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UNIVERSAL OPTIMALITY OF A CLASS OF TYPE 2 AND ALLIED SEQUENCES

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SUMMARY. This paper proves the universal optimality of a particular kind of serially balanced type 2 sequences for estimating the direct and first order residual effects when the treatments are applied sequentially to a single experimental unit. Universal optimality results have also been obtained for some more general types of sequences. A method of construction has been suggested.

1. Introduction

In some experiments each experimental unit receives a number of treatments in succession. In such situations the 'residual effect' of a treatment in the following period is also an important source of variation along with its 'direct effect' in the period in which it is applied. Williams (1949) considered such a problem with several experimental units. In some situations, specially in the field of biological assay, there is only one subject which receives each treatment several times. For such experiments, Finney and Outhwaite (1955, 1956) introduced serially balanced sequences of types 1 and 2. Sinha (1975) proved the optimality properties of type 1 sequences. The objective of this paper is to investigate the optimality properties of type 2 sequences. In fact, this paper proves the optimality of a larger class of sequences, of which the type 2 sequences are a particular subclass.

A serially balanced type 2 sequence of order v and index m is a closed chain of symbols such that (i) each of the v distinct symbols occurs $m(v-1)$ times in the sequence, (ii) the sequence falls into $m(v-1)$ blocks each containing the v symbols once each, (iii) the $v(v-1)$ possible ordered pairs of distinct symbols occur exactly m times each, no symbol following itself.

A type 2 sequence is called completely reversible if each block ends or begins with the same symbol (Sampford (1957)).

Definition 1.1 : A serially balanced completely reversible type 2 sequence will be called a type 2* sequence if

(i) the sequence is of index 1 and

(ii) each block ends with the same symbol.

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Example 1.1 : With blocks written as rows and symbols 0, 1, 2, ..., two type 2 sequences are shown below of which the second one is a type 2* sequence.

(i) $v = 4$, $m = 1$

1 2 3 0

2 1 0 3

1 3 2 0

(ii) $v = 5$, $m = 1$

1 2 3 4 0

2 4 1 3 0

3 1 4 2 0

4 3 2 1 0

Interpreting symbols as treatments, it is immediate that in a type 2* sequence the direct effect versus residual effect incidence matrix is $\boldsymbol{E}_{vv}-\boldsymbol{I}_v$ (where $\boldsymbol{I}_v$ is the identity matrix of order v and $\boldsymbol{E}_{vv}$ is a $v\times v$ matrix with all elements unity), which is, in fact, the incidence matrix of a symmetric balanced incomplete block (SBIB) design. Therefore, Definition 1.1 may be extended to yield the following.

Definition 1.2 : A type $2^*(u)$ sequence of order v and length vu ($u \leqslant v-1$) is a closed chain of symbols such that (i) each of the v distinct symbols occurs u times in the sequence, (ii) the sequence falls into u blocks each containing the v symbols once each, (iii) the direct effect versus first order residual effect incidence matrix is that of an SBIB design and (iv) each block ends with the same treatment.

Clearly for practical applications a type $2^*(u)$ sequence is usually more economic than a type 2* sequence (since the former is of a shorter length) and reduces to a type 2* sequence if $u = v-1$. A construction procedure, with illustrations, for type $2^*(u)$ sequences has been presented in Section 4.

Let $\mathcal{C}(n)$ be the class of all sequences with v symbols and length n. It will be shown in this paper that within $\mathcal{C}(vu)$ a type $2^*(u)$ sequence, if it exists, is universally optimal (Kiefer (1975)) for estimating both direct and residual effects. As a corollary, the universal optimality of a type 2* sequence within $\mathcal{C}(v(v-1))$ will follow. These optimality results are fairly general since the competing designs are all possible designs of the same length.

It may be noted that a similar problem was considered by Hedayat and Afsarinejad (1978) in the context of repeated measurements designs. The set-up here is, however, completely different as there is only one experimental unit.

2. Model and notations

Consider an arrangement of v symbols (treatments) 0, 1, ..., $v-1$ according to any sequence in $\mathcal{C}(n)$. Suppose the sequence consists of b blocks. As usual (cf. Sampford (1957)) it may be assumed that the last treatment in the last block is also applied as a conditioning treatment right in the beginning of the sequence, any observation arising out of this conditioning treatment being excluded from the analysis.

