ON THE HIERARCHICAL TWO-RESPONSE (CYCLIC PBIB) DESIGNS, COSTWISE OPTIMAL UNDER THE TRACE CRITERION

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1. Summary

Consider a general incomplete two-response design. Let S_1, S_2 and S_{12} be possible sets of units on which respectively, only response V_1, only response V_2, and both responses V_1 and V_2, are to be measured. Further suppose that under each of the two sets $(S_1 \cup S_{12})$ and $(S_2 \cup S_{12})$, a cyclic PBIB type of block-treatment design is going to be used. Then under a suitable cost restriction, and under the trace criterion for the comparison of designs, it is shown that the optimal two-response design will be such that at least one (and in most cases, only one) of the sets S_1 and S_2 would be empty. Also, methods are given to obtain the optimal design itself.

2. Introduction

Consider an experimental situation with p responses $(V_1, \cdots, V_p)$, v treatments $(\tau_1, \cdots, \tau_v)$ and a set S^* of experimental units, where the multiresponse design is possibly incomplete in the sense that all responses may not necessarily be measured on each experimental unit. Let $S^*(i_1, \cdots, i_k)$ denote the subset of S^* on each element of which the responses $V_{i_1}, \cdots, V_{i_k}$ (and these alone) are measured. Thus $U_r^* = \{S^*(i_1, \cdots, i_k) \mid r \in (i_1, \cdots, i_k)\}$ is the set of all units on which V_r is measured (alone or possibly with other responses). In a previous paper (Srivastava and McDonald [9]), heretofore, called paper I, the case where the sets $S^*(i_1, \cdots, i_k)$ are divided into randomized blocks (of v units each) was studied. However, if v is large, or if respect to any response (say V_r) there is a great deal of heterogeneity present in the experimental material, then as in the classical (univariate) experimental design theory, it would be advisable to use incomplete block designs rather than randomized blocks.

In paper I, it was shown that for the randomized block case, the hierarchical multiresponse (HM) (i.e. those where $U_1^* \supseteq \cdots \supseteq U_p^*$) designs are optimum in the general class of incomplete multiresponse designs, and a method of finding the optimal design was developed. In this paper, we develop a similar theory for the case when the designs defined on the set $S^*(i_1, \cdots, i_k)$ are cyclic PBIB designs of a very general type. This system of PBIB designs is very flexible in the sense that designs exist (in the combinatorial sense) for any given block size we wish. Also the number of replications of any treatment equals the block size, and therefore is not too large (unlike the BIB design in general). Of course, one could think of developing a theory of optimal multiresponse designs, where the designs on the sets $S^*(i_1, \cdots, i_k)$ are different from randomized block or cyclic PBIB designs. But this seems to necessarily involve complex combinatorial existential problems which we cannot discuss here for lack of space. Indeed, when $p>2$, even the cyclic PBIB gives rise to such difficulties, since the general incomplete multiresponse (GIM) design loses its structural balance. This paper is therefore restricted to $p=2$. Although the basic problem here is similar to that in paper I, the development is quite different. Here, the complexity arises not because of large p, but because the basic design used, viz. cyclic PBIB is mathematically more complex than the randomized blocks.

The notation is similar to that in paper I. Thus, under any design D, $\psi(D)$ denotes the associated 'cost'. A rival design D^* is at least as good as D, if $\psi(D^*) \leqq \psi(D)$ *and* $Q(D^*) \leqq Q(D)$; D^* is 'better' if one of the inequalities is strict. Here

$$Q(D) = \text{trace}\,[\text{Var}\,(P\hat{\boldsymbol{\tau}}^*)]\,, \tag{2.1}$$

where $\boldsymbol{\tau}^* = (\boldsymbol{\tau}_1', \cdots, \boldsymbol{\tau}_p')$, $\boldsymbol{\tau}_r' = (\tau_{r1}, \cdots, \tau_{tv})$, τ_{rj} denotes the true effect of τ_j on V_r, $\hat{\boldsymbol{\tau}}^*$ is the best linear unbiased estimate of $\boldsymbol{\tau}^*$ under the design, and P is a $p(v-1) \times pv$ matrix given by

$$P = \text{diag}\,(P_1, P_2, \cdots, P_p)\,, \tag{2.2}$$

where, for every r, $P_r(\overline{v-1} \times v)$ is an orthonormal matrix for which the sum of the elements in every row in zero.

The designs discussed in this paper should be useful in situations where the heterogeneity in the experimental material and/or the number of treatments is large, and where the measuring costs for the two responses (or the associated variances) differ appreciably from one another.

3. Determination of Q for certain response-wise incomplete cyclic PBIB designs

Consider the following cyclic PBIB design with v blocks and v treatments ($\tau_1, \cdots, \tau_v$ say).

