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OPTIMALITY OF BALANCED UNIFORM REPEATED MEASUREMENTS DESIGNS

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This paper continues the work of Hedayat and Afsarinejad (1978) and of Cheng and Wu (1980) on the optimality of balanced uniform repeated measurements designs. In addition to their well known optimality results over the class of designs which have no pairs of consecutive identical treatments, we compare the balanced uniform designs to all possible designs. Instances are given where they fail and where they succeed in being optimum.

1. Introduction. In repeated measurements designs, experimental units are exposed to a sequence of different or identical treatments. The experiment is based on t treatments, n experimental units and p periods, each unit being given one treatment during each period. The treatment applied to unit u during period k is determined by the repeated measurements design d and is called $d(k, u)$. The set of all such d is called $\Omega_{t,n,p}$. We measure the effect of the treatments by a random variable y. It is assumed that each measurement is influenced by an additive first-order residual effect of the treatment to which the unit under consideration has been exposed in the period before. (For details see Hedayat and Afsarinejad, 1975 and 1978.)

This paper deals with the optimality properties of balanced uniform designs. Hedayat and Afsarinejad (1978) and Cheng and Wu (1980) have shown that those designs are universally optimal over subclasses of $\Omega_{t,n,p}$ containing only designs d without pairs of consecutive identical treatments. Cheng and Wu (1980) have also shown that this restriction is essential. That is, if $p > t$ the optimal designs over $\Omega_{t,n,p}$ have pairs of identical treatments.

We deal with the situation where $t = p$. We show that, for the estimation of direct effects, balanced uniform designs d^* are universally optimal over $\Omega_{t,n,t}$ if $n = t$ or $2t$. If n is sufficiently large they are no longer optimal. For the estimation of residual effects, d^* can never be universally optimal over $\Omega_{t,2t,t}$ and cannot be universally optimal over $\Omega_{t,t,t}$, provided special other designs exist.

Formally, a repeated measurements design is a function d from $\{1, \cdots, p\} \times \{1, \cdots, n\}$ to $\{1, \cdots, t\}$. The observations are assumed to be uncorrelated with common variance and

$$E(y_{dku}) = \mu + \alpha_k + \beta_u + \tau_{d(k,u)} + \rho_{d(k-1,u)},$$

with $d(0, u) = 0$ and $\rho_0 = 0$, $1 \le k \le p$, $1 \le u \le n$. The unknown parameters have

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the following meanings (Cheng and Wu, 1980):

μ is the overall effect, α_k is the kth period effect, β_u is the uth unit effect, $\tau_{d(k,u)}$ is the direct effect of treatment $d(k, u)$ and $\rho_{d(k-1,u)}$ is the residual effect of treatment $d(k-1, u)$.

In vector notation we have

$$E(Y_d) = 1_{np}\mu + P\alpha + U\beta + T_d\tau + F_d\rho \tag{1.1}$$

(Kunert, 1983a) for the np observations Y_d. 1_{np} is the np-dimensional vector of ones. Given a matrix M, we write M' for the transpose and M^- for a generalized inverse and $\mathrm{pr}(M) = M(M'M)^-M'$ for the projection matrix onto the column span of M. I_x gives the identity matrix of order x and $\mathrm{pr}^\perp(M) = I_x - \mathrm{pr}(M)$, for appropriate x.

An important property of projection matrices is that, for any partitioned matrix $[A \mid B]$,

$$\mathrm{pr}([A \mid B]) = \mathrm{pr}(A) + \mathrm{pr}(\mathrm{pr}^\perp(A)B). \tag{1.2}$$

The information matrix for the estimation of direct effects,

$$\mathscr{C}_d = T_d'\mathrm{pr}^\perp([P \mid U \mid F_d])T_d,$$

and the information matrix for the estimation of residual effects,

$$\tilde{\mathscr{C}}_d = F_d'\mathrm{pr}^\perp([P \mid T_d])F_d,$$

both have row- and column-sums zero. This means that, in order to find optimal designs, we can use the tool introduced by Kiefer (1975).

A design d^* with the properties

(i) the information matrix of d^* for the estimation of direct (resp. residual) effects is completely symmetric (i.e. all diagonal elements are the same and all off-diagonal elements are identical),
(ii) this information matrix has maximal trace over $\Omega_{t,n,p}$,

is universally optimal over $\Omega_{t,n,p}$ for the estimation of direct (resp. residual) effects. The criterion of "universal optimality" includes the commonly applied criteria of D-, A-, and E-optimality (Kiefer, 1975).

