.15) holds because $v \geqslant 3 \Rightarrow 2v^{\frac{1}{2}}/3 > (v-3)/(v-2)$.

Consequently, (3.5) $\Rightarrow d^*$ is optimal with respect to any type 1 criterion. In this situation, if d is a design which is optimal with respect to some particular type 1 criterion ψ_f, then by Corollary 2.2.1, C_d has the same eigenvalues with the same multiplicities as C_{d^*}. This implies that C_d is also $(M\cdot S)$-optimal, and hence must be an extreme RGD of type 1. □

Similarly, we have

THEOREM 3.2. *For fixed v, b, k, let d^* be an extreme* RGD *of type* 2 *such that* $n(d^*) \leq v/2$; *then d^* is optimal with respect to any generalized type* 2 *criterion over all designs. If an extreme* RGD *of type* 2 *described above exists and if d is a design which is optimal with respect to some particular type* 2 *criterion ψ_f, then d must be an extreme* RGD *of type* 2.

PROOF. The proof is similar to that of Theorem 3.1. We only indicate the differences in the details.

We only need to verify (2.5), i.e.,

$$\text{tr } C_{d^*} - \text{tr } C_d \geq [(v-1)(v-2)]^{\frac{1}{2}}(P_{d^*} - P_d), \qquad \forall d \in \mathfrak{D}. \tag{3.16}$$

$P_{d^*}^2$ is again $k^{-2}(v-1)^{-1}vn(v-1-n)$. Hence $A_{d^*} - A_d \geq k^{-1}[(v-2)(v-1-n)vn]^{\frac{1}{2}} \Rightarrow$ (3.16). So we may again assume $A_d = A_{d^*} - k^{-1}\alpha$, where α is a positive integer such that $\alpha < [vn(v-1-n)(v-2)]^{\frac{1}{2}}$. Then

$$\begin{aligned} v^{-1}(v-1)^{-1}(A_{d^*} - k^{-1}\alpha) &> v^{-1}(v-1)^{-1}\left(A_{d^*} - k^{-1}[vn(v-1-n)(v-2)]^{\frac{1}{2}}\right) \\ &\geq v^{-1}(v-1)^{-1}A_{d^*} - k^{-1}(v-1)^{-1}(v-1-n) \\ &= k^{-1}\,\text{int}\left(v^{-1}(v-1)^{-1}kA_{d^*}\right). \end{aligned}$$

The last inequality follows from the assumption $n \leq v/2$ because

$$\begin{aligned} vn(v-1-n)(v-2) - [v(v-1-n)]^2 & \\ &= v(v-1-n)(v-1)(2n-v) \\ &\leq 0 \Rightarrow v(v-1-n) \geq [vn(v-1-n)(v-2)]^{\frac{1}{2}}. \end{aligned}$$

Therefore,

$$\begin{aligned} k^{-1}\,&\text{int}\left(kA_d v^{-1}(v-1)^{-1}\right) \\ &= v^{-1}(v-1)^{-1}A_{d^*} - k^{-1}(v-1)^{-1}(v-1-n). \end{aligned} \tag{3.17}$$

Hence, (3.9) still holds. Then (3.11) is replaced by

$$\left(k^{-1}\alpha - k^{-1}[vn(v-1-n)(v-2)]^{\frac{1}{2}}\right)^2 \leq (v-1)(v-2)P_d^2, \tag{3.18}$$

and instead of (3.12), we have

$$\begin{aligned} &\left(k^{-1}\alpha - k^{-1}[vn(v-1-n)(v-2)]^{\frac{1}{2}}\right)^2 \\ &\quad \leq k^{-2}vn(v-1-n)(v-2) \\ &\quad\quad + k^{-2}\alpha(v-1-2n)(v-2) - k^{-2}v^{-1}\alpha^2(v-2), \end{aligned} \tag{3.19}$$

which is equivalent to

$$\alpha - 2[vn(v-1-n)(v-2)]^{\frac{1}{2}} \leq (v-1-2n)(v-2) - \alpha v^{-1}(v-2). \tag{3.20}$$

This is the same as

$$2v^{-1}(v-1)\alpha \leq 2[vn(v-1-n)(v-2)]^{\frac{1}{2}} + (v-1-2n)(v-2). \tag{3.21}$$

A sufficient condition for (3.21) is

$$(3.22) \qquad 2v^{-1}[vn(v-1-n)(v-2)]^{\frac{1}{2}} \geqslant -(v-2)(v-1-2n).$$

Now, (3.22) holds for $n \leqslant (v-1)/2$. If $n > (v-1)/2$, then the left side of (3.22) is a decreasing function of n, and the right side is an increasing function of n. When $n = v/2$, both sides equal $v-2$. Therefore (3.22) is satisfied for any $n \leqslant v/2$. □

An important class of extreme RGD's satisfying the conditions of Theorem 3.1 and Theorem 3.2 are the MB GD PBBD's. Let d^* be an MB GD PBBD of type 1. If l_{d^*ij} is the off-diagonal element of C_{d^*} at position (i, j), then

$$(3.23) \qquad \begin{aligned} l_{d^*ij} &= -\lambda_1/k, \text{ if } i \text{ and } j \text{ are in the same group} \\ &= -(\lambda_1+1)/k \text{ if } i \text{ and } j \text{ are in different groups.} \end{aligned}$$

Therefore, C_{d^*} is of the form considered in Lemma 2.1 with $c > e$. Hence d^* is an extreme RGD of type 1. Similarly, an MB GD PBBD of type 2 is an extreme RGD of type 2. For an MB GD PBBD of type 1, $n(d^*) = v/2 - 1 < v/2$, and for an MB GD PBBD of type 2, $n(d^*) = v/2$. Therefore, by Theorem 3.1 and Theorem 3.2, we have

COROLLARY 3.1.1. *For fixed v, b, k, if there exists an* MB GD PBBD *of type* 1, *then it is optimal over all designs with respect to all generalized criteria of type* 1.