(3.1) Blocks

I	1	2	3	$\cdots$	$(v-1)$	v
II	2	3	4	$\cdots$	v	1
III	3	4	5	$\cdots$	1	2
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\cdots$	$\vdots$	$\vdots$
V	v	1	2	$\cdots$	$(v-2)$	$(v-1)$

Suppose that two responses, V_1 and V_2, are under study. Measure only V_1 on the first k_1 columns, both V_1 and V_2 on the next k columns and finally only V_2 on the next k_2 columns, where $2 \leqq k_r + k \leqq v$, $(r=1, 2)$, and $k_1+k+k_2 \leqq v$. Let $D=D(k_1, k, k_2)$ denote the above "response-wise incomplete" and "treatment-wise incomplete" design. The first (k_1+k) columns of (3.1) constitute a PBIB design (say D_1) for response V_1, and the last $(k+k_2)$ columns form a PBIB design D_2 for response V_2. Thus D_r $(r=1, 2)$ provides $(k+k_r)$ $(=\rho_r$, say) replications of the set of v treatments. Assume that for both D_1 and D_2, the jth associates of an element $x \in \{1, \cdots, v\}$ are $x \pm j$ (mod v). For odd v, there are $((v-1)/2+1)$ associate classes with, respectively, $n_0=1$, $n_1=\cdots=n_{(v-1)/2}=2$ elements; and for v even, there are $(v/2+1)$ classes with, respectively, $n_0=1$, $n_1=\cdots=n_{(v/2-1)}=2$, $n_{v/2}=1$ elements. Further, if any two treatments are jth associates under the design D_r, they occur together in exactly $\lambda_{r,j}$ blocks, where

$$(3.2) \qquad \lambda_{r,j}=\begin{cases} \rho_r-\min(j, \rho_r); & \rho_r=1, \cdots, (v-1)/2, \\ \rho_r-\min(j, v-\rho_r); & \rho_r=(v+1)/2, \cdots, v; \end{cases}$$

if v is odd; and

$$(3.3) \qquad \lambda_{r,j}=\begin{cases} \rho_r-\min(j, \rho_r); & \rho_r=1, \cdots, (v/2)-1; \\ \rho_r-\min(j, v-\rho_r); & \rho_r=(v/2), \cdots, v; \end{cases}$$

if v is even.

Consider now response V_1 ignoring V_2. The estimate $\hat{\boldsymbol{\tau}}_1$ of $\boldsymbol{\tau}_1$ under D_1 is given by the reduced normal equations $C_1\hat{\boldsymbol{\tau}}_1=\boldsymbol{Q}_1$, where (following the notation of Kempthorne ([1], p. 80), $\boldsymbol{Q}_1$ $(v \times 1)$ is the vector of adjusted yields, and C_1 $(v \times v)$ is a symmetric matrix of rank $v-1$ each row of which sums to zero. Also the (α, β) element $(\alpha, \beta=1, \cdots, v)$ of $C_1=((C_{1\alpha\beta}))$ is given by

$$(3.4) \qquad C_{1\alpha\alpha}=\rho_1-1; \quad C_{1\alpha\beta}=-(\rho_1^{-1})\lambda_{1\alpha\beta} \qquad (\alpha \neq \beta;\ \alpha, \beta=1, 2, \cdots, v),$$

where $\lambda_{1\alpha\beta}=\lambda_{1j}$ if $|\alpha-\beta| \equiv j$ (mod v). The matrix C_2 $(v \times v)$ corresponding to V_2 is similarly defined with the suffix 1 replaced by 2. Now, from (2.1), we have

$$Q(D)=\text{tr}\,(\text{Var}\,(P_1\hat{\tau}_1))+\text{tr}\,(\text{Var}\,(P_2\hat{\tau}_2)) \\ =\sigma_{11}\,\text{tr}\,(P_1C_1^{\dagger}P_1')+\sigma_{22}\,\text{tr}\,(P_2C_2^{\dagger}P_2')\,, \tag{3.5}$$

where σ_{rr} $(r=1, 2)$ is the variance (for response V_r) of the observation on any experimental unit, and where $C_r^{\dagger}=C_r^*C_rC_r^*$, C_r^* being a conditional inverse of C_r (i.e. C_r^* is any symmetrical matrix such that $C_rC_r^*C_r=C_r$). The following lemma can be easily established.

LEMMA 3.1. *If θ_{rj} $(r=1, 2)$ denotes the jth largest root of C_r, then*

$$\text{tr}\,(P_1C_1^{\dagger}P_1')=\sum_{j=1}^{v-1}\theta_{1j}^{-1}\,, \tag{3.6}$$

and

$$Q(D)=\sigma_{11}\sum_{j=1}^{v-1}\theta_{1j}^{-1}+\sigma_{22}\sum_{j=1}^{v-1}\theta_{2j}^{-1}\,. \tag{3.7}$$

The next step in the evaluation of $Q(D)$ is to find the θ_{1j} and θ_{2j}. Consider C_1, which is a circulant matrix in view of (3.4). Hence the roots θ_{1j} $(j=1,\cdots, v)$ of C_1 are given by

$$\theta_{1j}=\begin{cases} (\rho_1-1)-\rho_1^{-1}[\lambda_{11}(w_j+w_j^{v-1})+\cdots \\ \qquad +\lambda_{1(v-1)/2}(w_j^{(v-1)/2}+w_j^{(v-1)/2+1})]\,, & v \text{ odd}\,, \\ (\rho_1-1)-\rho_1^{-1}[\lambda_{11}(w_j+w_j^{v-1})+\cdots \\ \qquad +\lambda_{1,(v/2-1)}(w_j^{(v/2-1)}+w_j^{(v/2+1)})+\lambda_{1,v/2}w_j^{v/2}]\,, & v \text{ even}\,; \end{cases} \tag{3.8}$$

where w_j $(j=1,\cdots, v)$ denotes the v distinct vth roots of unity. Four cases arise. In case I, assume that v is odd and $0\leqq\rho_1\leqq(v-1)/2$. Here we have

$$\lambda_{l1}=\begin{cases} \rho_1-l\,, & l=1,\cdots, (v-\rho_1) \\ 2\rho_1-v\,, & l=(v-\rho_1+1),\cdots, (v-1)/2\,, \end{cases} \tag{3.9}$$

and

$$w_j^l+w_j^{v-l}=2\cos\,(2\pi jl/v)\,, \\ (j=1,\cdots, v-1\,;\ l=1,\cdots, (v-1)/2)\,. \tag{3.10}$$