We adopt the following notation from Cheng and Wu (1980). For any design $d \in \Omega_{t,n,p}$ the symbols ℓ_{dik}, n_{diu}, $\tilde{n}_{diu}$ and m_{dij} are, respectively, the number of appearances of treatment i in period k, on unit u, on the first $p-1$ periods of unit u, and preceded by treatment j $(1 \le u \le n,\ 1 \le k \le p,\ 1 \le i, j \le t)$. Observe that ℓ_{dik}, n_{diu}, $\tilde{n}_{diu}$ and m_{dij} are the elements of $T_d'P$, $T_d'U$, $F_d'U$ and $T_d'F_d$, respectively. The symbol ℓ_{dik-1} also gives the (i, k)th element of $F_d'P(2 \le k \le p,$ $1 \le i \le t)$. The first column of $F_d'P$ consists of zeroes. The diagonal elements r_{di} (resp. $\tilde{r}_{di}$) of $T_d'T_d$ (resp. $F_d'F_d$) are the total numbers of appearances of treatment i in d (in the first $p-1$ periods of d). Consider t and n such that n/t is integral. Then a design $d \in \Omega_{t,n,t}$ is

a) *uniform on the units*, if $n_{diu} = 1$ $(1 \le i \le t,\ 1 \le u \le n)$,

b) *uniform on the periods*, if $\ell_{dik} = n/t(1 \le i, k \le t)$,
c) *uniform*, if d is uniform on the periods as well as on the units. A uniform design $d \in \Omega_{t,t,t}$ is also called a *Latin square.*
d) If all $m_{dij}(i \neq j)$ are equal to n/t and all $m_{dii} = 0$ then $d \in \Omega_{t,n,t}$ is called *balanced.*

Some of the main technical problems of this paper are now briefly outlined. The information matrices can be split up as follows:

$$\text{(i)} \quad \mathscr{C}_d = T_d'\mathrm{pr}^{\perp}([P \mid U])T_d - T_d'\mathrm{pr}^{\perp}([P \mid U])F_d \cdot (F_d'\mathrm{pr}^{\perp}([P \mid U])F_d)^{-}F_d'\mathrm{pr}^{\perp}([P \mid U])T_d. = \mathscr{C}_{d11} - \mathscr{C}_{d12}\mathscr{C}_{d22}^{-}\mathscr{C}_{d21}$$

$$\text{(ii)} \quad \tilde{\mathscr{C}}_d = \mathscr{C}_{d22}\mathscr{C}_{d21}\mathscr{C}_{d11}^{-}\mathscr{C}_{d12} \quad \text{(see Cheng and Wu, 1980).}$$

Unfortunately, $\mathscr{C}_{d22}$ is dependent of d and no general form of $\mathscr{C}_{d22}^{-}$ can be found. This makes it impossible to write $\mathrm{tr}(\mathscr{C}_d)$ in terms of r_{di}, $\tilde{r}_{di}$, ℓ_{dik}, n_{diu}, $\tilde{n}_{diu}$ and m_{dij}. A solution is to search for an upper bound of $\mathscr{C}_{d22}$. One such bound is $F_d'F_d$ and thus

$$\mathrm{tr}(\mathscr{C}_d) \le \mathrm{tr}(\mathscr{C}_{d11} - \mathscr{C}_{d12}(F_d'F_d)^{-}\mathscr{C}_{d21}),$$

which can be computed for every d. Although the balanced uniform designs do not attain this bound, we can use it to prove their optimality in Theorems 2.1 and 2.2.

Another possibility is to use $\mathscr{C}_{d^*22}$, from the uniform design d^*, and to restrict the competing designs to those having $\mathscr{C}_{d^*22}$ as an upper bound of $\mathscr{C}_{d22}$. This was done by Cheng and Wu (1980, 1983) in their Theorem 4.3 and is done in Proposition 2.5 of this paper. For the estimation of residual effects we compute

$$\mathrm{tr}(\tilde{\mathscr{C}}_d) = \mathrm{tr}(\mathscr{C}_{d22} - \mathscr{C}_{d21}\mathscr{C}_{d11}^{-}\mathscr{C}_{d12}) \le \mathrm{tr}(\mathscr{C}_{d22} - \mathscr{C}_{d21}(T_d'T_d)^{-}\mathscr{C}_{d12}).$$

This upper bound is attained by the balanced uniform design d^*. That makes the computation for the residual effects a lot easier, although the results will turn out to be much less satisfying.