COROLLARY 3.2.1. *For fixed v, b, k, if there exists an* MB GD PBBD *of type* 2, *then it is optimal over all designs with respect to any generalized criterion of type* 2.

REMARK 1. A sufficient condition for (2.3) and (2.5) is (2.1) and that d^* minimizes $\operatorname{tr} C_d^2 - (\operatorname{tr} C_d)^2/(v-1)$ over all $d \in \mathfrak{D}$. But this is too stringent to be applied. For example, although an MB GD PBBD is optimal when it exists, it does not minimize $\operatorname{tr} C_d^2 - (\operatorname{tr} C_d)^2/(v-1)$ even over all connected designs. Take any MB GD PBBD, to which add a BBD with the same block size and the same number of varieties. Then the resulting design d^* is still an MB GD PBBD (with different parameters). Now, in the new design d^*, if we replace the original design by one with the same number of blocks each containing only one kind of variety, then the resulting design d' is connected, but with $\operatorname{tr} C_{d'}^2 - (\operatorname{tr} C_{d'})^2/(v-1) = 0 < \operatorname{tr} C_{d^*}^2 - (\operatorname{tr} C_{d^*})^2/(v-1)$. This is why we need weaker conditions like (2.3) and (2.5).

REMARK 2. When $k < v$, the condition "either $\lambda_1'(d^*) > 0$, or $\lambda_1'(d^*) = 0$ and $n(d^*) < v/2$" in Theorem 3.1 is equivalent to $(k-1)r \geqslant v/2 - 1$, where $r = bk/v$.

REMARK 3. Even in the cases where there is no extreme RGD of type 1, the result in Theorem 3.1 can still be used to establish a lower bound for ψ_f (ψ_f-optimal design) for any type 1 criterion ψ_f, as long as there is an RGD d s.t. $\lambda_1'(d) > 0$, or $\lambda_1'(d) = 0$ and $n(d) < v/2$. This lower bound is sharper than the classical one based on symmetric designs. This has been applied in Cheng (1977) to study the efficiencies of general regular graph designs. Similar comments hold for type 2 criteria.

4. Uniqueness of optimal designs. Takeuchi (1961, 1963) proved that for fixed parameters b, v, and k, if there are BIBD's, or GD PBIBD's with $\lambda_2 = \lambda_1 + 1$, then they are the only E-optimal designs. If we look at the proof carefully, we conclude that his result can be stated in a more general form which is not restricted to the setting of block designs.

That is, we have the following

THEOREM 4.1. *Let $\mathcal{C} = \{C_d : d \in \mathfrak{D}\}$ be a class of matrices in $\mathfrak{B}_{v,0}$. Suppose $\exists$ positive integer k such that kC has integral entries, $\forall C \in \mathcal{C}$, and $\exists C_{d^*} \in \mathcal{C}$ such that*

(1) *C_{d^*} maximizes* tr C_d *over $d \in \mathfrak{D}$,*
(2) *kC_{d^*} is completely symmetric or of the form*

$$\begin{bmatrix} (v^{-1}A + m)I_u - mJ_u & -(m+1)J_u & \cdots & -(m+1)J_u \\ -(m+1)J_u & (v^{-1}A + m)I_u - mJ_u & \cdots & -(m+1)J_u \\ \vdots & & \ddots & \vdots \\ -(m+1)J_u & \cdots & & (v^{-1}A + m)I_u - mJ_u \end{bmatrix},$$

where $m = \operatorname{int}(v^{-1}(v-1)^{-1}A)$, and $v = tu$ for some positive integer t. Eliminate one multiplicity of zero from the eigenvalues of the matrices in $\mathcal{C}$. Then except for a simultaneous rearrangement of rows and columns, C_{d^*} is the unique matrix in $\mathcal{C}$ which maximizes the minimum of the remaining eigenvalues over $\mathcal{C}$.

The proof is essentially the same as in Takeuchi's paper.

Therefore, Takeuchi's result on E-optimality is also true for $k \geqslant v$. That is, for fixed parameters k, b, and v, if there are BBD's or GD PBBD's with $\lambda_2 = \lambda_1 + 1$, then they are the only E-optimal designs.

We can also prove an interesting dual of Theorem 4.1.

THEOREM 4.2. *Let $\mathcal{C} = \{C_d : d \in \mathfrak{D}\}$ be a class of matrices in $\mathfrak{B}_{v,0}$. Suppose $\exists$ positive integer k such that kC has integral entries $\forall C \in \mathcal{C}$, and $\exists C_{d^*} \in \mathcal{C}$ such that*

(1) *C_{d^*} minimizes* tr C_d *over $d \in \mathfrak{D}$,*
(2) *kC_{d^*} is completely symmetric or of the form*

$$\begin{bmatrix} (v^{-1}A + m + 1)I_u - (m+1)J_u & -mJ_u & \cdots & -mJ_u \\ -mJ_u & (v^{-1}A + m + 1)J_u - (m+1)J_u & \cdots & -mJ_u \\ \vdots & & \ddots & \vdots \\ -mJ_u & \cdots & & (v^{-1}A + m + 1)I_u - (m+1)J_u \end{bmatrix},$$

where $m = \operatorname{int}(v^{-1}(v-1)^{-1}A)$, and $v = tu$ for some positive integer t.

Then except for a simultaneous rearrangement of rows and columns, C_{d^*} *is the unique matrix in* $\mathcal{C}$ *which minimizes the maximum eigenvalue over* $\mathcal{C}$.

This theorem can be proved by an easy modification of the proof of Theorem 4.1. One can multiply all the matrices in $\mathcal{C}$ by -1, and then follow the proof of Theorem 4.1.

