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OPTIMAL DESIGN AND REFINEMENT OF THE LINEAR MODEL WITH APPLICATIONS TO REPEATED MEASUREMENTS DESIGNS[1]

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The information matrices of one design in a finer and a simpler linear model are compared to each other. The orthogonality condition ensuring that both matrices are equal is examined in the model for repeated measurements designs which was considered e.g. by Cheng and Wu (1980). Examples of unbalanced designs fulfilling the orthogonality condition are shown to be optimum. Moreover, nearly strongly balanced generalized latin squares are introduced and their universal optimality is proved, if the numbers of units and periods are sufficiently large.

1. Introduction. Consider two linear models, the first containing exactly the set of parameters of the second and some additional nuisance parameters. Then we call the first model the finer and the second the simpler one. If an optimal design is investigated in the finer model, it often turns out to be optimal in the simpler model, too, and turns out to fulfil an orthogonality condition ensuring that the information matrices (for the estimation of the same effects) of the design are equal in both models. One example is the generalized Youden design in the so-called regular case of the two-way heterogeneity model which is a balanced block design in the one-way heterogeneity model and has the same information matrix in both models (see Kiefer, 1958). This result is due to an ordering property between the information-matrices in the finer and in the simpler model, which was shown by Magda (1980). We show an orthogonality condition which ensures equality of the two information-matrices for general linear models and apply it to the special case of repeated measurements design.

Our result is that this orthogonality condition for the estimation of direct effects in models with and without residual effects (and vice versa) is not so closely related to strong balance or balance as might be expected from the literature. Optimality has so far been shown exclusively for designs which either are strongly balanced (see Sinha, 1975, Sonnemann, 1982, Cheng and Wu, 1980 or Magda, 1980) or balanced (see Hedayat and Afsarinejad, 1978 or Cheng and Wu, 1980).

We give some examples of optimal and orthogonal designs which are neither balanced nor strongly balanced. To achieve orthogonality, we sometimes use a preperiod, i.e. residual effects even in the first period.

Finally we consider situations, where no designs exist, which on the one hand are optimal in the model without residual effects and on the other can fulfil their orthogonality conditions. We examine the situation where the numbers of units and of periods are divisible by the number of treatments and there is no preperiod. We prove the optimality of "nearly strongly balanced" designs over a subset of all possible designs; and in general if the numbers of units and periods are sufficiently large. This sufficient size is of some practical importance if the number of treatments does not exceed eight.

2. Strategies to find optimal designs. Consider a set of designs Δ. Each $d \in \Delta$ induces a linear model

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$$(2.1)\qquad Y = A_d\eta + B_d\xi + e,$$

where $A_d \in \mathbb{R}^{n\times p}$ and $B_d \in \mathbb{R}^{n\times q}$ depend on d, e is a n-dimensional random vector having uncorrelated components with common variance and expectation zero. η and ξ are unknown vectors of parameters.

In what follows A^- is a generalized inverse of the $n \times m$-matrix A, $im(A)$ is the column-spann of A, $\mathrm{pr}(A) = A(A'A)^-A'$ is the projector onto $im(A)$, and $\mathrm{pr}^\perp(A) = I_n - \mathrm{pr}(A)$ is the projector onto the space which is orthogonal to $im(A)$, where I_n is the identity matrix of order n. The matrix

$$\mathscr{C}_d = A'_d\mathrm{pr}^\perp(B_d)A_d$$

is called the *information matrix of d for the estimation of* η. Let 1_n be the n-dimensional vector of ones.

Assume that $A_d1_n \in im(B_d)$ for every $d \in \Delta$. Then $\mathrm{pr}^\perp(B_d)A_d1_n = 0$, the row- and column-sums of $\mathscr{C}_d$ are equal to zero and $1'_p\eta$ is not estimable. The set of all linear contrasts of η can be estimated if the rank of $\mathscr{C}_d$ is equal to $p - 1$ (see Kiefer, 1975). As optimality criterion, we use the concept of universal optimality. This criterion includes the criteria of A- and D-optimality (see Kiefer, 1975). We call a $n \times n$ matrix C completely symmetric, if all diagonal elements of C are the same and all off-diagonal elements are equal. Kiefer (1975) showed that a design $d^* \in \Delta$ with the properties that $\mathscr{C}_{d^*}$ is completely symmetric and has maximal trace over Δ is universally optimal for the estimation of η over Δ. Further, all designs which are also D- or A-optimal for the estimation of η over Δ must have an information matrix equal to $\mathscr{C}_{d^*}$. All proofs on optimality in this paper use this tool.

Now assume that for every $d \in \Delta$, $B_d \in \mathbb{R}^{n\times q}$ is partitioned into $B_d = [B_{1d} \mid B_{2d}]$, where $B_{1d} \in \mathbb{R}^{n\times r}$, $r < q$. Then $A'_d\,\mathrm{pr}^\perp(B_{1d})A_d$ is the information matrix of d for the estimation of η in the simpler model

$$(2.2)\qquad Y = A_d\,\eta + B_{1d}\phi + e.$$

We call model (2.1) *finer than* model (2.2).