Thus, for $j=1,\cdots, v-1$, we have

$$\theta_{1j}=(\rho_1-1)-2\rho_1^{-1}\left[\sum_{l=1}^{v-\rho_1}(\rho_1-l)\cos\,(l\alpha_j)-\sum_{l=v-\rho_1+1}^{(v-1)/2}(2\rho_1-v)\cos\,(l\alpha_j)\right]; \tag{3.11}$$

where $\alpha_j=2\pi j/v$. The following identities are well known:

(3.12) $$\sum_{l=1}^{n} \cos l\alpha = \frac{\cos((n+1)\alpha/2)\sin(n\alpha/2)}{\sin(\theta/2)},$$

(3.13) $$\sum_{l=1}^{n-1} l \cos l\alpha = \frac{n \sin((2n-1)\theta/2)}{2\sin(\theta/2)} - \frac{1-\cos(n\theta)}{4\sin^2(\theta/2)}.$$

Using these identities, (3.11) simplifies to (for $j=1,\cdots,v-1$):

(3.14) $$\theta_{1j} = \rho_1^{-1}\left[\rho_1^2 - \frac{1-\cos(\rho_1\alpha_j)}{1-\cos(\alpha_j)}\right] = f(\rho_1, j), \qquad \text{say.}$$

For the other cases (i.e., v odd and $\rho_1 > (v-1)/2$, and also v even), it can be checked that the above procedure leads to equation (3.14) again, as the formula for the $(v-1)$ nonzero roots of C_1. By the interchange of ρ_1 and ρ_2 we obtain the $(v-1)$ nonzero roots θ_{2j} of C_2. Thus, if $f(x, j)$ is defined by (3.14) by replacing ρ_1 by x $(x=2, 3, \cdots, v)$, then (3.1) gives

(3.15) $$Q(D) = \sigma_{11}G(\rho_1) + \sigma_{22}G(\rho_2),$$

where

(3.16) $$G(x) = \sum_{j=1}^{v-1} [f(x, j)]^{-1}.$$

For facility in obtaining the optimum design (see Sec. 3), the function $G(x)$, $(x=1, 2, 3, \cdots, 10, 12, 14, \cdots, v)$, $(v=1, 2, 3, \cdots, 18, 21, 24, \cdots, 45)$ is tabulated in Appendix I. For other values of v and x in this range, a good approximation can be obtained using a 4-point interpolation formula.

4. Optimality of the HM designs

Assume now that the 'cost' associated with the GIM design $D_0 = D(k_1, k, k_2)$ has the structure

(4.1) $$\psi(D_0) = \psi_0(k_1+k+k_2) + \psi_1(k_1+k) + \psi_2(k_2+k),$$

where ψ_0 is the overhead cost of including one column of v experimental units in the experiment and ψ_r, $(r=1, 2)$, is the additional cost of measuring response V_r on the experimental units of one column. We proceed to compare D_0 with the hierarchical design $D^* = D(k_1-k_2, k+k_2, 0)$ where we assume (without loss of generality) that $k_2 \leq k_1$. Recalling from (3.15) the value of $Q(D)$ for any design D, we notice that $Q(D_0) = Q(D^*)$. Since $\psi(D_0) - \psi(D^*) = \psi_0 k_2 \geq 0$, it is clear that D^* is at least as good as D_0. This shows that the subclass of HM designs is complete within the class of GIM designs. The main problem now is to find the optimal HM design D^* for which $\psi(D^*) = \psi'$ (a fixed positive number), and $Q(D^*)$ is a minimum. An investigation into this problem involves the following result concerning matrices, which is also of interest in the general theory of experimental designs.

THEOREM 4.1. *Let H_1 and H_2 be $(n\times n)$ symmetric matrices, which are respectively positive and non-negative definite. Also, for any matrix B given below, let $\phi(B)$ be defined by*

$$B=\begin{bmatrix} B_1 & B_2 \\ B_3 & B_4 \end{bmatrix}, \qquad \phi(B)=B_1-B_2B_4^{-1}B_3\,, \tag{4.2}$$

where B is $(n\times n)$, B_1 is $(n-m)\times(n-m)$, where $n>m$, and B_4 $(m\times m)$ is nonsingular. Let

$$\begin{aligned} \phi_1(H_1, H_2)&=[\phi(H_1)]^{-1}-[\phi(H_1+H_2)]^{-1}\,, \\ \phi_2(H_1, H_2)&=[\phi(H_1)]^{-1}-2[\phi(H_1+H_2)]^{-1}+[\phi(H_1+2H_2)]^{-1}\,. \end{aligned} \tag{4.3}$$

Then $\phi_1(H_1, H_2)$ and $\phi_2(H_1, H_2)$ are positive semidefinite.