EXAMPLE 1.3. Assume that $t = p = 2$ and n is even. This case can be solved entirely and therefore was chosen to start our computation. Without loss of generality, any design $d \in \Omega_{2,n,2}$ is of the form

$$d = \begin{bmatrix} 1 & & 1 & 1 & & 1 & 2 & & 2 & 2 & & 2 \\ & \cdot\cdot & & & \cdot\cdot & & & \cdot\cdot & & & \cdot\cdot & \\ 1 & \underbrace{\quad}_{w} & 1 & 2 & \underbrace{\quad}_{x} & 2 & 1 & \underbrace{\quad}_{y} & 1 & 2 & \underbrace{\quad}_{z} & 2 \end{bmatrix}.$$

(Rows will indicate periods and columns units throughout this paper.) Here w, $x, y, z \in \{0, 1, \cdots, n\}$ and $w + x + y + z = n$.

Let $E_x = I_x - x^{-1}1_x1_x'$, for every $x \in \mathbb{N}$. One easily computes
(i) $T_d'\mathrm{pr}^{\perp}([P \mid U])T_d = (x + y - (x-y)^2/n)E_2$
(ii) $F_d'\mathrm{pr}^{\perp}([P \mid U])F_d = (w + x)(y + z)/n\, E_2$
(iii) $T_d'\mathrm{pr}^{\perp}([P \mid U])F_d = -\,(x(y+z) + y(w+x))/n\, E_2$.

PART A. For the computation of $\mathscr{C}_d$ we distinguish among three situations.

SITUATION 1. Neither $w + x$ nor $y + z$ equals zero. Then

$$\mathscr{C}_d = E_2\left(\frac{wx}{w+x} + \frac{yz}{y+z}\right).$$

SITUATION 2. $w + x = 0$

$$\mathscr{C}_d = E_2\left(y - \frac{y^2}{n}\right) = E_2\left(\frac{yz}{y+z}\right).$$

SITUATION 3. $y + z = 0$

$$\mathscr{C}_d = E_2\left(x - \frac{x^2}{n}\right) = E_2\left(\frac{xw}{x+w}\right).$$

It follows that $\mathrm{tr}(\mathscr{C}_d) \le n/4$, with equality holding iff $w = x$ and $y = z$. Thus the optimal designs for the estimation of direct effects are of the form

$$d_1 = \begin{bmatrix} 1 & & 1 & 1 & & 1 & 2 & & 2 & 2 & & 2 \\ & \ddots & & & \ddots & & & \ddots & & & \ddots & \\ 1 & \underbrace{}_{a} & 1 & 2 & \underbrace{}_{a} & 2 & 1 & \underbrace{}_{b} & 1 & 2 & \underbrace{}_{b} & 2 \end{bmatrix},$$

which includes

$$d_2 = \begin{bmatrix} 1 & & 1 & 1 & & 1 \\ & \ddots & & & \ddots & \\ 1 & \underbrace{}_{n/2} & 1 & 2 & \underbrace{}_{n/2} & 2 \end{bmatrix}.$$

PART B. For the computation of $\tilde{\mathscr{C}}_d$, we use the fact that $F_d'\mathrm{pr}^{\perp}([P \mid U])F_d \ge \tilde{\mathscr{C}}_d$, with equality holding iff $T_d'\mathrm{pr}^{\perp}([P \mid U])F_d = 0$.

STEP (i).

$$F_d'\mathrm{pr}^{\perp}([P \mid U])F_d = \frac{(w+x)(y+z)}{n} E_2 \le \frac{n}{4} E_2;$$

equality holds for $w + x = y + z = n/2$.

STEP (ii). If $w + x = y + z = n/2$ then $T_d'\mathrm{pr}^{\perp}([P \mid U])F_d = 0$ if and only if $x + y = 0$.

Altogether it follows that $\tilde{\mathscr{C}}_d \le (n/4)E_2$ and equality holds iff $w = z = n/2$ and $y = x = 0$, for which d is of the form

$$d = \begin{bmatrix} 1 & & 1 & 2 & & 2 \\ & \ddots & & & \ddots & \\ 1 & \underbrace{}_{n/2} & 1 & 2 & \underbrace{}_{n/2} & 2 \end{bmatrix}.$$

REMARKS.

(i) Example 1.3 already indicates one main problem of this paper: the optimal designs for the estimation of direct and of residual effects are not the same.

(ii) Both classes of optimal designs use pairs of identical treatments and are not uniform. The uniform design usually applied (Grizzle, 1965) allows no estimation of the contrast of the direct effects in model (1.1). This explains the bad performance of the design in Grizzle's paper.