PROPOSITION 2.3. (cf. Magda, 1980). *Let $\mathscr{C}_d$ be the information matrix of $d \in \Delta$ for the estimation of η in model* (2.1). *Then $\mathscr{C}_d \le A'_d\mathrm{pr}^\perp(B_{1d})A_d$ with equality holding if and only if*

$$(2.4)\qquad A'_d\mathrm{pr}^\perp(B_{1d})B_{2d} = 0.$$

PROOF. It can easily be checked that

$$\mathrm{pr}([B_{1d} \mid B_{2d}]) = \mathrm{pr}(B_{1d}) + \mathrm{pr}(\mathrm{pr}^\perp(B_{1d})B_{2d}).$$

Proposition 2.3 is an immediate consequence of this equation. □

This proposition implies two strategies to find optimal designs which we shall use in the following sections. Let Δ^* denote the set of all $d \in \Delta$ for which $A'_d\mathrm{pr}^\perp(B_{1d})A_d$ is completely symmetric and has maximal trace over Δ. (We conclude that Δ^* is the set of all designs which are universally optimal in the simpler model (2.2).)

STRATEGY 1. Assume there is a $d^* \in \Delta^*$ such that $A'_{d^*}\mathrm{pr}^\perp(B_{1d^*})B_{2d^*} = 0$. It follows for the finer model (2.1) that (i) d^* is universally optimal for the estimation of η over Δ, and (ii) the set of all D- or A-optimal designs for the estimation of η is equal to the subset of Δ^* consisting of all designs $d \in \Delta^*$ which fulfil the orthogonality condition (2.4).

We point out that the orthogonality condition (2.4) depends on d and in general is not the same for all $d \in \Delta^*$. If no design $d \in \Delta^*$ fulfils its orthogonality condition, we can generalize Strategy 1 in the following way.

STRATEGY 2. Find a $d^* \in \Delta^*$ with the properties (i) $\mathscr{C}_{d^*}$ is completely symmetric and has maximal trace over Δ^*, (ii) $\operatorname{tr}(\mathscr{C}_{d^*}) \geq \operatorname{tr}(A_d'\operatorname{pr}^{\perp}(B_{1d})A_d)$ for all d in a subset $\tilde{\Delta}$ of Δ. Then d^* is universally optimal for the estimation of η over $\Delta^* \cup \tilde{\Delta}$.

3. Description of the model. In a setting of repeated measurements design each of a set of n experimental units is, in each of p periods, exposed to one of t treatments. The treatment which is applied to unit j at period i is determined by the repeated measurements design d and is called $d(i, j)$. At each period we measure the effect of the treatments applied to each unit 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, 1978.) We distinguish between designs with no residual effects on the first period (cf. Hedayat and Afsarinejad, 1978 or Cheng and Wu, 1980) and designs with residual effects on the first period, i.e. with a preperiod (cf. Sinha, 1975, Sonnemann, 1982, Magda, 1980). For designs with preperiod we assume that either the preperiod can be chosen freely, i.e. that the experimenter can apply a treatment to each unit before the experiment begins, or that the preperiod is consisting only of ones, as might be the case if one of the treatments (say number one) is a control and none of the units has been treated before the beginning of the experiment.

Formally speaking a repeated measurements design is a function d from $\{0, 1, \cdots, p\} \times \{1, \cdots, n\}$ to $\{0, 1, \cdots, t\}$. The set of all such d with

$$d(0, j) = 0 \quad \text{and} \quad d(i, j) \neq 0, \qquad 1 \leq i \leq p, \qquad 1 \leq j \leq n,$$

is denoted by $\Omega_{t,n,p}$ and called the set of all repeated measurements designs without preperiod. The set of all such d with

$$d(i, j) \neq 0, \qquad 0 \leq i \leq p, \qquad 1 \leq j \leq n,$$

is called $\tilde{\Omega}_{t,n,p}$ the set of all repeated measurements designs with preperiod.

Let y_{dij} be the response obtained from the jth unit in the ith period under $d \in \Omega_{t,n,p} \cup \tilde{\Omega}_{t,n,p}$. Then the observations are assumed uncorrelated with common variance and

$$E(y_{dij}) = \mu + \alpha_i + \beta_j + \tau_{d(i,j)} + \rho_{d(i-1,j)}, \qquad 1 \leq i \leq p, \qquad 1 \leq j \leq n, \quad \text{with} \quad \rho_0 = 0.$$

We refer to the unknown parameters as follows: μ is the overall effect, α_i is the ith period effect, β_j is the jth experimental unit effect, $\tau_{d(i,j)}$ is the direct effect of treatment $d(i, j)$, and $\rho_{d(i-1,j)}$ is the residual effect of treatment $d(i-1, j)$ (cf. Hedayat and Afsarinejad, 1978 or Cheng and Wu, 1980).

In vector notation we have

$$E(Y_d) = 1_{np}\mu + P\alpha + U\beta + T_d\tau + F_d\rho \tag{3.1}$$

for the np observations Y_d. It can easily be seen that $1_{np} = T_d 1_t = P1_p = U1_n$ for every $d \in \Omega_{t,n,p} \cup \tilde{\Omega}_{t,n,p}$. If $\otimes$ indicates the Kronecker product of matrices, then $F_d 1_t = 1_n \otimes [0 \mid 1_{p-1}']' = P[0 \mid 1_{p-1}']'$ for every design $d \in \Omega_{t,n,p}$ without preperiod, while $F_d 1_t = 1_{np}$ for every design $d \in \tilde{\Omega}_{t,n,p}$ with preperiod.