Denoting by g_{ij}, h_{ij} the treatments whose direct and first order residual effects occur in y_{ij}, the j-th observation from the i-th block, one may take the following fixed-effects additive linear model,

$$y_{ij} = \mu+\beta_i+\delta_{g_{ij}}+\xi_{h_{ij}}+e_{ij}, \qquad \ldots \quad (2.1)$$

where μ is the general mean, β_i is the i-th block effect and δ_w, ξ_w are respectively the direct and first order residual effects due to the w-th treatment ($w = 0, 1, \ldots, v-1$), β_i, δ_w, ξ_w being measured from the general mean. The random disturbances e_{ij} are uncorrelated with means zero and a constant variance σ^2.

Let $\boldsymbol{N}^{(v\times b)}$ ($\boldsymbol{N}^{*(v\times b)}$) be the incidence matrix considering direct (first order residual) effects of treatments with respect to blocks. Denote by r_w the number of replications of the w-th treatment ($w = 0, 1, \ldots, v-1$) and by k_i the i-th block size ($i = 1, 2, \ldots, b$). Let $\boldsymbol{r}^\delta = \text{Diag}(r_0, \ldots, r_{v-1})$, $\boldsymbol{k}^\delta = \text{Diag}\,(k_1, \ldots, k_b)$. Also define $\boldsymbol{Z}^{(v\times v)} = ((z_{ww'}))$, where $z_{ww'}$ is the number of times the direct effect of the w-th treatment occurs with the first order residual effect of the w'-th treatment.

Then for any sequence in $\mathcal{C}(n)$, under the model (2.1), it can be easily seen that the coefficient matrices of the reduced normal equations for direct and first order residual effects are respectively given by

$$\begin{aligned} \boldsymbol{G}_1 &= \boldsymbol{r}^\delta-[\boldsymbol{Z}\;\boldsymbol{N}]\begin{bmatrix} \boldsymbol{r}^\delta & \boldsymbol{N}^* \\ \boldsymbol{N}^{*\prime} & \boldsymbol{k}^\delta \end{bmatrix}^-\begin{bmatrix} \boldsymbol{Z}' \\ \boldsymbol{N}' \end{bmatrix} \\ \boldsymbol{G}_2 &= \boldsymbol{r}^\delta-[\boldsymbol{Z}'\;\boldsymbol{N}^*]\begin{bmatrix} \boldsymbol{r}^\delta & \boldsymbol{N} \\ \boldsymbol{N}' & \boldsymbol{k}^\delta \end{bmatrix}^-\begin{bmatrix} \boldsymbol{Z} \\ \boldsymbol{N}^{*\prime} \end{bmatrix} \end{aligned} \qquad \ldots \quad (2.2)$$

3. The optimality results

In this section some universal optimality results will be obtained following a method due to Kiefer (1975). For that the following three lemmas will be required. The proof of the first lemma is trivial and hence omitted.

Lemma 3.1 : *Let* $\boldsymbol{X} = [\boldsymbol{X}_1, \boldsymbol{X}_2, \boldsymbol{X}_3]$. *Then*

$$[\boldsymbol{X}_1'\boldsymbol{X}_1 - \boldsymbol{X}_1'\boldsymbol{X}_2(\boldsymbol{X}_2'\boldsymbol{X}_2)^{-}\boldsymbol{X}_2'\boldsymbol{X}_1]$$
$$-\left[\boldsymbol{X}_1'\boldsymbol{X}_1 - (\boldsymbol{X}_1'\boldsymbol{X}_2 \;\; \boldsymbol{X}_1'\boldsymbol{X}_3)\begin{pmatrix}\boldsymbol{X}_2'\boldsymbol{X}_2 & \boldsymbol{X}_2'\boldsymbol{X}_3 \\ \boldsymbol{X}_3'\boldsymbol{X}_2 & \boldsymbol{X}_3'\boldsymbol{X}_3\end{pmatrix}^{-}\begin{pmatrix}\boldsymbol{X}_2'\boldsymbol{X}_1 \\ \boldsymbol{X}_3'\boldsymbol{X}_1\end{pmatrix}\right]$$

is nonnegative definite.

Lemma 3.2 : *Considering* $n = vu$ $(u \leqslant v-1)$, *for any sequence in* $\mathscr{C}(vu)$,

(i) $tr(\boldsymbol{G}_1) \leqslant v(u-1)$, (ii) $tr(\boldsymbol{G}_2) \leqslant v(u-1)$.