Therefore, for fixed parameters v, b, and k, if there are BBD's or GD PBBD's with $\lambda_1 = \lambda_2 + 1$, then they are the only designs which minimize the maximum eigenvalue of C_d over the set $\{d : d$ maximizes tr C_d over $\mathfrak{D}\}$. While (unlike E-optimality) the minimization of the maximum eigenvalue has no intuitive merit as an optimality criterion, we will use the above result to obtain the uniqueness of optimal designs for the meaningful type 2 criteria.

If there is an MB GD PBBD of type 1, say d^*, and d' is a design which is optimal w.r.t. some particular type 1 criterion ψ_f, then by Corollary 2.2.1, $C_{d'}$ has the same set of eigenvalues as C_{d^*}. This implies that d' is also E-optimal. Then by Theorem 4.1, d' must be an MB GD PBBD of type 1.

Similarly, if there is an MB GD PBBD of type 2, say d^*, and d' is a design which is optimal w.r.t. some particular type 2 criterion ψ_f, then d' also minimizes the maximum eigenvalue of C_d over the set $\{d : d$ maximizes tr C_d over $\mathfrak{D}\}$. Therefore, by Theorem 4.2, d' must be an MB GD PBBD of type 2.

We state these results as

THEOREM 4.3. *For fixed* v, b, k, *if there is an* MB GD PBBD *of type* i ($i = 1, 2$), *and* d' *is optimal* w.r.t. *some particular type* i *criterion, then* d' *must be an* MB GD PBBD *of type* i.

Note that Theorem 4.3 is also true for BBD's.

5. Existence and nonexistence of MB GD PBBD. If $v < k$, and $k = v \cdot \text{int}(k/v) + k'$, then the existence of an MB GD PBIBD with parameters v, b, k' is equivalent to that of an MB GD PBBD with parameters v, b, k. An MB GD PBIBD plus several complete block designs adjoined to the incomplete blocks is easily seen to be an MB GD PBBD, and conversely. Thus, for the construction of an MB GD PBBD, it suffices to consider the case $k < v$. It is also clear that for fixed k, b, v, if there is an MB GD PBBD, then there is no BBD with these parameters.

An important necessary condition for the existence of an MB GD PBIBD of type 1 is that $(v-1)^{-1}(k-1)r - v/2(v-1)$ should be an integer. One can derive an analogous condition for type 2 designs.

By Theorem 2 of Shah-Raghavarao-Khatri (1976), and our Theorem 4.3, we have the following simple result about the nonexistence of BBD and MB GD PBBD:

THEOREM 5.1. *Let* d^* *be a* BBD *or an* MB GD PBBD *of type* 1 *with parameters* b, k, v. *If the dual design of* d^* *is not a* BBD, *then there is no* BBD *with parameters* $b' = v$, $v' = b$, *and* $k' = r$; *also, if the dual design of* d^* *is not an* MB GD PBBD *of* *type* 1, *then there is no* MB GD PBBD *of type* 1 *with parameters* $b' = v$, $v' = b$, *and* $k' = r$.

PROOF. Let d^* be an MB GD PBBD of type 1 with parameters v, b, k. If there is a BBD with parameters $b' = v$, $v' = b$, and $k' = r$, say $\bar{d}$, then by Theorem 2 of Shah-Raghavarao-Khatri, the dual design of d^* is at least as good as $\bar{d}$ under the E-criterion. Consequently, the dual design of d^* must be a BBD. The rest can be proved similarly. □

So, e.g., combining this theorem with Theorem 10.3.1 and Theorem 10.3.2 of Raghavarao (1971, pages 204–205), we conclude that if there is a BIBD with parameters v, b, r, k, $\lambda = 1$, or $v = \binom{r-1}{2}$, $b = \binom{r}{2}$, $k = r - 2$, $\lambda = 2$, then there is no MB GD PBBD of type 1 with parameters $v' = b$, $b' = v$, and $k' = r$.

Theorem 8.6.3 of Raghavarao (1971, page 139) provides us with a method for constructing many MB GD PBIBD's of both types from a resolvable or partly resolvable BIBD with $v = 2k$. For convenience of later use, we restate it as

THEOREM 5.2. *If a resolvable solution or at least a solution with one complete replication exists for a* BIBD *with parameters* v^*, b^*, r^*, k^*, λ^*, *in which* $k^*|v^*$, *then there always exists a* GD PBIBD *with the parameters* $v = v^*$, $b = tb^* + av^*/k^*$, $r = \mathrm{tr}^* + a$, $k = k^*$, $\lambda_1 = t\lambda^* + a$, $\lambda_2 = t\lambda^*$, *number of groups* $= v^*/k^*$, *and number of varieties in each group* $= k^*$, *where* a *and* t *are integers* ($t > 0$, $a \geqslant -t\lambda^*$).

Note that an MB GD PBIBD of type 1 (resp., 2) is obtained by taking $v^* = 2k^*$, and $a = -1$ (resp., $+1$).

For example, let d be the resolvable BIBD (1, 2), (1, 3), (1, 4), (2, 3), (2, 4), (3, 4) with parameters $v^* = 4$, $b^* = 6$, $r^* = 3$, $k^* = 2$, and $\lambda^* = 1$. Then there exists an MB GD PBIBD of type 1 with parameters $v = 4$, $b = 6t - 2$, $r = 3t - 1$, $k = 2$, $\lambda_1 = t - 1$, $\lambda_2 = t$, where $t > 0$; and there exists an MB GD PBIBD of type 2 with parameters $v = 4$, $b = 6t + 2$, $r = 3t + 1$, $k = 2$, $\lambda_1 = t + 1$, and $\lambda_2 = t$.

For the method of construction, see the proof of the above theorem in Raghavarao's book.

Because of the appealing optimality property which an MB GD PBBD possesses, more developments on the construction of such designs would be useful. It is also desirable, if possible, to investigate the conditions under which an RGD is extreme. For a PBBD with two associate classes, the corresponding C-matrix has two distinct nonzero eigenvalues. The question is, when do these two eigenvalues have extreme multiplicities? Except for group divisible designs, there seems at present to be no systematic study in this respect. The applicability of Theorem 3.1 and Theorem 3.2 will be enhanced by significant research along this line.