Thus the information-matrix for the estimation of direct effects

$$\mathscr{C}_d = T_d'\operatorname{pr}^{\perp}([1_{np} \mid P \mid U \mid F_d])T_d = T_d'\operatorname{pr}^{\perp}([P \mid U \mid F_d])T_d \tag{3.2}$$

and the information-matrix for the estimation of residual effects

$$\tilde{\mathscr{C}}_d = F_d'\operatorname{pr}^{\perp}([1_{np} \mid P \mid U \mid T_d])F_d = F_d'\operatorname{pr}^{\perp}([P \mid U \mid T_d])F_d \tag{3.3}$$

each have row and column sums zero.

We adopt the following notation from Cheng and Wu (1980). For a design $d \in \Omega_{t,n,p} \cup \tilde{\Omega}_{t,n,p}$ the symbols $\ell_{dik}, \tilde{\ell}_{dik}, n_{diu}, \tilde{n}_{diu}, m_{dij}, r_{di}, \tilde{r}_{di}$ are, respectively, the number of appearances of treatment i in period k, in period $k-1$, on unit u in the periods 1 to p, on unit u in the period 0 to $p-1$, preceded by treatment j, in the periods 1 to p, in the periods 0 to $p-1$, where $1 \leq u \leq n$, $1 \leq k \leq p$, $1 \leq i, j \leq t$. Observe that ℓ_{dik}, $\tilde{\ell}_{dik}$, n_{diu}, $\tilde{n}_{diu}$ and m_{dij} are the elements of T'_dP, F'_dP, T'_dU, F'_dU and T'_dF_d, respectively, and r_{di} (resp. $\tilde{r}_{di}$) are the diagonal elements of T'_dT_d (resp. F'_dF_d).

Now consider t, n, p such that npt^{-1} is integral, i.e. $t \mid np$ (say). Then a design $d \in \Omega_{t,n,p} \cup \tilde{\Omega}_{t,n,p}$ is called

(a) *balanced block design* (BBD) *on the units*, if (i) $T'_d\text{pr}^{\perp}(U)T_d$ is completely symmetric, and (ii) $n_{diu} \in \{[pt^{-1}], [pt^{-1}] + 1\}$, $1 \le i \le t$, $1 \le u \le n$, where $[x]$ is the integral part of the real number x,
(b) *uniform on the units*, if d is a BBD on the units and $t \mid p$,
(c) BBD *on the periods*, if (i) $T'_d\text{pr}^{\perp}(P)T_d$ is completely symmetric, and (ii) $\ell_{dik} \in \{[nt^{-1}], [nt^{-1}] + 1\}$, $1 \le i \le t$, $1 \le k \le p$,
(d) *uniform on the periods*, if d is a BBD on the periods and $t \mid n$,
(e) *generalized Youden design* (GYD), if d is a BBD on the units and a BBD on the periods,
(f) *generalized latin square* (GLS), if d is a GYD and $t|p$ and $t \mid n$.

It should be noted that if $t = 2$ our definition of a BBD is more general than the usual definition.

4. Designs fulfilling the orthogonality condition. All proofs in this section will be done with Strategy 1. We concentrate on searching optimal designs for the estimation of direct effects. The problem of designs for the estimation of residual effects is only shortly treated. The examples of optimal designs are restricted to such which are not balanced or strongly balanced.

THEOREM 4.1. *Let $t \mid n$ and $t \mid p$. Assume there is a* GLS $d^* \in \Omega_{t,n,p} \cup \tilde{\Omega}_{t,n,p}$, *such that*

$$m_{d^*ij} = t^{-1} r_{d^*j}, \qquad 1 \le i \le t, 1 \le j \le t. \tag{4.2}$$

Then d^* is universally optimal for the estimation of direct effects over $\Omega_{t,n,p} \cup \tilde{\Omega}_{t,n,p}$. Every design $d \in \Omega_{t,n,p} \cup \tilde{\Omega}_{t,n,p}$ which is also D- or A-optimal for the estimation of direct effects over $\Omega_{t,n,p} \cup \tilde{\Omega}_{t,n,p}$ must also be a GLS *and fulfil the orthogonality condition analogous to* (4.2).

PROOF. (i) From Proposition 2.3 and Equation (3.2) $\mathscr{C}_d \le T'_d\text{pr}^{\perp}(1_{np})T_d$ with equality holding iff

$$T'_d\text{pr}^{\perp}(1_{np})[P \mid U \mid F_d] = 0 \tag{a}$$

(ii) $T'_d\text{pr}^{\perp}(1_{np})T_d$ is completely symmetric and has maximal trace, if and only if d is equally replicated, i.e. if all r_{di} are equal. This is true for the GLS d^*.

(iii) The orthogonality condition (a) can be split up into

$$T'_d pr^{\perp}(1_{np})[P \mid U] = 0 \tag{b}$$

and

$$T'_d\text{pr}^{\perp}(1_{np})F_d = 0. \tag{c}$$

For an equally replicated design (b) is fulfilled if the design is a GLS and (c) is equivalent to (4.2). □

If all $\tilde{r}_{di}$ are equal, then Condition (4.2) is just strong balance, i.e. all m_{dij} are equal. This holds for generalized latin squares without preperiod. But for designs with preperiod, Condition (4.2) is more general.