(iii) Example 1.3 indicates that balanced uniform designs will not in general be optimal even when $p = t$, if designs with pairs of identical treatments are competing.

2. Optimality for direct effects. It is well known (Hedayat and Afsarinejad, 1978) that the information matrix for the estimation of direct effects, $\mathscr{C}_{d^*}$, of every balanced uniform design is completely symmetric. Cheng and Wu (1980) have shown that d^* maximizes tr $\mathscr{C}_d$ over a subset of $\Omega_{t,t,t}$. We now show that tr $\mathscr{C}_{d^*}$ is maximum over the remaining designs. The idea is to use a more tractable upper bound of tr $\mathscr{C}_d$. We use two different upper bounds, both of which are not attained by d^*. It thus remains to show that, for every remaining design, at least one of the bounds is smaller than tr $\mathscr{C}_{d^*}$.

To maximize the two upper bounds over the competing designs, we can use Cheng and Wu's (1980) methods. However, one important point in their proofs is that $m_{dii} = 0$. This is not true for our designs but fortunately we can make use of limits for the m_{dii} instead.

In this section we will summarize the optimality results for the estimation of direct effects and leave the proofs to Section 4.

THEOREM 2.1. *If $t = n = p \neq 2$ and if a balanced Latin square $d^* \in \Omega_{t,t,t}$ exists, this d^* is universally optimal for the estimation of direct effects over $\Omega_{t,t,t}$.*

The result of Theorem 2.1 is not surprising, since in a balanced uniform design in $\Omega_{t,t,t}$ the m_{dij} are as nearly equal as possible. In a balanced uniform design with more than t units, this is no longer true. We have, however, almost the same strong result in the situation of practical interest where $n = 2\,t$.

THEOREM 2.2. *Assume that $t \ge 6$. A balanced uniform design $d^* \in \Omega_{t,2t,t}$ is universally optimal for the estimation of direct effects over $\Omega_{t,2t,t}$.*

If the number of units is very large, then there are designs which are universally better than the balanced uniform designs. The following class of designs helps to construct them.

DEFINITION 2.3. Assume $n = t(t-1)$. Construct a balanced uniform design $d \in \Omega_{t,n,t}$ with the property that every ordered pair of distinct treatments appears exactly once between the last and second to last period. Then construct a design $f \in \Omega_{t,n,t}$ consisting of the first $t-1$ periods of d and a last period equal to the second to last. We call f an *orthogonal residual effects design.* An example of such a design is

$$f = \begin{bmatrix} 123123 \\ 231312 \\ 231312 \end{bmatrix}.$$

Although not all m_{fij} are equal in an orthogonal residual effects design, residual and direct effects are orthogonal, i.e. $\mathscr{C}_{f12} = 0$. These designs are not optimal for the estimation of direct effects, but will be shown to be optimal for residual effects in Section 3.

PROPOSITION 2.4. *Take $t = p > 2$ and $n = \lambda t$, with an integer*

$$\lambda > t(t-1)^2/2.$$

Assume there is a design $g \in \Omega_{t,n,t}$ with the following properties.

(i) *The first $(t-1)t$ units of g are an orthogonal residual effects design $f \in \Omega_{t,t(t-1),t}$.*
(ii) *The other $n - t(t-1)$ units of g are a balanced uniform design $d \in \Omega_{t,n-t(t-1),t}$.*

Then g is universally better than any balanced uniform design $d^* \in \Omega_{t,n,t}$ for the estimation of direct effects.

The number of units required in Proposition 2.4 is very large, and increases much faster than t. This is one reason why Theorem 2.2 could only be shown for $t \geq 6$. The other reason lies in the fact that we used $t/(n(t-1))I_t$ as a lower bound of $(F'_{d^*}\mathrm{pr}^{\perp}([P \mid U])F_{d^*})^-$, while one true g-inverse is $t/(n(t-1-1/t))I_t$. The difference decreases for larger t.

In the following proposition we consider the optimality properties of balanced uniform designs $d^* \in \Omega_{t,n,t}$ for which

$$2t < n < (t-1)^2t^2/2.$$

To make the computation easier, we restrict attention to the class of designs d with the property

$$F'_d\mathrm{pr}^{\perp}(U)F_d = F'_{d^*}\mathrm{pr}^{\perp}(U)F_{d^*}.$$

Define $\mathscr{A}_{t,n,t}$ as the set of all designs $d \in \Omega_{t,n,t}$ which can be transformed to be uniform on the units and on the last period by exchanging the last period. The orthogonal residual effects designs are elements of $\mathscr{A}_{t,n,t}$.