PROOF. Define $\phi_1^*=H_1^{-1}-(H_1+H_2)^{-1}$ and $\phi_2^*=H_1^{-1}-2(H_1+H_2)^{-1}+(H_1+2H_2)^{-1}$. Since, $\phi_i(H_1, H_2)$ is a principal submatrix of ϕ_i^* $(i=1, 2)$, the result will be proved if the ϕ_i^* are both p.s.d. Now, there exists a nonsingular matrix T such that $H_i=TE_iT'$, where E_i are diagonal matrices with non-negative elements, and E_1 is nonsingular. Hence, putting $\Delta_1=E_1^{-1}-(E_1+E_2)^{-1}$, and $\Delta_2=E_1^{-1}-2(E_1+E_2)^{-1}+(E_1+2E_2)^{-1}$, we have $\phi_i^*=T'^{-1}\Delta_iT^{-1}$. Thus it is enough to show that the Δ_i are p.s.d. However, if e_{ji} and δ_{ji} respectively represent the jth diagonal element of E_i and Δ_i for $(i=1, 2)$, then $\delta_{j1}=e_{j1}^{-1}-(e_{j1}+e_{j2})^{-1}$, $\delta_{j2}=e_{j1}^{-1}-2(e_{j1}+e_{j2})^{-1}+(e_{j1}+2e_{j2})^{-1}$. Thus $\delta_{j1}\geqq 0$, $\delta_{j2}\geqq 0$, and the proof is completed.

Consider now one response, and three disjoint sets U_i $(i=1, 2, 3)$ of experimental units. Here all units of all sets are assumed mutually independent, and any observation on any unit has the same variance σ^2. Let U_i give rise to a vector of (independent) observations $\boldsymbol{y}_i$, and let

$$\mathrm{E}(\boldsymbol{y}_1)=A_1\boldsymbol{\tau}^*+A_2\boldsymbol{\beta}^*\,, \qquad \mathrm{E}(\boldsymbol{y}_2)=\mathrm{E}(\boldsymbol{y}_3)=A_3\boldsymbol{\tau}^*+A_4\boldsymbol{\beta}^*\,, \tag{4.4}$$

where $\boldsymbol{\tau}^*$ and $\boldsymbol{\beta}^*$ are unknown parameters, which without any essential loss of generality can be assumed to be estimable from $\boldsymbol{y}_i$. Let $U_1^*=U_1$, $U_2^*=U_1+U_2$, $U_3^*=U_1+U_2+U_3$; where + denotes union. Let $\hat{\boldsymbol{\tau}}_i^*$ denote the best linear unbiased estimate of $\boldsymbol{\tau}^*$ obtained from the observations on the units in U_i^* $(i=1, 2, 3)$. Then W_i, the variance-matrix of $\hat{\boldsymbol{\tau}}_i^*$ is given by $W_i=[\phi(H_i^*)]^{-1}$, where $H_1^*=H_1$, $H_2^*=H_1+H_2$, and $H_3^*=H_1+2H_2$, and where

$$H_1=\begin{bmatrix} A_1'A_1 & A_1'A_2 \\ A_2'A_1 & A_2'A_2 \end{bmatrix}, \qquad H_2=\begin{bmatrix} A_3'A_3 & A_3'A_4 \\ A_4'A_3 & A_4'A_4 \end{bmatrix}. \tag{4.5}$$

In this context, Theorem 4.1 tells us that the matrices ϕ_i, where $\phi_1 = (W_1 - W_2)$ and $\phi_2 = [(W_1 - W_2) - (W_2 - W_3)]$ are both positive definite. Now $W_1 - W_2$, and $(W_2 - W_3)$ can be interpreted as the "decrease in the variance" due to the addition of U_2 or U_3. (Note that U_2 and U_3 are, in view of (4.4), 'equivalent' sets of units.) Thus ϕ_1 being p.s.d. means "variance decreases" by the addition of U_2, and ϕ_2 p.s.d. implies that 'variance' has the 'convexity property' in the generalized sense that the 'decrease in variance' is 'more' at the first addition of U_2, than at the next addition of the equivalent set of units U_3.

Notice that ϕ_1 being p.s.d. implies $\operatorname{tr} W_1 \geqq \operatorname{tr} W_2$. Recalling the definition of $G(x)$ from (3.16), this gives

$$G(x) \geqq G(x+1), \qquad x = 2, 3, \cdots, v-1. \tag{4.6}$$

Again, suppose in the above discussion, we let the first x columns of (3.1) correspond to U_1, the $(x+1)$th column to U_2, and the $(x+2)$th column to a *new* set U_3'. Notice that U_2^* would then involve the first $(x+1)$ columns, and U_3^* will be U_2^* with the $(x+1)$th column occuring twice. Let U_3^{**} correspond to the first $(x+2)$ columns. Assume there is only one response. Let Γ_1 and Γ_2 respectively be the covariance matrix $\operatorname{Var}(P_1\hat{\tau}_1)$ based on the designs U_3^* and U_3^{**}. Then (recall (3.14)) $[f(x+2, j)]^{-1}$ is the jth root of Γ_2. Also, correspondingly the jth root of Γ_1 is $[f^*(x+2), j)]^{-1}$ where

$$f^*(x+2, j) = (x+2) - (x+2)^{-1}\lambda_{2j} \tag{4.7}$$

$$\lambda_{2j} = 2 + \frac{\sin[(x+1/2)\alpha_j]}{\sin(\alpha_j/2)} + \frac{1-\cos[(x+1)\alpha_j]}{2\sin^2(\alpha_j/2)} \tag{4.8}$$

with $\alpha_j = 2\pi j/v$. A proof of this is out of place here, and would be found in McDonald [3]. Thus it is easily checked that $[f(x+2, j)]^{-1} \leqq [f^*(x+2, j)]^{-1}$, for all permissible j. This shows that our method of using a new column is better than repeating the same column more than once.

Furthermore, we now show that U_3^{**} (like U_3^*) also has a kind of convexity property.