EXAMPLE 4.3. Assume that $d^* \in \Omega_{t,n,p}$ is a strongly balanced GLS without preperiod. Now construct a GLS $\tilde{d}^* \in \tilde{\Omega}_{t,n,p}$ by taking a preperiod with all entries equal to ones and the other periods like d^*. Then $\tilde{d}^*$ fulfils Condition (4.2).

THEOREM 4.4. *Let $t \nmid n$ and $t \mid p$. Assume there is a* GYD $d^* \in \Omega_{t,n,p} \cup \tilde{\Omega}_{t,n,p}$ *such that*

$$m_{d^*ij} = n^{-1} \sum_{k=1}^{p} \ell_{d^*ik} \tilde{\ell}_{d^*jk}, \qquad 1 \le i \le t,\ 1 \le j \le t. \tag{4.5}$$

Then d^* is universally optimal for the estimation of direct effects over $\Omega_{t,n,p} \cup \tilde{\Omega}_{t,n,p}$. Every design $d \in \Omega_{t,n,p} \cup \tilde{\Omega}_{t,n,p}$ which is also D- or A-optimal for the estimation of direct effects over $\Omega_{t,n,p} \cup \tilde{\Omega}_{t,n,p}$ must also be a GYD *and fulfil the orthogonality condition analogous to* (4.5).

PROOF. (i) $\mathscr{C}_d \le T_d' \mathrm{pr}^\perp(P) T_d$ with equality holding iff

$$T_d' \mathrm{pr}^\perp(P)[U \mid F_d] = 0 \tag{a}$$

(ii) $T_d' \mathrm{pr}^\perp(P) T_d$ is completely symmetric and has maximal trace if and only if d is a BBD on the periods (see Kiefer, 1958).

(iii) Condition (a) is split up into

$$T_d' \mathrm{pr}^\perp(P) U = 0 \tag{b}$$

and

$$T_d' \mathrm{pr}^\perp(P) F_d = 0. \tag{c}$$

For a BBD on the periods (b) is fulfilled if and only if it is uniform on the units, i.e. if it is a GYD. (c) then is equivalent to (4.5). □

EXAMPLE 4.6. Consider the GYD without preperiod $d \in \Omega_{t,n,p}$, where $t = 3$, $n = 4$, $p = 15$ and

$$d' = \underbrace{\begin{bmatrix} 1\,2\,3 & 2\,3\,1 & 2\,3\,1 & 1\,2\,3 & 1\,2\,3 \\ 1\,3\,2 & 2\,1\,1 & 3\,3\,2 & 2\,2\,1 & 1\,3\,3 \\ 2\,1\,3 & 3\,1\,2 & 2\,1\,3 & 1\,1\,3 & 3\,2\,2 \\ 3\,2\,1 & 1\,2\,3 & 1\,2\,3 & 3\,3\,2 & 2\,1\,1 \end{bmatrix}}_{\text{periods}} \Bigg\} \text{units}$$

The matrix with entries m_{dij} is

$$T_d' F_d = \begin{bmatrix} 6 & 6 & 6 \\ 7 & 6 & 6 \\ 6 & 7 & 6 \end{bmatrix}$$

and is equal to the matrix with entries

$$4^{-1} \sum_{k=1}^{p} \ell_{dik} \tilde{\ell}_{djk} = 4^{-1} \sum_{k=2}^{p} \ell_{dik} \ell_{djk-1}.$$

EXAMPLE 4.7. Let $t \mid n+1$ or $t \mid n-1$ and assume that $p = nt\lambda$, $\lambda \in N$. Define

$$r = \begin{cases} (n+1)t^{-1} - 1, & \text{if } t \mid n+1, \\ (n-1)t^{-1} + 1, & \text{if } t \mid n-1, \end{cases}$$

$$q = \begin{cases} (n+1)t^{-1}, & \text{if } t \mid n+1, \\ (n-1)t^{-1}, & \text{if } t \mid n-1. \end{cases}$$

If there is a GYD $d \in \tilde{\Omega}_{t,n,p}$ with preperiod, such that

$$\ell_{dik} = \begin{cases} r, & \text{if } i = k + xt \text{ (where } x = 0, 1, \cdots, n\lambda - 1), \\ q, & \text{else,} \end{cases} \tag{i}$$

(ii) the preperiod of d is equal to the last period,
(iii) there are integers a and b, $a - b = \lambda$, such that

$$m_{dij} = \begin{cases} a, & \text{if } 1 \le i \le t-1 \text{ and } j - i = 1, \text{ or } i = t \text{ and } j = 1, \\ b, & \text{else,} \end{cases}$$

then d fulfils the orthogonality condition (4.5).

As an example consider $d \in \tilde{\Omega}_{3,4,12}$, where

$$d' = \left[\begin{array}{c|cccc} 3 & 1\,2\,3 & 1\,2\,3 & 1\,2\,3 & 1\,2\,3 \\ 2 & 1\,2\,3 & 3\,2\,1 & 1\,1\,3 & 3\,2\,2 \\ 3 & 2\,3\,1 & 1\,3\,2 & 2\,2\,1 & 1\,3\,3 \\ 1 & 3\,1\,2 & 2\,1\,3 & 3\,3\,2 & 2\,1\,1 \end{array}\right]\Bigg\}\text{units}$$

preperiod periods

THEOREM 4.8. *Let $t \mid n$ and $t \nmid p$. Assume there exists a* GYD $d^* \in \Omega_{t,n,p} \cup \tilde{\Omega}_{t,n,p}$ *such that*

$$(4.9) \qquad m_{d^*ij} = p^{-1} \textstyle\sum_{u=1}^{n} n_{diu}\tilde{n}_{dju}, \qquad 1 \le i \le t, \qquad 1 \le j \le t.$$

Then d^* is universally optimal for the estimation of direct effects over $\Omega_{t,n,p} \cup \tilde{\Omega}_{t,n,p}$. Every design $d \in \Omega_{t,n,p} \cup \tilde{\Omega}_{t,n,p}$ which is also D- or A-optimal for the estimation of direct effects over $\Omega_{t,n,p} \cup \tilde{\Omega}_{t,n,p}$ must also be a GYD *and fulfil the orthogonality condition analogous to* (4.9).