PROPOSITION 2.5. *A balanced uniform design $d^* \in \Omega_{t,n,t}$ is universally optimal for the estimation of direct effects over $\mathscr{A}_{t,n,t}$ provided $n < t(t-1)/2$.*

The result of Proposition 2.5 does not imply that, for n not much greater than $t(t-1)/2$, there actually are designs f with $\operatorname{tr}(\mathscr{C}_f) > \operatorname{tr}(\mathscr{C}_{d^*})$.

It is not very useful from a practical viewpoint to determine such designs if $t > 2$. The following proposition implies that the d^* are highly efficient for every n and for every optimality criterion.

PROPOSITION 2.6. *Assume that a balanced uniform design $d^* \in \Omega_{t,n,t}$ exists. Then*

$$\frac{\operatorname{tr}(\mathscr{C}_{d^*})}{\sup_{d\in\Omega_{t,n,t}}(\operatorname{tr}(\mathscr{C}_d))} \geq \frac{(t-1)^2 - 2(t-1)t^{-1}}{(t-1)^2 - 2(t-1)t^{-1} + t^{-2}}$$

for any $n = \lambda t$, $\lambda \in \mathbb{N}$.

3. Nonoptimality for residual effects. For the estimation of residual effects the balanced uniform designs d^* do not perform so well. Even if $t = n = p$, $\tilde{\mathscr{C}}_{d^*}$ has not, in general, a maximal trace.

PROPOSITION 3.1. *Assume $t = n = p$ and a design $f \in \Omega_{t,t,t}$ exists with the following properties*:

(i) *by exchanging the last period we can transform f to be uniform*;
(ii) *the last and the second to last period are the same*;
(iii) *for every treatment i there is exactly one $j(i)$, such that treatment i is never preceded by treatment $j(i)$, (it follows that i is exactly once preceded by every other treatment including itself)*
(iv) *in the one unit in which treatment i appears twice in the last two periods, treatment $j(i)$ does not appear at all.*

Then no balanced Latin square $d^* \in \Omega_{t,t,t}$ can be universally optimal for the estimation of residual effects over $\Omega_{t,t,t}$ i.e. $\operatorname{tr} \tilde{\mathscr{C}}_{d^*} < \operatorname{tr} \tilde{\mathscr{C}}_f$.

The proof is straightforward and is therefore omitted. To give Proposition 3.1 any meaning, it is necessary to show that there are such t that a balanced Latin square d^* exists in $\Omega_{t,t,t}$ as well as a design f as defined in Proposition 3.1. Unfortunately the author could only construct such designs for odd values of t.

EXAMPLE 3.2. The smallest balanced Latin square d^* with an odd t is in

$\Omega_{9,9,9}$ and was found by Mertz and Sonneman (1978). We compare it with

$$f = \begin{bmatrix} 123456789 \\ 567891234 \\ 345678912 \\ 234567891 \\ 789123456 \\ 456789123 \\ 678912345 \\ 912345678 \\ 912345678 \end{bmatrix}$$

This f is better than d^* even for the E-criterion. We have thus shown that, for the estimation of residual effects, d^* is not D-, A- or E-optimal over $\Omega_{9,9,9}$.

If $n = 2t$ we get, by the construction method of Williams (1949), balanced uniform designs with the following property: if, in any unit, treatment i appears in the last period preceded by treatment j, then there is another unit with treatment j in the last period preceded by treatment i. An obvious generalization of Proposition 3.1 shows that no balanced uniform design $d^* \in \Omega_{t,2t,t}$ can be universally optimal for the estimation of residual effects over $\Omega_{t,2t,t}$ (the same can be shown for any n with n/t even).

We will now show the optimality of orthogonal residual effects designs.

PROPOSITION 3.3. *Assume $n = t(t-1)$. An orthogonal residual effects design $f \in \Omega_{t,n,t}$ is universally optimal for the estimation of residual effects over $\Omega_{t,n,t}$.*

PROOF. The proof can be constructed by the strategy indicated in Example 1.3. It is easy to show that (i) $\mathscr{L}_{f22}$ is completely symmetric and has maximal trace over $\Omega_{t,n,t}$ and (ii) $\mathscr{L}_{f12} = 0$. Note that $\operatorname{tr} \tilde{\mathscr{L}}_f > \operatorname{tr} \tilde{\mathscr{L}}_{d^*}$ for a balanced uniform design $d^* \in \Omega_{t,n,t}$. □