6. Situation where BBD and extreme RGD do not exist. When both BBD and extreme RGD of type 1 do not exist, and if we are considering type 1 criteria, then intuitively there seem to be two most likely candidates for the optimal designs: a

GD PBBD $\bar{d}$ with 2 groups and $\lambda_2 = \lambda_1 + 2$, or a connected RGD d* such that C_{d^*} has two distinct nonzero eigenvalues $\mu > \mu'$, and μ has multiplicity 2.

Although we cannot presently prove either of these is optimum, we can compare the performances of $\bar{d}$ and d^* when both of them exist. In order to do this, we need a property of convex functions.

For any given n-tuples $(x_1, \cdots, x_n)$ and $(y_1, \cdots, y_n)$ of nonnegative numbers, we say that $(x_1, \cdots, x_n)$ majorizes $(y_1, \cdots, y_n)$ if $\Sigma_{i=1}^n x_i = \Sigma_{i=1}^n y_i$, and $\Sigma_{i=1}^k x_{[i]} \geq \Sigma_{i=1}^k y_{[i]}$, $\forall k \leq n$, where $x_{[1]} \geq x_{[2]} \geq \cdots \geq x_{[n]}$, and $y_{[1]} \geq y_{[2]} \geq \cdots \geq y_{[n]}$ are rearrangements of $(x_1, \cdots, x_n)$ and $(y_1, \cdots, y_n)$, respectively. It is well known (see, e.g., Mirsky (1963)) that the majorization of $(y_1, \cdots, y_n)$ by $(x_1, \cdots, x_n)$ is equivalent to $\Sigma_{i=1}^n f(x_i) \geq \Sigma_{i=1}^n f(y_i)$ for each real continuous convex function f defined on some real interval.

We now compare the two designs $\bar{d}$ and d^*. Firstly, we look at the E-criterion.

Both of $\bar{d}$ and d^* maximize $\operatorname{tr} C_d$ over all possible designs. Let $A = \operatorname{tr} C_{\bar{d}} = \operatorname{tr} C_{d^*}$. Then $c_{\bar{d}ii} = c_{d^*ii} = A/v$, $\forall i$. It is easily seen that for $i \neq j$, there are $v(v/2 - 1)$ of the $c_{\bar{d}ij}$'s $= -[v^{-1}(v-1)^{-1}A - k^{-1}(v-1)^{-1}v]$, and $v^2/2$ of the $c_{\bar{d}ij}$'s $= -[v^{-1}(v-1)^{-1}A + k^{-1}(v-1)^{-1}(v-2)]$. By a straightforward computation, $P_{\bar{d}}^2 = k^{-2}(v-1)^{-1}v^2(v-2)$. Also, by the computation in Section 3, $\exists$ positive integer n s.t. $P_{d^*}^2 = k^{-2}(v-1)^{-1}vn(v-1-n)$.

We claim that

(6.1) $v > 4 \Rightarrow R_2(1; A, B_{\bar{d}}) < R_2(2; A, B_{d^*})$, where R_2 is defined in Lemma A2; i.e., d^* is E-better than $\bar{d}$.

Note that (6.1) is equivalent to

$$v > 4 \Rightarrow \left[(v-2)^{-1}(v-1)\right]^{\frac{1}{2}} P_{\bar{d}} > \left[2(v-3)^{-1}(v-1)\right]^{\frac{1}{2}} P_{d^*}. \tag{6.2}$$

Now, the left side of the above inequality equals v/k, and the right side equals $k^{-1}[2vn(v-1-n)(v-3)^{-1}]^{\frac{1}{2}}$, which is less than or equal to $k^{-1}(v-1)[v/2(v-3)]^{\frac{1}{2}}$. So it suffices to show $v^2 > 2^{-1}(v-3)^{-1}v(v-1)^2$, i.e., $v^2 > 4v + 1$. It is easily seen that this is true for any $v \geq 5$.

Therefore, $v > 4 \Rightarrow d^*$ is E-better than $\bar{d}$ if both of them exist. Since $C_{\bar{d}}$ has two distinct nonzero eigenvalues and the smaller has multiplicity $v - 2$, the nonzero eigenvalues of $C_{\bar{d}}$ majorize those of C_{d^*}. Consequently, for $v > 4$, d^* is also ψ_f-better than $\bar{d}$ for any continuous strictly convex function f defined on $(0, \bar{c}_{\mathcal{D}})$.

A similar result holds for type 2 analogues of $\bar{d}$ and d^*. An example of d^* is a GD PBBD with 3 groups and $\lambda_2 = \lambda_1 + 1$ (which exists only for $v \geq 6$). By Takeuchi's result, this design is E-optimal, but we do not know whether it is optimal with respect to other generalized criteria of type 1.

John and Mitchell (1977) conjectured that if an RGD exists, then a D-optimal (or A-optimal, or E-optimal) design should be an RGD. This is the same as saying that an optimal design should be $(M \cdot S)$-optimal if an RGD exists. We have seen in Section 3 that this is true for many extreme RGD's. Since we are considering criteria ψ_f where f is a strictly decreasing function, seeking for optimal designs among those which maximize tr C_d seems reasonable. The next step is then to find a design which is closest to the ideal minimum. Unfortunately, except for designs with certain structures like complete symmetry or those considered in Section 3, it is difficult to prove that this can produce designs which are optimal with respect to any meaningful criterion. But a design which is too far away from the ideal minimum (with a big value of P_d) certainly is bad. Therefore, as suggested by the comparison of $\bar{d}$ with d^*, Mitchell and John's conjecture might be true for large v.