PROOF. The proof uses $T_d'\mathrm{pr}^{\perp}(U)T_d$ as an upper bound of $\mathscr{C}_d$ and is analogous to the proof of Theorem 4.4. □

EXAMPLE 4.10. Consider the GYD $d \in \Omega_{3,12,5}$ where

$$d = \begin{bmatrix} 2\,1\,1 & 3\,1\,3 & 1\,2\,3 & 2\,2\,3 \\ 1\,2\,1 & 2\,3\,1 & 1\,3\,2 & 3\,2\,3 \\ 1\,2\,3 & 2\,3\,1 & 2\,3\,2 & 3\,1\,1 \\ 2\,1\,2 & 1\,1\,3 & 3\,1\,3 & 2\,3\,2 \\ 3\,3\,2 & 1\,2\,2 & 3\,1\,1 & 1\,3\,2 \end{bmatrix}\Bigg\}\text{periods}$$

units

The matrix with entries m_{dij} is

$$T_d'F_d = \begin{bmatrix} 6 & 5 & 5 \\ 5 & 6 & 5 \\ 5 & 5 & 6 \end{bmatrix}$$

and is equal to the matrix with entries $5^{-1} \sum_{u=1}^{n} n_{diu}\tilde{n}_{dju}$.

EXAMPLE 4.11. Let $t \mid n$ and $t \mid p-1$. Take the strongly balanced GYD without preperiod $d^* \in \Omega_{t,n,p}$ considered by Cheng and Wu (1980) in their Theorem 3.3. Construct a design $\tilde{d} \in \tilde{\Omega}_{t,n,p}$ with preperiod by adding a preperiod consisting only of ones.

If one is interested in the estimation of residual effects, then designs with preperiod are in general preferable, as they have more observations of the residual effects. For designs with preperiods, the theorems analogous to Theorems 4.2, 4.5 and 4.9 are obvious. It thus can be shown that the designs in Example 4.7 are also optimal for the estimation of residual effects.

For designs without preperiods, a difficulty arises from the fact that $F_d 1_t$ in general is neither in $im(T_d)$ nor in $im(U)$. So we have that e.g. $F_d'\mathrm{pr}^{\perp}(U)F_d$ has row- and column-sums, which are not zero, and thus cannot be equal to $\tilde{\mathscr{C}}_d$. We circumvent this problem in the following way:

$$\tilde{\mathscr{C}}_d = F_d'\mathrm{pr}^{\perp}([P \mid U \mid T_d \mid F_d 1_t])F_d \le F_d'\mathrm{pr}^{\perp}([U \mid F_d 1_t])F_d$$

with equality holding iff

$$(4.12) \qquad F_d'\mathrm{pr}^{\perp}([U \mid F_d 1_t])[P \mid T_d] = 0.$$

EXAMPLE 4.13. The design $d \in \Omega_{3,18,6}$, where

$$d = \underbrace{\begin{bmatrix} 2\,3\,1 & 2\,3\,1 & 2\,3\,1 & 2\,3\,1 & 1\,2\,3 & 1\,2\,3 \\ 2\,3\,1 & 2\,3\,1 & 2\,3\,1 & 2\,3\,1 & 2\,3\,1 & 3\,1\,2 \\ 3\,1\,2 & 1\,2\,3 & 3\,1\,2 & 1\,2\,3 & 3\,1\,2 & 2\,3\,1 \\ 3\,1\,2 & 3\,1\,2 & 3\,1\,2 & 3\,1\,2 & 3\,1\,2 & 2\,3\,1 \\ 1\,2\,3 & 3\,1\,2 & 1\,2\,3 & 3\,1\,2 & 2\,3\,1 & 3\,1\,2 \\ 2\,3\,1 & 2\,3\,1 & 2\,3\,1 & 2\,3\,1 & 2\,3\,1 & 2\,3\,1 \end{bmatrix}}_{\text{units}} \Bigg\} \text{periods}$$

fulfils the condition (4.12) and is universally optimal for the estimation of residual effects over $\Omega_{3,18,6}$, the set of all designs *without* preperiod. (Note the existence of a strongly balanced GLS without preperiod in $\Omega_{3,18,6}$, which is as good as d for the estimation of residual effects.) d is not uniform on the units and the matrix with entries m_{dij} is

$$T'_d F_d = \begin{bmatrix} 11 & 10 & 9 \\ 9 & 11 & 10 \\ 10 & 9 & 11 \end{bmatrix}.$$

5. Designs which nearly fulfil the orthogonality conditions. It should be realized by the reader that in a great many combinations of t, n, p the orthogonality conditions from Section 4 cannot be verified by integral m_{dij} for any GYD or GLS $d \in \Omega_{t,n,p} \cup \tilde{\Omega}_{t,n,p}$. The value of the knowledge of the orthogonality conditions in such situations is exemplified in this section.