EXAMPLE 3.4. Take $t = 5$ and $n = 20$. Then the orthogonal residual effects design

$$f = \begin{bmatrix} 51423 & 34251 & 52341 & 13452 \\ 12534 & 23145 & 24513 & 41235 \\ 45312 & 45312 & 35124 & 35124 \\ 23145 & 12534 & 41235 & 24513 \\ 23145 & 12534 & 41235 & 24513 \end{bmatrix}$$

is universally optimal for the estimation of residual effects over $\Omega_{5,20,5}$, according to Proposition 3.3. Note that the first ten units of f form a design $\tilde{f} \in \Omega_{5,10,5}$ with the property

$$\operatorname{tr}(\tilde{\mathscr{L}}_{\tilde{f}}) > \operatorname{tr}(\tilde{\mathscr{L}}_{d^*})$$

where $d^* \in \Omega_{5,10,5}$ is a balanced uniform design.

4. Proofs of Section 2. As Theorems 2.1 and 2.2 are the main part of the paper, we will give complete proofs.The proofs of the other propositions are briefly sketched, except the proof of Proposition 2.4 which is completely omitted, to save space. For technical details see Kunert (1983b).

The single steps of the proofs are given by Propositions 4.1 to 4.6. The first proposition introduces the upper bounds already mentioned.

PROPOSITION 4.1. *For any t and n and for any $d \in \Omega_{t,n,t}$, the following relations hold. Define $1/\tilde{r}_{dj} = 0$ if $\tilde{r}_{dj} = 0$. Then*

$$\text{(i)} \quad \begin{aligned} \operatorname{tr} \mathscr{C}_d \le nt &- \textstyle\sum_{i=1}^t \sum_{u=1}^n n_{diu}^2/t \\ &- \textstyle\sum_{i=1}^t \sum_{j=1}^t (m_{dij} - \sum_{u=1}^n n_{diu}\tilde{n}_{dju}/t)^2/\tilde{r}_{dj}, \end{aligned}$$

$$\text{(ii)} \quad \begin{aligned} \operatorname{tr} \mathscr{C}_d \le nt &- \textstyle\sum_{i=1}^t \sum_{k=1}^t \ell_{dik}^2/n \\ &- \textstyle\sum_{i=1}^t \sum_{j=1}^t (m_{dij} - \sum_{k=2}^t \ell_{dik}\ell_{djk-1}/n)^2/\tilde{r}_{dj}. \end{aligned}$$

PROOF. We only prove inequality (i). The proof of the second inequality is analogous. With the help of equation (1.2) we can show that

$$\mathscr{C}_d \le T_d'\mathrm{pr}^\perp(U)T_d - T_d'\mathrm{pr}^\perp(U)F_d(F_d'\mathrm{pr}^\perp(U)F_d)^- F_d'\mathrm{pr}^\perp(U)T_d.$$

The fact that we can choose a g-inverse such that

$$\operatorname{diag}(1/\tilde{r}_{dj}) \le (F_d'\mathrm{pr}^\perp(U)F_d)^-$$

completes the proof. □

PROPOSITION 4.2. *Assume that $\sum_{i=1}^t x_i = 0$ and the $x_i (1 \le i \le t)$ are integral. The sum of all positive x_i is assumed to equal the integer z. Then the minimum of $\sum_{i=1}^t x_i^2$ equals $2z$.*

PROOF. Let I be the set of all indices $i \in \{1, \cdots, t\}$ with $x_i > 0$. Then

$$\textstyle\sum_{i=1}^t x_i^2 = \sum_{i\in I} x_i^2 + \sum_{i\notin I} (-x_i)^2 \ge \sum_{i\in I} x_i + \sum_{i\notin I} (-x_i) = 2z. \quad \square$$

PROPOSITION 4.3. *Assume that $t = p > 2$, n/t is integral and $d \in \Omega_{t,n,t}$. Defining $x_{diu} = n_{diu} - 1$ for every (i, u), we assume that the sum of all positive x_{diu} equals the integer z. If $d^* \in \Omega_{t,n,t}$ is a balanced uniform design, a necessary condition for $\operatorname{tr}(\mathscr{C}_d)$ to be not smaller than $\operatorname{tr}(\mathscr{C}_{d^*})$ is that*

$$z < n/2 + n/(2t).$$

PROOF. As in Proposition 4.1,

$$\operatorname{tr}(\mathscr{C}_d) \le \operatorname{tr}(T_d'\mathrm{pr}^\perp(U)T_d) = nt - \textstyle\sum_{i=1}^t \sum_{u=1}^n n_{diu}^2/t \le n(t-1) - 2z/t.$$