For $v = 4$, their conjecture is false, at least for the E-criterion. They used a computer to search for the best RGD for many parameter values. If their conjecture is true, then the designs they obtained should be optimal. For $v = 4$, we can construct several examples of $\bar{d}$ which are not RGD's but have the same performance as the best RGD under the E-criterion.

For example, there is a BIBD with parameters $v^* = 4$, $b^* = 18$, $r^* = 9$, $k^* = 2$, $\lambda^* = 3$ (take three replications of (1, 2), (1, 3), (1, 4), (2, 3), (2, 4), (3, 4)). Then by Theorem 5.2, taking $t = 1$ and $a = -2$, there is a GD PBIBD d' with parameters $v = 4$, $b = 14$, $r = 7$, $k = 2$, $\lambda_1 = 1$, and $\lambda_2 = 3$. By Lemma 2.10, the nonzero eigenvalues of $C_{d'}$ are 4 (multiplicity = 2) and 6 (multiplicity = 1). Looking up the best RGD with the same parameters listed in John and Mitchell (1977), we see that it has the same E-performance as d'. This rules out the uniqueness part of Mitchell and John's conjecture. But it is still possible that the best RGD's are optimal.

The problem of finding optimal designs when both BBD and extreme RGD do not exist seems very difficult. At least the method we developed for proving the optimality of extreme RGD's failed. A GD PBBD with 3 groups and $\lambda_2 = \lambda_1 + 1$ might be a reasonable candidate to study. We hope that research along this line can be carried out in the future.

APPENDIX

In what follows, a complete proof of Theorem 2.2 is given. We begin with some terminology and a series of lemmas.

Given any two positive numbers A and B such that $A^2 \geqslant B \geqslant A^2/(v-1)$, we define the number P as before. Such a pair (A, B) is called *regular* if $\sum_{i=1}^{v-1} \mu_i = A$, $\sum_{i=1}^{v-1} \mu_i^2 = B$, and $\mu_i \geqslant 0$, $\forall i \Rightarrow \mu_i \neq 0$, $\forall i$; otherwise, (A, B) is called *singular*.

In Lemmas A1 through A9, we always assume $A^2 \geqslant B \geqslant A^2/(v-1)$.

LEMMA A1. *If (A, B) is singular, then $B \geqslant A^2/(v-2)$. Or, equivalently, $A^2/(v-1) \leqslant B < A^2/(v-2) \Rightarrow (A, B)$ is regular.*

LEMMA A2. *For any fixed positive number n, $1 \leqslant n \leqslant v-2$, the solution of $nR_1 + (v-1-n)R_2 = A$, $nR_1^2 + (v-1-n)R_2^2 = B$, and $R_1 \geqslant R_2$ is given by*

$$R_1(n; A, B) = \left(A + \left[n^{-1}(v-1)(v-1-n)\right]^{\frac{1}{2}} P\right) / (v-1),$$

$$R_2(n; A, B) = \left(A - \left[(v-1-n)^{-1} n(v-1)\right]^{\frac{1}{2}} P\right) / (v-1).$$

For fixed A and B, both of R_1 and R_2 are strictly decreasing functions of n.

The easy proofs of Lemma A1 and Lemma A2 are omitted.

For convenience, we define $F(n; A, B)$ to be $nf(R_1(n; A, B)) + (v - 1 - n) f(R_2(n; A, B))$.

LEMMA A3. *Assume* $A^{*2} \geqslant B^* \geqslant A^{*2}/(v-1)$, $f' < 0$, *and* $f'' > 0$ *on* $(0, A^*)$. *Let* n^* *be a number in* $[1, v-2]$ *such that* $R_2(n^*; A^*, B^*) \geqslant 0$. *Then*:

(i) *For fixed* $n \in [1, n^*]$, $F(n; A^*, B)$ *is a strictly increasing function of* B (*and the corresponding* P) *on* $[A^{*2}/(v-1), B^*]$.

(ii) *For fixed* $n \in [1, n^*]$, $F(n; A, B^*)$ *is a strictly decreasing function of* A *on* $[A^*, A^{**}]$, *provided* $A^{**} \leqslant [(v-1)B^*]^{\frac{1}{2}}$, *and* $f' < 0$ *on* $(0, A^{**})$.

(iii) *Furthermore, if* f' *is strictly concave on* $(0, A^*)$, *then* $F(n; A^*, B^*)$ *is a strictly increasing function of* n *on* $[1, n^*]$.

(iv) *If* f' *is strictly convex on* $(0, A^*)$, *then* $F(n; A^*, B^*)$ *is a strictly decreasing function of* n *on* $[1, n^*]$.

PROOF. We only give the proof of (iii). (iv) can be similarly proved, and (i) and (ii) are trivial.

We have

$$
\begin{aligned}
&\partial F(n; A^*, B^*)/\partial n \\
&\quad = f\Big(\big(A^* + [n^{-1}(v-1)(v-1-n)]^{\frac{1}{2}} P^*\big)/(v-1)\Big) \\
&\qquad - f\Big(\big(A^* - [(v-1-n)^{-1} n(v-1)]^{\frac{1}{2}} P^*\big)/(v-1)\Big) \\
&\qquad - (P^*/2)\big[n^{-1}(v-1-n)^{-1}(v-1)\big]^{\frac{1}{2}} \\
&\qquad \times \Big[f'\Big(\big(A^* + [n^{-1}(v-1)(v-1-n)]^{\frac{1}{2}} P^*\big)/(v-1)\Big) \\
&\qquad + f'\Big(\big(A^* - [(v-1-n)^{-1} n(v-1)]^{\frac{1}{2}} P^*\big)/(v-1)\Big)\Big] \\
&\quad = f\Big(\big(A^* + [n^{-1}(v-1)(v-1-n)]^{\frac{1}{2}} P^*\big)/(v-1)\Big) \\
&\qquad - f\Big(\big(A^* - [(v-1-n)^{-1} n(v-1)]^{\frac{1}{2}} P^*\big)/(v-1)\Big) \\
&\qquad - (1/2)\Big[f'\Big(\big(A^* + [n^{-1}(v-1)(v-1-n)]^{\frac{1}{2}} P^*\big)/(v-1)\Big) \\
&\qquad + f'\Big(\big(A^* - [(v-1-n)^{-1} n(v-1)]^{\frac{1}{2}} P^*\big)/(v-1)\Big)\Big] \\
&\qquad \times \Big[\big(A^* + [n^{-1}(v-1)(v-1-n)]^{\frac{1}{2}} P^*\big)/(v-1) \\
&\qquad - \big(A^* - [(v-1-n)^{-1} n(v-1)]^{\frac{1}{2}} P^*\big)/(v-1)\Big] > 0,
\end{aligned}
$$