THEOREM 4.2. *Let* $h(x, j) = (1-\cos\alpha_j)f(x, j)$, *where* $\alpha_j = 2\pi j/v$; $j = 1, 2, \cdots, v-1$; *and* $x = 2, 3, \cdots, v$. *Then for all permissible* x *and* j, *we have*

$$[h(x, j)]^{-1} - [h(x+1, j)]^{-1} \geqq [h(x+1, j)]^{-1} - [h(x+2, j)]^{-1}. \tag{4.9}$$

PROOF. Let $\zeta_1(x) = h(x+2, j)[h(x+1, j) - h(x, j)]$, $\zeta_2(x) = h(x, j)[h(x+2, j) - h(x+1, j)]$, and $\zeta_3(x) = \zeta_1(x) - \zeta_2(x)$. Then it is enough to show that $\zeta_3(x) \geqq 0$. Let $\cos\alpha_j = c$, $\sin\alpha_j = s$, $\cos\alpha_j(x+1) = c_1$, and $\sin\alpha_j(x+1) = s_1$; and $\zeta_4(x) = (1/2)x(x+1)\zeta_3(x)$. Then it can be checked that

$$\begin{aligned}(4.10)\qquad \zeta_4(x)&=(1-c)(1-c_1)x^2(x+2)(x+1)^{-1}+(1+c_1)(1-c)^2x(x+2)\\&\quad+(1-c_1^2)+(1-c^2)+(1-cc_1)(2-c_1-3c)\\&\quad-3ss_1(1-c)(x+1)-ss_1(1-c_1)(x+1)^{-1}.\end{aligned}$$

Note that $\zeta_4(0)=0$. Thus it is enough to show that $\zeta_5(x)\geqq 0$, where $\zeta_5(x)=\zeta_4(x+1)-\zeta_4(x)$, for $x=0,\cdots,v-3$. Putting $\varepsilon_x=(x+1)^{-1}(x+2)^{-1}$ we find

$$\begin{aligned}(4.11)\qquad \zeta_5(x)&=(1-c)(1-c_1)[(2x+2)-\varepsilon_x]+(1+c_1)(1-c)^2(2x+3)\\&\quad+ss_1(1-c_1)\varepsilon_x-3ss_1(1-c).\end{aligned}$$

We consider three cases. In case 1, assume $ss_1=0$; then clearly $\zeta_5(x)\geqq 0$. In case 2, assume $ss_1<0$. The only negative term in $\zeta_5(x)$ is $ss_1(1-c_1)\varepsilon_x$. Let

$$\begin{aligned}(4.12)\qquad \zeta_6(x)&=(1-c)^{-1}(1-c_1)^{-1}\zeta_5(x)\\&=(2x+2-\varepsilon_x)+(2x+3)(1+c_1)(1-c)/(1-c_1)\\&\quad-3[ss_1/(1-c_1)]+\varepsilon_x ss_1/(1-c).\end{aligned}$$

Now $|\varepsilon_x ss_1/(1-c)|\leqq|\varepsilon_x\sin 2(x+1)\gamma_j(\sin\gamma_j)^{-1}|$, where $\gamma_j=\pi j/v$. Since $|(\sin u\theta)(\sin\theta)^{-1}|\leqq u$ when u is positive, we have $|\varepsilon_x ss_1(1-c)^{-1}|\leqq\varepsilon_x 2(x+1)$. Thus $\zeta_6(x)\geqq(2x+2)-\varepsilon_x-\varepsilon_x(2x+2)>0$. In the third and final case, assume $ss_1>0$. Consider

$$\begin{aligned}(4.13)\qquad \zeta_7(x)&=(2x+3)(1+c_1)(1-c)(1-c_1)^{-1}-3ss_1(1-c_1)^{-1}\\&=(2x+3)(1-c)u^2-3su,\end{aligned}$$

where $u=\cot(x+1)\pi j/v$. Consider $\zeta_7(x)$ as a function of u and call it $\zeta_7^*(u)$. Differentiating $\zeta_7^*(u)$ with respect to u, we find that $\zeta_7^{*\prime}(u)=2(2x+3)(1-c)u-3s=0$ implies that $u=u_0$ (say)$=3s/2(2x+3)(1-c)$. Secondly, $\zeta_7^{*\prime\prime}(u_0)=2(2x+3)(1-c)\geqq 0$, so the minimum value of $\zeta_7^*(u)$, under variation of u, is $\zeta_7^*(u_0)=-9s^2/4(2x+3)(1-c)=[-9\cos^2\gamma_j]/[2(2x+3)]$. Now $\zeta_5(x)\geqq(2x+2)-\varepsilon_x-9\cos^2\gamma_j/2(2x+3)\geqq(2x+2)-\varepsilon_x-9/2(x+3)$. Thus $\zeta_5(x)\geqq 0$ for $x=0,1,2,\cdots,v$. This completes the proof.

We now return to the problem of the determination of the optimum HM design assuming that the variances σ_{11} and σ_{22} are known (or good estimates are available) and that ψ_0,ψ_1,ψ_2 are given. The problem is to find the design $D^*=D(k_1,k,k_2)$ which minimizes Q, defined in equation (3.15), subject to the linear constraints $2\leqq k_r+k$, $(r=1,2)$, $k_1+k_2+k\leqq v$ and $\psi(D^*)\leqq\psi'$, where ψ' is the total capital available for conducting the experiment. Since the subclass of HM designs is complete the procedure will be to evaluate Q for the optimum HM design of the type $D(k_1,k,0)$ and compare it with Q evaluated for the optimum design of the type $D(0,k,k_2)$. In what follows, we let

(4.14) $$\gamma_1=\psi_0+\psi_1\,,\qquad \gamma_2=\psi_0+\psi_2\,,\qquad \gamma_{12}=\psi_0+\psi_1+\psi_2\,,$$

and denote by $[x]$, the largest integer less than or equal to x. Also, to avoid unessential complications, we make the (mild) assumption that $N=\psi'/\gamma_{12}$ is an integer.