EXAMPLE 5.1. For simplicity of computation, we restrict our attention to designs without preperiod. Assume $t = 3$, $n = 3$, $p = 8$. Any GYD $d \in \Omega_{3,3,8}$ can be gained from a GLS by skipping one period. This omitted period determines three types of GYD d in $\Omega_{3,3,8}$ as follows.

Type 1: The last period of d is equal to the omitted period.

Type 2: The last period of d applies exactly one treatment to the same unit as the omitted period does.

Type 3: The last period of d applies no treatment to the same unit as the omitted period.

We first consider the model without period effect which is simpler than (3.1). Without loss of generality, we get the following orthogonality conditions for the three types of designs. The matrix with entries m_{dij} should be equal to

$$8^{-1}\begin{bmatrix} 20 & 18 & 18 \\ 18 & 20 & 18 \\ 18 & 18 & 20 \end{bmatrix}, \quad 8^{-1}\begin{bmatrix} 19 & 19 & 18 \\ 19 & 19 & 18 \\ 18 & 18 & 20 \end{bmatrix}, \quad 8^{-1}\begin{bmatrix} 19 & 18 & 19 \\ 19 & 19 & 18 \\ 18 & 19 & 19 \end{bmatrix}$$

for designs of type 1, 2, 3 respectively.

From the restriction $\sum_{j=1}^{t} m_{dij} = r_{di} - \ell_{di1} = 7$ for every GYD $d \in \Omega_{3,3,8}$ we conclude that $\operatorname{tr}\{T'_d \operatorname{pr}(\operatorname{pr}^{\perp}(U)F_d)T_d\}$ is minimized by taking the matrix with entries m_{dij} equal to

$$T'_d F_d = \begin{bmatrix} 3 & 2 & 2 \\ 2 & 3 & 2 \\ 2 & 2 & 3 \end{bmatrix}$$

for all three types of designs. The minimum of the three minima is attained by Type 1. We conclude that the design d, where

$$d' = \begin{bmatrix} 1 & 2 & 3 & 3 & 3 & 2 & 2 & 1 \\ 2 & 3 & 1 & 1 & 1 & 3 & 3 & 2 \\ 3 & 1 & 2 & 2 & 2 & 1 & 1 & 3 \end{bmatrix},$$

is universally optimal for the estimation of direct effects over the set of all GYD without preperiod in $\Omega_{3,3,8}$. (This is done by realizing that $T'_d \operatorname{pr}^{\perp}([U \mid F_d])P = 0$.)

EXAMPLE 5.2. Assume $t = 3$, $n = 12$, $p = 2$. Compare the design

$$d = \begin{bmatrix} 1\,2\,3 & 2\,3\,1 & 1\,2\,3 & 2\,3\,1 \\ 2\,3\,1 & 1\,2\,3 & 2\,3\,1 & 1\,2\,3 \end{bmatrix},$$

which is balanced (i.e. all $m_{dii} = 0$, all other m_{dij} are equal) and is a GYD, with the design

$$f = \begin{bmatrix} 1\,2\,3 & 1\,2\,3 & 1\,2\,3 & 2\,3\,1 \\ 1\,2\,3 & 2\,3\,1 & 1\,2\,3 & 1\,2\,3 \end{bmatrix},$$

which is neither balanced (or strongly balanced) nor a GYD. In the model with neither period nor residual effects, the design d is better ($T'_d\mathrm{pr}^\perp(U)T_d \geq T'_f\,\mathrm{pr}^\perp(U)T_f$). None of the designs fulfils the orthogonality conditions on the m_{dij} (but in the model without period effects both have respectively the same information matrices as in the one with period effects).

The orthogonality conditions on the matrix with entries m_{dij} (respectively m_{fij}) are

$$T'_fF_f \text{ should be equal to } 2^{-1}\begin{bmatrix} 6 & 1 & 1 \\ 1 & 6 & 1 \\ 1 & 1 & 6 \end{bmatrix} \text{ and is } \begin{bmatrix} 2 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 2 \end{bmatrix},$$

$$T'_dF_d \text{ should be equal to } \begin{bmatrix} 2 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 2 \end{bmatrix} \text{ and is } \begin{bmatrix} 0 & 2 & 2 \\ 2 & 0 & 2 \\ 2 & 2 & 0 \end{bmatrix}.$$

We find that f comes so much nearer to its orthogonality condition that $\mathscr{C}_f = 15/8\,\mathrm{pr}^\perp(1_3) \geq 3/2\,\mathrm{pr}^\perp(1_3) = \mathscr{C}_d$.

In the following we consider the situation that $t\,|\,n$ and $t\,|\,p$ and that we have only designs without preperiod to compare. We have seen in Section 4 that for generalized latin squares without preperiod, the orthogonality condition (4.2) is equivalent to strong balance. Strongly balanced generalized latin squares can only exist if $t^2\,|\,n$ and $p \geq 2t$ (see Cheng and Wu, 1980). If $p = t$, the nearest to strong balance one can get (for a design being uniform on the units) is balance. In this situation balanced designs are universally optimal for the estimation of direct effects over the class of designs which are uniform on the units and the last period.

We treat the situation that $p \geq 2$, but $t^2 \nmid n$. In order to come near to strong balance we make the following definition.