since $f' < 0$, and f' is strictly concave. □

LEMMA A4. *$R_2(v-2; A, B) > 0 \Leftrightarrow B < A^2/(v-2)$, and hence $R_2(v-2; A, B) > 0 \Rightarrow (A, B)$ is regular. Similarly, $R_2(1; A, B) \geqslant 0 \Leftrightarrow B \leqslant A^2$. So we always have $R_2(1; A, B) \geqslant 0$.*

PROOF. $R_2(v-2; A, B) = (A - [(v-1)(v-2)]^{\frac{1}{2}}P)/(v-1) > 0$ if and only if $A^2 > (v-1)(v-2)[B - A^2/(v-1)]$.

This is equivalent to $B < A^2/(v-2)$.

The other part is similar. □

LEMMA A5. *Let f be strictly convex on $[0, A]$. If (A, B) is singular, and $\Sigma_{i=1}^{v-1}\mu_i = A$, $\Sigma_{i=1}^{v-1}\mu_i^2 = B$, with $\mu_1 = 0$, $\mu_i \geqslant 0$, $\forall i = 2, \cdots, v-1$, then for $0 < \mu \leqslant A^2/2(v-2)^2$, $\exists \mu_1', \cdots, \mu_{v-1}' \geqslant 0$ s.t. $\Sigma_{i=1}^{v-1}\mu_i' = A$, $\Sigma_{i=1}^{v-1}(\mu_i')^2 = B - \mu$, and $\Sigma_{i=1}^{v-1}f(\mu_i) > \Sigma_{i=1}^{v-1}f(\mu_i')$.*

PROOF. There is at least one $\mu_i \geqslant A/(v-2)$, say μ_2.

Take $0 < \varepsilon \leqslant A/2(v-2)$, then $\varepsilon \leqslant \mu_2/2$. Let $\mu_1' = \varepsilon$, $\mu_2' = \mu_2 - \varepsilon$, $\mu_i' = \mu_i$, $\forall i > 2$. Then $\Sigma_{i=1}^{v-1}\mu_i' = A$, and, by convexity of f, $\Sigma_{i=1}^{v-1}f(\mu_i) > \Sigma_{i=1}^{v-1}f(\mu_i')$.

Now, $\Sigma\,\mu_i'^2 = B + 2\varepsilon^2 - 2\mu_2\varepsilon$; also, $\varepsilon = 0 \Rightarrow 2\mu_2\varepsilon - 2\varepsilon^2 = 0$, and $\varepsilon = A/2(v-2) \Rightarrow 2\mu_2\varepsilon - 2\varepsilon^2 \geqslant A^2/2(v-2)^2$. So, by appropriate choice of ε, $\Sigma\,\mu_i'^2$ can be $B - \mu$ for any μ with $0 < \mu \leqslant A^2/2(v-2)^2$. □

LEMMA A6. *Let f be continuous on $[0, A]$, $f' < 0$ and $f'' > 0$ on $(0, A)$ (allowing $\lim_{x\to 0^+} f(x) = f(0) = +\infty$). Also, let $S(A, B) = \{(\mu_1, \cdots, \mu_{v-1}) : \Sigma_{i=1}^{v-1}\mu_i = A, \Sigma_{i=1}^{v-1}\mu_i^2 = B, \mu_i \geqslant 0, \forall i\}$.*

If $f''' < 0$ on $(0, A)$, then the minimum of $\Sigma_{i=1}^{v-1}f(\mu_i)$ on $S(A, B)$ occurs at a point with some coordinate equal to zero or the point $(R_1(1; A, B), R_2(1; A, B), \cdots, R_2(1; A, B))$. If $f''' > 0$ on $(0, A)$, then this minimum value occurs at a point with some coordinate equal to zero or the point

$$\Big(\underbrace{R_1(n^*; A, B), \cdots, R_1(n^*; A, B)}_{n^*}, R_2(n^*; A, B), \cdots, R_2(n^*; A, B)\Big),$$

where n^* is the largest integer $\leqslant v-2$ s.t. $R_2(n^*; A, B) > 0$.

PROOF. The minimum of $\Sigma_{i=1}^{v-1}f(\mu_i)$ on $S(A, B)$ occurs either at a point with some coordinate $= 0$, or in the subset $S(A, B) \cap \{(\mu_1, \cdots, \mu_{v-1}) : \mu_i > 0\ \forall i\}$.

Now, consider the subproblem of minimizing $\Sigma_{i=1}^{v-1}f(\mu_i)$ subject to $\Sigma_{i=1}^{v-1}\mu_i = A$, $\Sigma_{i=1}^{v-1}\mu_i^2 = B$, and $\mu_i > 0$, $\forall i$. This is equivalent to minimizing $\Sigma_{i=1}^{v-2}f(\mu_i) + f(A - \Sigma_{i=1}^{v-2}\mu_i)$ subject to

$$\Sigma_{i=1}^{v-2}\mu_i^2 + \left(A - \Sigma_{i=1}^{v-2}\mu_i\right)^2 = B,$$

$$\mu_i > 0, \forall i = 1, \cdots, v-2, \text{ and } \Sigma_{i=1}^{v-2}\mu_i < A.$$

By Lagrange's theorem (see Apostol (1974, page 381)), it suffices to compare $\Sigma_{i=1}^{v-2}f(\mu_i) + f(A - \Sigma_{i=1}^{v-2}\mu_i)$ among the stationary points.