Two cases arise. Under case I, assume $k_2=0$. Now $k\leqq N$. Let $N-k=m$, then $k_1=m+[m\psi_2/\gamma_1]$. For any given m, denote the corresponding HM design D by $D_{1,m}$. The problem is to find the optimum value of m. Since the optimum HM design must be connected with respect to response V_2, we must have $\rho_2=k\geqq 2$. Thus the admissible values of m are $m=0, 1,\cdots, N-2$.

Now

(4.15) $$Q(D_{1,m})=\sigma_{11}G(N+[m\psi_2/\gamma_1])+\sigma_{22}G(N-m)\,.$$

Thus $Q(D_{1,m})\leqq Q(D_{1,m+1})$, if and only if

(4.16) $$\frac{\sigma_{22}}{\sigma_{11}}\geqq\frac{G(N+[m\psi_2/\gamma_1])-G(N+[(m+1)\psi_2/\gamma_1])}{G(N-(m+1))-G(N-m)}=\beta_{1,m}\,,\qquad \text{(say)}.$$

Now consider subcase Ia where $\psi_2/\gamma_1\geqq 1$. Here $[(m+1)\psi_2/\gamma_1]-[m\psi_2/\gamma_1]\geqq 1$. Hence by (4.6) and (4.9), $\beta_{1,m}$ is a monotone decreasing function of m and

(4.17) $$\max_m \beta_{1,m}=\beta_{1,0}=\frac{G(N)-G(N+[\psi_2/\gamma_1])}{G(N-1)-G(N)}\,.$$

Hence if $\sigma_{22}/\sigma_{11}\geqq\beta_{1,0}$, then $D_{1,0}=D(0, N, 0)$ is optimum. If $\sigma_{22}/\sigma_{11}<\beta_{1,0}$ then $D_{1,m_0}=D(m_0+[m_0\psi_2/\gamma_1], N-m_0, 0)$ is optimum where m_0 is the least value of m for which $\sigma_{22}/\sigma_{11}\geqq\beta_{1,m}$. If $\sigma_{22}/\sigma_{11}<\beta_{1,N-3}$ then $D_{1,N-2}$ is optimum. For subcase Ib, where $\psi_2/\gamma_1<1$ the procedure is more complicated since $\beta_{1,m}$ is no longer a monotone function of m. However, $[(m+1)\psi_2/\gamma_1]-[m\psi_2/\gamma_1]\leqq 1$. Thus when $[(m+1)\psi_2/\gamma_1]=[m\psi_2/\gamma_1]$, we have $\sigma_{22}/\sigma_{11}>\beta_{1,m}=0$, and $D_{1,m}$ is better than $D_{1,m+1}$. The procedure is to find the set M of values of $m=0, 1,\cdots, N-2$ such that $[(m+1)\psi_2/\gamma_1]-[m\psi_2/\gamma_1]=1$. Let $M=\{m_{i_1},\cdots, m_{i_l}\}$ where $m_{i_1}<m_{i_2}<\cdots<m_{i_l}$. By (4.6) and (4.9) $\beta_{1,m_{i_1}}\geqq\beta_{1,m_{i_2}}\geqq\cdots\geqq\beta_{1,m_{i_l}}$. If $\sigma_{22}/\sigma_{11}\geqq\beta_{1,m_{i_1}}$ or M is empty, then $D_{1,0}$ is optimum. If $\sigma_{22}/\sigma_{11}<\beta_{1,m_{i_1}}$ then find the smallest value of $m\in M$, (say) m_{i_h}, such that $\sigma_{22}/\sigma_{11}\geqq\beta_{1,m_{i_h}}$. If $\sigma_{22}/\sigma_{11}<\beta_{1,m_{i_l}}$ then set $h-1=l$ in the following. Evaluate Q for the designs $D_{1,m}$ corresponding to the values of m equal to $(m_{i_{h-1}}+1)$, $(m_{i_{h-2}}+1),\cdots, (m_{i_1}+1)$ and 0 and select the one for which Q is a minimum. Clearly, in practice this number $(h-1)$ should be expected to be small. Hence using Appendix I, the evaluation of Q and their comparison would be quite easy.

For case II, assume $k_1=0$. Subcases IIa ($\psi_1/\gamma_2\geqq 1$) and IIb ($\psi_1/\gamma_2<1$) arise as for case I. Exactly the same results as above, with the subscripts 1 and 2 interchanged, are applicable.

The procedure that suggests itself is to obtain the best design from each of cases I and II and compare Q calculated for each. Usually this procedure can be shortened.

If $\psi_2/\gamma_1<2$ and $\psi_1/\gamma_2<2$ (as will be the case in most applications), then by (4.6) and (4.9), all of the β's in cases I and II are less than 1. Thus if $\sigma_{22}/\sigma_{11}=1$, the optimum design is $D^*=D(0, N, 0)$. If $\sigma_{22}/\sigma_{11}<1$, then the optimum design will come from case I, while if $\sigma_{11}/\sigma_{22}<1$ the optimum design will come from case II.