A design $d \in \Omega_{t,n,p}$ is *nearly strongly balanced*, if
(i) $T'_dF_dF'_dT_d$ is completely symmetric, and
(ii) for all $1 \leq i, j \leq t: m_{dij} \in \{[n(p-1)t^{-2}], [n(p-1)t^{-2}] + 1\}$.
T'_dF_d is the incidence matrix of a BBD with equal numbers of treatments and blocks. Theorem 5.2.1 of Raghavarao (1971) implies that $F'_dT_dT'_dF_d$ is also completely symmetric.

THEOREM 5.3. *Assume $n = at^2 + bt$, $1 \leq b \leq t-1$, $p = \lambda t$. A nearly strongly balanced* GLS $d^* \in \Omega_{t,n,p}$ *without preperiod is universally optimal for the estimation of direct effects over the class of all designs $f \in \Omega_{t,n,p}$ without preperiod which are uniform on the units and the last period.*

PROOF. (i) $\mathscr{C}_{d^*} = T'_{d^*}\mathrm{pr}^\perp([U\,|\,F_{d^*}])T_{d^*}$, as $T'_{d^*}\mathrm{pr}^\perp([U\,|\,F_{d^*}])P = 0$. Using Strategy 1, it suffices to show that $T'_{d^*}\mathrm{pr}^\perp([U\,|\,F_{d^*}])T_{d^*}$ is completely symmetric and has maximal trace.

(ii) For every competing design f

$$T'_f\mathrm{pr}^\perp(U)T_f = npt^{-1}\mathrm{pr}^\perp(1_t), \qquad T'_f\mathrm{pr}(U)F_f = n(p-1)t^{-2}1_t1'_t,$$

$$F'_f\mathrm{pr}^\perp(U)F_f = n(p-1-p^{-1})t^{-1}I_t - n(p-2)t^{-2}1_t1'_t \leq n(p-1-p^{-1})t^{-1}I_t.$$

Thus

$$T_f'\mathrm{pr}^\perp([U \mid F_f])T_f \le npt^{-1}\mathrm{pr}^\perp(1_t) - tn^{-1}(p-1-p^{-1})^{-1}(T_f'F_f - n(p-1)t^{-2}1_t1_t') \cdot (F_f'T_f - n(p-1)t^{-2}1_t1_t').$$

Equality holds for designs g which are also uniform on the first period, as then $T_g'F_g - n(p-1)t^{-2}1_t1_t'$ has row-sums zero. For such g, $T_g'\mathrm{pr}^\perp([U \mid F_g])T_g$ is completely symmetric iff $T_g'F_gF_g'T_g$ is.

It remains to minimize

$$\mathrm{tr}[\{T_f'F_f - n(p-1)t^{-2}1_t1_t'\}\{F_f'T_f - n(p-1)t^{-2}1_t1_t'\}] = \textstyle\sum_{i=1}^t \sum_{j=1}^t (m_{fij} - npt^{-1} + a + bt^{-1})^2,$$

subject to the constraints

$$\textstyle\sum_{i=1}^t (m_{fij} - npt^{-2} + a + bt^{-1}) = 0$$

for every j, as

$$1_t'T_f'\mathrm{pr}^\perp(U)F_f = 0.$$

The minimum is attained if exactly b of the m_{dij} are (for every j) equal to $npt^{-2} - a - 1$ and $(t-b)$ are equal to $npt^{-2} - a$. The minimum is $\sum_{j=1}^t \{(bt^{-1})^2(t-b) + (1-bt^{-1})^2 b\} = b(t-b)$ and is attained by d^*. □

THEOREM 5.4. *Assume that $n = at^2 + bt$, $1 \le b \le t-1$, $p = \lambda t$. A nearly strongly balanced* GLS *$d^* \in \Omega_{t,n,p}$ without preperiod is universally optimal for the estimation of residual effects over the set of all designs without preperiod which are uniform on the units and the first and last periods.*

PROOF. (i) $F_{d^*}'\mathrm{pr}^\perp([U \mid T_{d^*} \mid F_{d^*}1_t])P = 0$ and it thus remains to show that $F_{d^*}'\mathrm{pr}^\perp([U \mid T_{d^*} \mid F_{d^*}1_t])F_{d^*}$ is completely symmetric and has maximal trace.

(ii) For every competing design f

$$F_f'\mathrm{pr}^\perp([U \mid T_f])F_f1_t = F_f'\mathrm{pr}^\perp(U)F_f1_t = p^{-1}t^{-1}n(p-1)1_t.$$

It follows that

$$F_f'\mathrm{pr}^\perp([U \mid T_f \mid F_f1_t])F_f = F_f'\mathrm{pr}^\perp(U)F_f - F_f'\mathrm{pr}(\mathrm{pr}^\perp(U)T_f)F_f - n(p-1)p^{-1}t^{-2}1_t1_t'.$$

Complete symmetry holds iff $F_f'T_fT_f'F_f$ is completely symmetric. This is true for d^*.