Differentiating $\Sigma_{i=1}^{v-2}f(\mu_i) + f(A - \Sigma_{i=1}^{v-2}\mu_i) + \mu[B - \Sigma_{i=1}^{v-2}\mu_i^2 - (A - \Sigma_{i=1}^{v-2}\mu_i)^2]$ w.r.t. each μ_i, and setting the derivatives equal to zero, we get

(A1) $$f'(\mu_i) - f'(\mu_{v-1}) + \mu[-2\mu_i + 2\mu_{v-1}] = 0.$$

If $\mu_i \neq \mu_{v-1}$, then (A1) can be written as

$$[f'(\mu_i) - f'(\mu_{v-1})]/(\mu_i - \mu_{v-1}) = 2\mu. \tag{A2}$$

For fixed μ_{v-1}, the strict convexity or concavity of f' implies that (A2) has a unique solution $\mu_i \in (0, A)$. Therefore, all the stationary points can have at most two distinct coordinates. The rest follows from Lemma A2 and (iii), (iv) of Lemma A3. □

For any $A, B > 0$, $A^2 \geqslant B \geqslant A^2/(v-1)$, we now denote the minimum of $\sum_{i=1}^{v-1} f(\mu_i)$ on $S(A, B)$ by $M_f(A, B)$.

LEMMA A7. *Assume $A^2 \geqslant B' > B \geqslant A^2/(v-1)$, and that (A, B') is regular; also, f satisfies the conditions in Lemma* A6. *Then $M_f(A, B') > M_f(A, B)$.*

PROOF. (i) Firstly, we consider the case $f''' > 0$ on $(0; A)$.

By Lemma A6, $\exists n, n' \in [1, v-2]$, $n \geqslant n'$ s.t. $R_2(n; A, B) > 0$, $R_2(n'; A, B') > 0$, $M_f(A, B) \leqslant F(n; A, B)$ and $M_f(A, B') = F(n'; A, B')$.

By Lemma A3, $F(n'; A, B') > F(n'; A, B) \geqslant F(n; A, B)$.

(ii) If $f''' < 0$ on $(0, A)$, then $M_f(A, B') = F(1; A, B') > F(1; A, B) \geqslant M_f(A, B)$. □

LEMMA A8. *If (A, B') is singular, $B' > B \geqslant B' - A^2/2(v-2)^2$, $B \geqslant A^2/(v-1)$, and f satisfies the conditions in Lemma* A6, *then $M_f(A, B') > M_f(A, B)$.*

PROOF. We only consider the case $f''' > 0$ on $(0, A)$. The case $f''' < 0$ can be proved similarly.

Then $M_f(A, B')$ either equals $F(n^*; A, B')$ for some $n^* \in [1, v-2]$, or occurs at a point with some coordinate equal to zero.

By an argument similar to that of Lemma A7, $F(n^*; A, B') > M_f(A, B)$.

On the other hand, if $\sum_{i=1}^{v-1} \mu_i = A$, $\sum_{i=1}^{v-1} \mu_i^2 = B'$, $\mu_i \geqslant 0$, $\forall i$, and some $\mu_i = 0$, then by Lemma A5, $\sum_{i=1}^{v-1} f(\mu_i) > \sum_{i=1}^{v-1} f(\mu_i^*)$ for some $\mu_1^*, \cdots, \mu_{v-1}^*$ s.t. $\sum_{i=1}^{v-1} \mu_i^* = A$, $\sum_{i=1}^{v-1} \mu_i^{*2} = B$, and $\mu_i^* \geqslant 0$, $\forall i$. Therefore, $M_f(A, B') > M_f(A, B)$. □

By a finite number of repeated applications of Lemma A7 and Lemma A8, we get

LEMMA A9. *If $A^2 \geqslant B' > B \geqslant A^2/(v-1)$, and f satisfies the conditions in Lemma A6, then $M_f(A, B') > M_f(A, B)$.*

Now we are ready to prove Theorem 2.2.

PROOF OF THEOREM 2.2. We will only give the proof of part (b) in detail, and briefly indicate the major differences in the proof of part (a).

For convenience, we write P_d instead of $[\text{tr } C_d^2 - (\text{tr } C_d)^2/(v-1)]^{\frac{1}{2}}$; also, $A_d = \text{tr } C_d$, and $B_d = \text{tr } C_d^2$. It suffices to prove the optimality with respect to any type 2 criterion ψ_f.

By Lemma A4, the existence of the matrix C_{d^*} in part (b) implies that (A_{d^*}, B_{d^*}) is regular. So by Lemma A6,

$$\psi_f(C_{d^*}) = M_f(A_{d^*}, B_{d^*}) \text{ for any type 2 criterion } \psi_f. \tag{A3}$$

For any $d \in \mathcal{D}$, there are five possible cases:

(i) $A_d = A_{d^*}$. Then (2.5) $\Rightarrow B_d \geqslant B_{d^*}$. Hence we may assume $B_d > B_{d^*}$. Then Lemma A9 $\Rightarrow \psi_f(C_d) \geqslant M_f(A_{d^*}, B_d) > M_f(A_{d^*}, B_{d^*}) = \psi_f(C_{d^*})$.

(ii) $A_d < A_{d^*}(A_d, B_d)$ is regular, and $P_{d^*} \geqslant P_d$.