Proof : Since, by Lemma 3.1,

$$\boldsymbol{r}^{\delta} - \boldsymbol{Z}r^{-\delta}\boldsymbol{Z}' - \left[\boldsymbol{r}^{\delta} - (\boldsymbol{Z} \;\; \boldsymbol{N})\begin{pmatrix}\boldsymbol{r}^{\delta} & \boldsymbol{N}^* \\ \boldsymbol{N}^{*\prime} & \boldsymbol{k}^{\delta}\end{pmatrix}^{-}\begin{pmatrix}\boldsymbol{Z}' \\ \boldsymbol{N}'\end{pmatrix}\right]$$

is nonnegative definite, it follows by (2.2) that

$$\mathrm{tr}(\boldsymbol{G}_1) \leqslant \mathrm{tr}(\boldsymbol{r}^{\delta} - \boldsymbol{Z}\boldsymbol{r}^{-\delta}\boldsymbol{Z}') = n - \sum_{w=0}^{v-1}\sum_{w'=0}^{v-1}(z_{ww'}^2/r_{w'})$$
$$\leqslant n - \sum_{w=0}^{v-1}\sum_{w'=0}^{v-1}(z_{ww'}/r_{w'}) = v(u-1),$$

since $n = vu$ and $\sum_{w} z_{ww'} = r_{w'}$ for each w'. This proves (i). The proof of (ii) is similar.

Lemma 3.3 : *Considering* $n = vu(u \leqslant v-1)$, *for a type* 2^* (u) *sequence (if it exists)*

$$tr(\boldsymbol{G}_1) = tr(\boldsymbol{G}_2) = v(u-1).$$

Proof : By Definition 1.2, for a type $2^*(u)$ sequence the direct effect versus block and the first order residual effect versus block incidence matrices are those of a randomised block design. Thus $\boldsymbol{N} = \boldsymbol{N}^* = \boldsymbol{E}_{vu}$ and $\boldsymbol{r}^{\delta} = u\boldsymbol{I}_v$, $\boldsymbol{k}^{\delta} = v\boldsymbol{I}_u$, where $\boldsymbol{I}_m$ is the $m \times m$ identity matrix and $\boldsymbol{E}_{mm'}$, is an $m \times m'$ matrix with all elements unity. Further, the direct effect versus first order residual effect incidence matrix $\boldsymbol{Z}$ is that of an SBIB design and hence

$$\boldsymbol{Z}\boldsymbol{Z}' = (u-\lambda)\boldsymbol{I}_v + \lambda\boldsymbol{E}_{vv}, \qquad \ldots (3.1)$$

λ being the usual λ parameter of the SBIB design given by $\boldsymbol{Z}$. Hence by (2.2), for such a sequence

$$\boldsymbol{G}_1 = u\boldsymbol{I}_v - [\boldsymbol{Z} \; \boldsymbol{E}_{vu}]\begin{bmatrix}u\boldsymbol{I}_v & \boldsymbol{E}_{vu} \\ \boldsymbol{E}_{uv} & v\boldsymbol{I}_u\end{bmatrix}^{-}\begin{bmatrix}\boldsymbol{Z}' \\ \boldsymbol{E}_{uv}\end{bmatrix}.$$

Since

$$\begin{bmatrix} u\boldsymbol{I}_v & \boldsymbol{E}_{vu} \\ \boldsymbol{E}_{uv} & v\boldsymbol{I}_u \end{bmatrix}^{-} = \begin{bmatrix} u^{-1}\boldsymbol{I}_v & -(vu)^{-1}\boldsymbol{E}_{vu} \\ -(vu)^{-1}\boldsymbol{E}_{uv} & v^{-1}\boldsymbol{I}_u+(vu)^{-1}\boldsymbol{E}_{uu} \end{bmatrix}$$

one ultimately obtains, applying (3.1),

$$\boldsymbol{G}_1 = (\lambda/u)(v\boldsymbol{I}_v-\boldsymbol{E}_{vv}). \qquad \ldots \quad (3.2)$$

Hence, the fact that $\lambda(v-1) = u(u-1)$, leads to $\mathrm{tr}(\boldsymbol{G}_1) = v(u-1)$. Similarly one can check that $\mathrm{tr}(\boldsymbol{G}_2) = v(u-1)$.

Note that if $v = 2$, then the relation $v > u > \lambda$ makes $\boldsymbol{G}_i$ $(i = 1, 2)$ as in (3.2) a null matrix. To avoid such trivialities, consider hereafter $v > 2$. Then the matrix $\boldsymbol{G}_i$ $(i = 1, 2)$ for a type $2^*(u)$ sequence is completely symmetric (by (3.2)) and has maximum trace (by Lemmas 3.2, 3.3) in $\mathcal{C}(vu)$. Therefore, by Proposition 1 in Kiefer (1975), the following universal optimality result holds.