For every competing design

$$\mathrm{tr}(F_f'\mathrm{pr}^\perp([U \mid T_f \mid F_f1_t])F_f) = n(p-1) - p^{-1}\textstyle\sum_{i=1}^t \sum_{u=1}^n \tilde{n}_{fiu}^2 - tn^{-1}p^{-1}\sum_{i=1}^t \sum_{j=1}^t \{m_{fij} - n(p-1)t^{-1}\}^2 - n(p-1)p^{-1}t^{-1}.$$

Under the constraints

$$\textstyle\sum_{i=1}^t m_{dij} = \tilde{r}_{dj} = t^{-1}n(p-1), \qquad \sum_{i=1}^t \sum_{u=1}^n \tilde{n}_{diu} = n(p-1)$$

the maximal trace is attained by d^*.□

We use Strategy 2 to extend the result of Theorem 5.3 to optimality for the estimation of direct effects over all designs without preperiod. We see that with our rough methods this can only be shown for numbers of periods and units which are large.

PROPOSITION 5.5. *Consider the function $f(x) = \sum_{i=1}^m x_i^2$ with the constraints* (i) *$x_i (1 \le i \le m)$ is an integer,* (ii) $\sum_{i=1}^m x_i = m\lambda$, (iii) *at least z of the components x_i of x are not equal to λ. Then $c = m\lambda^2 + z$ is a lower bound of $f(x)$.*

PROOF. Define $d_i = \lambda - x_i (1 \le i \le m)$. Then $\sum_{i=1}^m d_i = 0$ and

$$\sum_{i=1}^{m} x_i^2 = \sum_{i=1}^{m} (\lambda - d_i)^2 = m\lambda^2 + \sum_{i=1}^{m} d_i^2 \geq m\lambda^2 + z. \qquad \square$$

PROPOSITION 5.6. *Let $t \mid p$ and assume that $d \in \Omega_{t,n,p}$ is not uniform on the units. Then*

$$\operatorname{tr}(\mathscr{C}_d) \leq \operatorname{tr}\{T_d' \operatorname{pr}^{\perp}(U) T_d\} \leq np(t-1)t^{-1} - 2p^{-1}.$$

PROOF. $\operatorname{tr}\{T_d' \operatorname{pr}^{\perp}(U) T_d\} = np - p^{-1} \sum_{i=1}^{t} \sum_{u=1}^{n} n_{diu}^2$. d is not uniform on the units. As $\sum_{i=1}^{t} n_{diu} = p$ for every u, at least two of the n_{diu} are not equal to pt^{-1}. Proposition 5.5 implies the conjecture. □

PROPOSITION 5.7. *Let $t \mid p$ and $t \mid n$. Assume that $d \in \Omega_{t,n,p}$ is uniform on the units but not on the periods. Then*

$$\operatorname{tr}(\mathscr{C}_d) \leq \operatorname{tr}(T_d' \operatorname{pr}^{\perp}(P) T_d) \leq np(t-1)t^{-1} - 4n^{-1}.$$

PROOF. Uniformity on the units but not on the periods implies that at least four of the ℓ_{dik} are not equal to nt^{-1}. □

THEOREM 5.8. *Assume that $n = at^2 + bt$ $(1 \leq b \leq t-1)$ and $p = \lambda t$, such that $a \geq b(t - b - 1)t^{-1}$ and $\lambda \geq \max\{2, 4^{-1}b(t-b) + 2t^{-1}\}$. A nearly strongly balanced* GLS *without preperiod $d^* \in \Omega_{t,n,p}$ is universally optimal for the estimation of direct effects over the set of all designs without preperiod.*

PROOF. From Theorem 5.3 it follows that

$$\operatorname{tr}(\mathscr{C}_{d^*}) = np(t-1)t^{-1} - n^{-1}(p - 1 - p^{-1})^{-1} tb(t-b)$$

and that d^* is optimal over the set of all GLS. The conditions on n and p and Propositions 5.6 and 5.7 ensure that $\operatorname{tr}(\mathscr{C}_{d^*}) \geq \operatorname{tr}(\mathscr{C}_d)$ for every design $d \in \Omega_{t,n,p}$ which is no generalized latin square. □

If $t \leq 8$ and $b = t - 1$, the conditions on n and p imply that $n \in \{(t-1)t, t^2 + (t-1)t, \cdots\}$ and $p \in \{2t, 3t, \cdots\}$. Then the smallest nearly strongly balanced GLS for which we have proved optimality over $\Omega_{t,n,p}$ needs the same number of periods and t units less than the smallest strongly balanced GLS. If $t = 9$ the minimum number of periods is already $p = 3t$. For larger t it is still increasing.

EXAMPLE 5.9. If $t = 3$ and $n = p = 6$, then $b = 2$ and the nearly strongly balanced GLS

$$d^* = \underbrace{\begin{bmatrix} 1 & 2 & 3 & 1 & 2 & 3 \\ 2 & 3 & 1 & 1 & 2 & 3 \\ 3 & 1 & 2 & 2 & 3 & 1 \\ 3 & 1 & 2 & 3 & 1 & 2 \\ 2 & 3 & 1 & 3 & 1 & 2 \\ 1 & 2 & 3 & 2 & 3 & 1 \end{bmatrix}}_{\text{units}} \Bigg\} \text{periods, where} \quad T_{d^*}' F_{d^*} = \begin{bmatrix} 3 & 3 & 4 \\ 4 & 3 & 3 \\ 3 & 4 & 3 \end{bmatrix},$$

is universally optimal for the estimation of direct effects over $\Omega_{3,6,6}$. The first six units of d from example 4.13 form a design $d \in \Omega_{3,6,6}$ which is universally better for the estimation of residual effects than d^*

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