If $\psi_2/\gamma_1\geqq 2$, but $\beta_{10}\leqq 1$, the same remarks as in the preceding paragraph are applicable. However if $\beta_{10}>1$, we must compare the optimum designs from each of cases I and II. A similar remark as above with the subscripts 1 and 2 interchanged is also applicable.

Example. We now illustrate the preceding theory using some artificial data. Suppose that $v=40$ varieties of wheat are to be compared with respect to two responses: V_1=total yield of grain in lbs. per acre and V_2=total yield, in terms of protein, in lbs. per acre. Assume that it is known from past experience that $\sigma_{11}=32{,}400$, $\sigma_{22}=3{,}600$, $\psi_1=40$, $\psi_2=600$, and $\psi_0=800$. Further assume that $\psi'=7{,}200$, so that if the SM design is used we will have $N=\psi'/\gamma_{12}=5$ replications of each variety. Now $\psi_2/\gamma_1=600/840<2$, $\psi_1/\gamma_2=40/1400<2$, and $\sigma_{22}/\sigma_{11}=.11<1$ so that the optimum design will come from case I (i.e., $k_2=0$). Also since $\psi_2/\gamma_1<1$ we are under subcase Ib. The admissible values of m such that $[(m+1)600/840]-[m600/840]=1$ are $m_{i_1}=1$ and $m_{i_2}=2$. From (4.16) and using Appendix I, we get $\beta_{1,1}=.157$ and $\beta_{1,2}=.017$. Thus $(\beta_{1,1}=.157)>(\sigma_{22}/\sigma_{11}=.11)>(\beta_{1,2}=.017)$, and we evaluate Q corresponding to $m=m_{i_1}+1=2$ and $m=0$. Using (4.15) and Appendix I, we have $Q(D_{1,0})=674{,}100$ and $Q(D_{1,2})=664{,}815$. Thus the optimum design is $D_{1,2}=D(3, 3, 0)$.

Appendix I

Values of the Function $G(x)$, $(x=1, 2, \cdots, 10, 12, 14, \cdots, V)$.

$V=3$	$G(2)=1.333$	$G(3)=.667$			
$V=4$	$G(2)=2.500$	$G(3)=1.125$	$G(4)=.750$		
$V=5$	$G(2)=4.000$	$G(3)=1.636$	$G(4)=1.067$	$G(5)=.800$	
$V=6$	$G(2)=5.833$	$G(3)=2.242$	$G(4)=1.399$	$G(5)=1.042$	$G(6)=.833$
$V=7$	$G(2)=8.000$	$G(3)=2.927$	$G(4)=1.761$	$G(5)=1.289$	$G(6)=1.029$
	$G(7)=.857$				
$V=8$	$G(2)=10.500$	$G(3)=3.696$	$G(4)=2.162$	$G(5)=1.549$	$G(6)=1.227$
	$G(7)=1.021$	$G(8)=.875$			
$V=9$	$G(2)=13.333$	$G(3)=4.549$	$G(4)=2.594$	$G(5)=1.827$	$G(6)=1.431$
	$G(7)=1.186$	$G(8)=1.016$	$G(9)=.889$		