We know from Cheng and Wu (1980) that

$$\operatorname{tr}(\mathscr{C}_{d^*}) = n(t-1) - (t-1-1/t)^{-1}t^{-1}n(t-1).$$

Assume

$$2z \geq n + n/t.$$

Then

$$\begin{aligned} 2z/t \geq n/t + n/t^2 &> n/t + nt^{-2}(t-1-1/t)^{-1} \\ &= (t-1-1/t)^{-1}t^{-1}n(t-1) \end{aligned}$$

and $\operatorname{tr}(\mathscr{C}_d) < \operatorname{tr}(\mathscr{C}_{d^*})$. □

PROPOSITION 4.4. *Consider a design $d \in \Omega_{t,n,t}$ such that the sum of all positive $x_{diu} = n_{diu} - 1$ equals z, where $1 \leq z \leq t$. Then*

$$\operatorname{tr} \mathscr{C}_d \leq n(t-1) - n/t - z(t-1)/((n+1)t).$$

PROOF. We use bound (i) of Prop. 4.1. Then

$$\operatorname{tr} \mathscr{C}_d \leq n(t-1) - 2z/t - \textstyle\sum_{i=1}^t \sum_{j=1}^t (m_{dij} - \sum_{u=1}^n n_{diu}\tilde{n}_{dju}/t)^2/\tilde{r}_{dj}.$$

Without loss of generality we assume that for every treatment j in $\{z+1, \cdots, t\}$ all $n_{dju} \leq 1$ (which implies $m_{djj} = 0$). Note that $\{z+1, \cdots, t\}$ can be empty. Now apply the methods of Cheng and Wu (1980) in their Theorem 4.1. It follows that

$$\begin{aligned} &\textstyle\sum_{i=1}^t \sum_{j=1}^t (m_{dij} - \sum_{u=1}^n n_{diu}\tilde{n}_{dju}/t)^2/\tilde{r}_{dj} \\ &\quad \geq (\textstyle\sum_{j=1}^z \sum_{u=1}^n n_{dju}\tilde{n}_{dju}/t - \sum_{j=1}^z m_{djj})^2 t/((t-1)\sum_{j=1}^z \tilde{r}_{dj}) \\ &\quad\quad + (\textstyle\sum_{j=z+1}^t \sum_{u=1}^n n_{dju}\tilde{n}_{dju})^2/(t(t-1)\sum_{j=z+1}^t \tilde{r}_{dj}). \end{aligned}$$

Define $a = \sum_{j=1}^z \tilde{r}_{dj}$. It can be shown that $\sum_{j=1}^z m_{djj} \leq z$ and $\sum_{j=1}^z \sum_{u=1}^n n_{dju}\tilde{n}_{dju} \geq a + z$, while $\sum_{j=z+1}^t \sum_{u=1}^n n_{dju}\tilde{n}_{dju} \geq n(t-1) - a$.

SITUATION 1. $a < (t-1)z$.
In this case $z < t$ and $\{z+1, \cdots, t\}$ is not empty. We restrict the summation to $j \in \{z+1, \cdots, t\}$. Thus

$$\begin{aligned} \operatorname{tr}(\mathscr{C}_d) &\leq n(t-1) - 2z/t - (n(t-1) - a)/(t(t-1)) \\ &< n(t-1) - n/t - z/t. \end{aligned}$$

SITUATION 2. $a \geq (t-1)z$.
Then the bound is maximized if $\sum_{j=1}^z m_{djj} = z$ and

$$\begin{aligned} \operatorname{tr}(\mathscr{C}_d) &\leq n(t-1) - \frac{2z}{t} - \frac{(a-(t-1)z)^2}{t(t-1)a} - \frac{n(t-1)-a}{t(t-1)} \\ &= n(t-1) - \frac{n}{t} - \frac{(t-1)z^2}{ta}. \end{aligned}$$

The fact that $a \leq (n+1)z$ completes the proof. □

PROPOSITION 4.5. *Consider a design $d \in \Omega_{t,n,t}$ which is uniform on the units but not on the periods; i.e. the sum of all positive $z_{dik} = \ell_{dik} - n/t$ equals z, where $2 \le z$. Then*

$$\mathrm{tr}\ \mathscr{C}_d \le n(t-1) - n/t - z(2t(t-1) - 4n)/(nt(t-1)).$$

PROOF. We use bound (ii) of Proposition 4.1. As d is uniform on the units, $m_{djj} = 0$, for all j. As in Proposition 4.4 we get

$$\mathrm{tr}(\mathscr{C}_d) \le n(t-1) - \frac{2z}{n} - \frac{t\left(\sum_{j=1}^{t} \sum_{k=2}^{t} \ell_{djk}\ell_{djk-1}\right)^2}{n^3(t-1)^2}.$$