In this case, $\exists n^* \in [1, v-2]$ s.t. $\psi_f(C_d) \geqslant F(n^*; A_d, B_d)$. On the other hand, $\psi_f(C_{d^*}) = F(v-2; A_{d^*}, B_{d^*}) \leqslant F(n^*; A_{d^*}, B_{d^*})$. Now, compare $F(n^*; A_d, B_d)$ with $F(n^*; A_{d^*}, B_{d^*})$. Since f is strictly decreasing, it is easily seen that $\psi_f(C_d) > \psi_f(C_{d^*})$ in case (ii) if

$$\text{(A4)} \quad A_d - \left[(v-1-n^*)^{-1} n^*(v-1)\right]^{\frac{1}{2}} P_d \leqslant A_{d^*} - \left[(v-1-n^*)^{-1} n^*(v-1)\right]^{\frac{1}{2}} P_{d^*}.$$

Now, (2.5) $\Rightarrow A_{d^*} - A_d \geqslant [(v-1)(v-2)]^{\frac{1}{2}}(P_{d^*} - P_d) \geqslant [(v-1-n^*)^{-1}n^*(v-1)]^{\frac{1}{2}}(P_{d^*} - P_d)$, where the last inequality follows from $(v-1)(v-2) \geqslant (v-1-n^*)^{-1}n^*(v-1)$ and $P_{d^*} \geqslant P_d$. This gives (A4).

(iii) $A_d < A_{d^*}$, (A_d, B_d) is regular, and $P_{d^*} < P_d$.

Then $\exists n^* \in [1, v-2]$ s.t. $R_2(n^*; A_d, B_d) > 0$ and

$$\begin{aligned}\psi_f(C_d) &\geqslant F(n^*; A_d, B_d) > F(n^*; A_d, B_{d^*}) \text{ (by Lemma A3(i))} \\ &> F(n^*; A_{d^*}, B_{d^*}) \text{ (by Lemma A3(ii))} \\ &\geqslant F(v-2; A_{d^*}, B_{d^*}) \text{ (by Lemma A3(iv))} \\ &= \psi_f(C_{d^*}).\end{aligned}$$

(iv) $A_d < A_{d^*}$, (A_d, B_d) is singular, and $A_d < A_{d^*} - [(v-1)(v-2)]^{\frac{1}{2}} P_{d^*}$.

Then

$$\begin{aligned}\psi_f(C_d) &\geqslant M_f(A_d, B_d) \\ &\geqslant M_f\big(A_d, A_d^2/(v-1)\big) \text{ (by Lemma A9)} \\ &= (v-2)f(A_d/(v-1)) + f(A_d/(v-1)) \\ &> (v-2)f(A_{d^*}/(v-1)) + f\Big(\big(A_{d^*} - \left[(v-1)(v-2)\right]^{\frac{1}{2}} P_{d^*}\big)/(v-1)\Big) \\ &> \psi_f(C_{d^*}).\end{aligned}$$

The last two inequalities follow from the fact that f is strictly decreasing.

(v) $A_d < A_{d^*}$, (A_d, B_d) is singular, and $A_d \geqslant A_{d^*} - [(v-1)(v-2)]^{\frac{1}{2}} P_{d^*}$.

By Lemma A4, we have

$$\text{(A5)} \qquad A_{d^*} > \left[(v-1)(v-2)\right]^{\frac{1}{2}} P_{d^*}.$$

Hence $A_d = A_{d^*} - (A_{d^*} - A_d) > (v-1)^{\frac{1}{2}}(v-2)^{\frac{1}{2}} P_{d^*} - (A_{d^*} - A_d) \geqslant 0$. Therefore $A_d^2 > \{[(v-1)(v-2)]^{\frac{1}{2}} P_{d^*} - (A_{d^*} - A_d)\}^2$, which implies

$$\text{(A6)} \qquad A_d^2/(v-2) > A_d^2/(v-1) + \left\{\left[(v-1)(v-2)\right]^{\frac{1}{2}} P_{d^*} - (A_{d^*} - A_d)\right\}^2 (v-1)^{-1}(v-2)^{-1}.$$

Choose a number B' such that

$$\text{(A7)}\qquad A_d^2/(v-2) > B' > A_d^2/(v-1) + \left\{[(v-1)(v-2)]^{\frac{1}{2}}P_{d^*} - (A_{d^*} - A_d)\right\}^2 (v-1)^{-1}(v-2)^{-1}.$$

Then (A_d, B_d) is singular $\Rightarrow B_d > B'$. Hence by Lemma A9, $\psi_f(C_d) \geq M_f(A_d, B_d) > M_f(A_d, B')$. Now (A_d, B') is regular, and (A7) $\Rightarrow A_{d^*} - A_d > (v-1)^{\frac{1}{2}}(v-2)^{\frac{1}{2}}\{P_{d^*} - [B' - A_d^2/(v-1)]^{\frac{1}{2}}\}$. Thus, the proof is reduced to case (ii) and (iii).

For the proof of part (a), we replace $A_d < A_{d^*} - [(v-1)(v-2)]^{\frac{1}{2}}P_{d^*}$ by $A_d < A_d{}^* - [(v-1)/(v-2)]^{\frac{1}{2}}P_{d^*}$ in (iv), and make similar changes in (v). Then instead of (A6), we need

$$\text{(A8)}\qquad A_d^2/(v-2) > A_d^2/(v-1) + (v-1)^{-1}(v-2) \times \left\{[(v-1)/(v-2)]^{\frac{1}{2}}P_{d^*} - (A_{d^*} - A_d)\right\}^2$$

or, equivalently,

$$\text{(A9)}\qquad A_d > [(v-1)(v-2)]^{\frac{1}{2}}P_{d^*} - (v-2)(A_{d^*} - A_d).$$

Now, (2.2) $\Rightarrow$ (A 5). Therefore, $A_d \geq A_{d^*} - (v-2)(A_d{}^* - A_d) > [(v-1)(v-2)]^{\frac{1}{2}}P_{d^*} - (v-2)(A_{d^*} - A_d)$, which gives (A9). □

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