$V=10$	$G(2)=16.500$	$G(3)=5.485$	$G(4)=3.059$	$G(5)=2.123$	$G(6)=1.643$
	$G(7)=1.354$	$G(8)=1.158$	$G(9)=1.013$	$G(10)=.900$	
$V=11$	$G(2)=20.000$	$G(3)=6.504$	$G(4)=3.558$	$G(5)=2.434$	$G(6)=1.866$
	$G(7)=1.527$	$G(8)=1.301$	$G(9)=1.137$	$G(10)=1.010$	
$V=12$	$G(2)=23.833$	$G(3)=7.607$	$G(4)=4.090$	$G(5)=2.763$	$G(6)=2.099$
	$G(7)=1.706$	$G(8)=1.447$	$G(9)=1.262$	$G(10)=1.121$	$G(12)=.917$
$V=13$	$G(2)=28.000$	$G(3)=8.793$	$G(4)=4.656$	$G(5)=3.108$	$G(6)=2.342$
	$G(7)=1.892$	$G(8)=1.597$	$G(9)=1.389$	$G(10)=1.232$	$G(12)=1.007$
$V=14$	$G(2)=32.500$	$G(3)=10.062$	$G(4)=5.255$	$G(5)=3.470$	$G(6)=2.593$
	$G(7)=2.084$	$G(8)=1.751$	$G(9)=1.518$	$G(10)=1.344$	$G(12)=1.098$
	$G(14)=.929$				
$V=15$	$G(2)=37.333$	$G(3)=11.415$	$G(4)=5.887$	$G(5)=3.848$	$G(6)=2.855$
	$G(7)=2.281$	$G(8)=1.910$	$G(9)=1.650$	$G(10)=1.458$	$G(12)=1.188$
	$G(14)=1.005$				
$V=16$	$G(2)=42.500$	$G(3)=12.851$	$G(4)=6.553$	$G(5)=4.243$	$G(6)=3.126$
	$G(7)=2.485$	$G(8)=2.072$	$G(9)=1.785$	$G(10)=1.573$	$G(12)=1.280$
	$G(14)=1.082$	$G(16)=.938$			
$V=17$	$G(2)=48.000$	$G(3)=14.370$	$G(4)=7.252$	$G(5)=4.655$	$G(6)=3.406$
	$G(7)=2.694$	$G(8)=2.239$	$G(9)=1.923$	$G(10)=1.691$	$G(12)=1.372$
	$G(14)=1.159$	$G(16)=1.004$			
$V=18$	$G(2)=53.833$	$G(3)=15.973$	$G(4)=7.984$	$G(5)=5.083$	$G(6)=3.696$
	$G(7)=2.909$	$G(8)=2.409$	$G(9)=2.064$	$G(10)=1.811$	$G(12)=1.465$
	$G(14)=1.236$	$G(16)=1.070$	$G(18)=.944$		
$V=21$	$G(2)=73.333$	$G(3)=21.281$	$G(4)=10.381$	$G(5)=6.468$	$G(6)=4.623$
	$G(7)=3.591$	$G(8)=2.944$	$G(9)=2.503$	$G(10)=2.183$	$G(12)=1.750$
	$G(14)=1.470$	$G(16)=1.271$	$G(18)=1.121$	$G(20)=1.003$	
$V=24$	$G(2)=95.833$	$G(3)=27.339$	$G(4)=13.078$	$G(5)=8.004$	$G(6)=5.636$
	$G(7)=4.327$	$G(8)=3.514$	$G(9)=2.966$	$G(10)=2.573$	$G(12)=2.047$
	$G(14)=1.710$	$G(16)=1.473$	$G(18)=1.298$	$G(20)=1.160$	$G(22)=1.050$
	$G(24)=.958$				
$V=27$	$G(2)=121.333$	$G(3)=34.147$	$G(4)=16.074$	$G(5)=9.689$	$G(6)=6.734$
	$G(7)=5.116$	$G(8)=4.120$	$G(9)=3.455$	$G(10)=2.982$	$G(12)=2.355$
	$G(14)=1.956$	$G(16)=1.680$	$G(18)=1.476$	$G(20)=1.319$	$G(22)=1.192$
	$G(24)=1.089$	$G(26)=1.001$			
$V=30$	$G(2)=149.833$	$G(3)=41.705$	$G(4)=19.371$	$G(5)=11.524$	$G(6)=7.918$
	$G(7)=5.958$	$G(8)=4.762$	$G(9)=3.969$	$G(10)=3.409$	$G(12)=2.672$
	$G(14)=2.210$	$G(16)=1.892$	$G(18)=1.658$	$G(20)=1.479$	$G(22)=1.336$
	$G(24)=1.219$	$G(26)=1.121$	$G(28)=1.038$	$G(30)=.967$	
$V=33$	$G(2)=181.333$	$G(3)=50.013$	$G(4)=22.968$	$G(5)=13.510$	$G(6)=9.188$
	$G(7)=6.854$	$G(8)=5.440$	$G(9)=4.508$	$G(10)=3.853$	$G(12)=3.000$
	$G(14)=2.470$	$G(16)=2.108$	$G(18)=1.843$	$G(20)=1.641$	$G(22)=1.481$
	$G(24)=1.350$	$G(26)=1.242$	$G(28)=1.149$	$G(30)=1.070$	$G(32)=1.001$
$V=36$	$G(2)=215.833$	$G(3)=59.071$	$G(4)=26.865$	$G(5)=15.645$	$G(6)=10.543$
	$G(7)=7.804$	$G(8)=6.153$	$G(9)=5.072$	$G(10)=4.316$	$G(12)=3.339$
	$G(14)=2.737$	$G(16)=2.328$	$G(18)=2.031$	$G(20)=1.805$	$G(22)=1.627$
	$G(24)=1.482$	$G(26)=1.362$	$G(28)=1.261$	$G(30)=1.174$	$G(32)=1.098$
	$G(34)=1.031$	$G(36)=.972$			
$V=39$	$G(2)=253.333$	$G(3)=68.879$	$G(4)=31.062$	$G(5)=17.930$	$G(6)=11.985$
	$G(7)=8.807$	$G(8)=6.902$	$G(9)=5.661$	$G(10)=4.798$	$G(12)=3.688$
	$G(14)=3.010$	$G(16)=2.553$	$G(18)=2.222$	$G(20)=1.972$	$G(22)=1.775$
	$G(24)=1.615$	$G(26)=1.484$	$G(28)=1.372$	$G(30)=1.277$	$G(32)=1.195$
	$G(34)=1.122$	$G(36)=1.058$	$G(38)=1.001$		

$V=42$	$G(2)=293.833$	$G(3)=79.437$	$G(4)=35.558$	$G(5)=20.365$	$G(6)=13.512$
	$G(7)=9.864$	$G(8)=7.687$	$G(9)=6.274$	$G(10)=5.297$	$G(12)=4.048$
	$G(14)=3.290$	$G(16)=2.782$	$G(18)=2.417$	$G(20)=2.141$	$G(22)=1.925$
	$G(24)=1.750$	$G(26)=1.606$	$G(28)=1.485$	$G(30)=1.381$	$G(32)=1.292$
	$G(34)=1.213$	$G(36)=1.144$	$G(38)=1.082$	$G(40)=1.026$	$G(42)=.976$
$V=45$	$G(2)=337.333$	$G(3)=90.745$	$G(4)=40.355$	$G(5)=22.951$	$G(6)=15.124$
	$G(7)=10.974$	$G(8)=8.508$	$G(9)=6.913$	$G(10)=5.815$	$G(12)=4.418$
	$G(14)=3.577$	$G(16)=3.015$	$G(18)=2.614$	$G(20)=2.312$	$G(22)=2.076$
	$G(24)=1.886$	$G(26)=1.729$	$G(28)=1.598$	$G(30)=1.486$	$G(32)=1.389$
	$G(34)=1.304$	$G(36)=1.229$	$G(38)=1.163$	$G(40)=1.103$	$G(42)=1.049$
	$G(44)=1.001$				

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