Since $\sum_{j=1}^{t} \sum_{k=2}^{t} \ell_{djk}\ell_{djk-1} \ge (n/t)(n(t-1) - 2z)$ it follows that

$$\mathrm{tr}\ \mathscr{C}_d \le n(t-1) - \frac{n}{t} - \frac{z(2t(t-1) - 4n)}{nt(t-1)} - \frac{4z^2}{nt(t-1)^2}. \quad \square$$

PROPOSITION 4.6. *If $t = p > 2$ and if a balanced uniform design $d^* \in \Omega_{t,n,t}$ exists, this d^* is universally optimal for the estimation of the direct effects over the class of designs $d \in \Omega_{t,n,t}$ which are uniform on the units and the last period.*

Proposition 4.6 is an immediate consequence of Theorem 4.3 of Cheng and Wu (1980).

PROOF OF THEOREM 2.1. Assume there is a design $f \in \Omega_{t,t,t}$ such that $\mathrm{tr}\ \mathscr{C}_f > \mathrm{tr}\ \mathscr{C}_{d^*}$.

Proposition 4.6 implies that f must be (i) not uniform on the units, or (ii) uniform on the units but not on the periods. Assume $t > 3$.

(i) In case (i) Proposition 4.3 and 4.4 imply that $\mathrm{tr}\ \mathscr{C}_f < \mathrm{tr}\ \mathscr{C}_{d^*}$.
(ii) In case (ii) Proposition 4.5 implies that

$$\mathrm{tr}\ \mathscr{C}_f \le n(t-1) - 1 - \frac{2(t-3)}{t(t-1)} < \mathrm{tr}\ \mathscr{C}_{d^*}.$$

No balanced Latin square exists if $t = 3$ (Hedayat and Afsarinejad, 1978). □

PROOF OF THEOREM 2.2. The proof is completely analogous to the proof of Theorem 2.1 when $t \ge 7$. For $t = 6$ in the case $z = 1$, a slight variation of Proposition 4.4 is necessary, taking into account the fact that

$$\textstyle\sum_{u=1}^{n} n_{d1u}\tilde{n}_{d1u} \ge a + 3 \quad \text{if} \quad z = 1 \quad \text{and} \quad a = \tilde{r}_{d1} = 2t + 1. \quad \square$$

PROOF OF PROPOSITION 2.5. It can be shown that, for every competing design,

$$\mathrm{tr}\ \mathscr{C}_d \le n(t-1) - \frac{2z}{t} - \frac{\left(\sum_{j=1}^{t} \sum_{u=1}^{n} n_{dju}\tilde{n}_{dju}/t - \sum_{j=1}^{t} m_{djj}\right)^2 t}{n(t-1)(t-1-1/t)}.$$

if the sum of the positive $x_{diu} = n_{diu} - 1$ equals $z \ge 0$. As in Proposition 4.4 we proceed by showing that $\sum m_{djj} \le \sum \sum n_{dju}\tilde{n}_{dju}/t$ and thus

$$\begin{aligned}\operatorname{tr} \mathscr{C}_d &\le n(t-1) - 2z/t - (t-1)(n-z)^2/(nt(t-1-1/t)) \\ &= n(t-1) - n(t-1)/(t(t-1-1/t)) \\ &\qquad - z(zt(t-1)-2n)/(nt^2(t-1-1/t)) \\ &\le n(t-1) - n(t-1)/(t(t-1-1/t)) = \operatorname{tr} \mathscr{C}_{d^*}. \quad \square\end{aligned}$$

PROOF OF PROPOSITION 2.6. Using bound (i) of Proposition 4.1 we find that, for every design $d \in \Omega_{t,n,t}$

$$\operatorname{tr} \mathscr{C}_d \le n(t-1) - \frac{2z}{t} - \frac{t(\sum_{j=1}^{t} \sum_{u=1}^{n} n_{dju}\tilde{n}_{dju}/t - \sum_{j=1}^{t} m_{djj})^2}{(t-1)\sum \tilde{r}_{dj}}.$$

Using the same arguments as in Proposition 2.5, we conclude that

$$\operatorname{tr} \mathscr{C}_d \le n(t-1) - n/t - z^2/(nt)$$

which completes the proof. $\square$

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