Theorem 3.1 : *Within the class $\mathcal{C}(vu)$ if a type $2^*(u)$ sequence exists then it is universally optimal for both direct and first order residual effects, under the model assumed, provided $v > 2$.*

Since a type 2^* sequence is nothing but a type $2^*(u)$ sequence of length $v(v-1)$, the following corollary is immediate.

Corollary 3.1 : *Within the class $\mathcal{C}$ $(v(v-1))$ if a type 2^* sequence exists then it is universally optimal for both direct and first order residual effects, under the model assumed, provided $v > 2$.*

4. A METHOD OF CONSTRUCTION

This section considers the problem of construction of type 2^* and type $2^*(u)$ sequences. Recall that a type 2^* sequence is nothing but a serially balanced completely reversible type 2 sequence of index unity, where each block ends with the same treatment. For the details of construction of such sequences, reference is made to Sampford (1957). Following Sampford, a type 2^* sequence in v symbols for every odd $v (v \geqslant 3)$ and also for some even v can always be constructed.

As for type $2^*(u)$ sequences, which are generalisations of type 2^* sequences, the constructional aspects pose more stringent combinatorial problems. A method of construction, obtained by suitably modifying the method of differences for the construction of balanced incomplete block designs (Raghavarao (1971, Ch. 5)) and having a satisfactory coverage, is described below.

Suppose v is a prime and let M be a module $\{0, 1, \ldots, v-1\}$ and $S = \{a_1, \ldots, a_u\}$ be a set of u distinct nonzero elements of M such that among the ordered differences arising out of S, each nonzero element of M is repeated a constant number (say, λ) of times. Then

$$\begin{matrix} a_1 & 2a_1 & \ldots & (v-1)a_1 & 0 \\ a_2 & 2a_2 & \ldots & (v-1)a_2 & 0 \\ & & \vdots & & \\ a_u & 2a_u & \ldots & (v-1)a_u & 0 \end{matrix}, \qquad \ldots \quad (4.1)$$

where each entry is reduced mod v, can be seen to be a type $2^*(u)$ sequence (with blocks, as usual, given by rows) in v symbols and length vu. This is because, with notations as before, clearly $\boldsymbol{N} = \boldsymbol{N}^* = \boldsymbol{E}_{vu}$. Further, for $0 \leqslant w \leqslant v-1$, in (4.1), the symbol w is followed by the symbols $w+a_i$ $(1 \leqslant i \leqslant u)$. Hence Z is the incidence matrix of the SBIB design generated by the method of differences from the initial set $\{a_1, \ldots, a_u\}$, proving our assertion.

In particular, if $v = 4t+3$ be a prime then S may be taken as any block (not containing the symbol zero) of the SBIB design, constructed by the method of differences, involving $(4t+3)$ symbols, having block size $(2t+1)$ and the usual parameter $\lambda = t$ (Raghavarao (1971), p. 83). This gives a type $2^*(u)$ sequence with $v = 4t+3$, $u = 2t+1$. For example, if $v = 7$ or 11 one may take $S = \{1, 2, 4\}$ or $S = \{1, 3, 4, 5, 9\}$ respectively. Apart from this series, other SBIB designs, obtained by the method of differences, can be reoriented to yield type $2^*(u)$ sequences, as illustrated by the following example.

Example 4.1 : Let $v = 13$. Then $M = \{0, 1, \ldots, 12\}$. Taking $S = \{1, 2, 4, 10\}$, among the ordered differences arising out of S, each non-zero member of M is repeated λ $(= 1)$ times. On developing S, as in (4.1) as

$$\begin{matrix} 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 & 11 & 12 & 0 \\ 2 & 4 & 6 & 8 & 10 & 12 & 1 & 3 & 5 & 7 & 9 & 11 & 0 \\ 4 & 8 & 12 & 3 & 7 & 11 & 2 & 6 & 10 & 1 & 5 & 9 & 0 \\ 10 & 7 & 4 & 1 & 11 & 8 & 5 & 2 & 12 & 9 & 6 & 3 & 0 \end{matrix},$$

one gets a type 2^* (u) sequence with $v = 13$, $u = 4$. Incidentally, S is as well an initial block from which, by the method of differences, one can construct an SBIB design in 13 symbols having block size 4 and the usual parameter $\lambda = 1$.

5. Concluding remarks

As Definition 1.1 indicates, a type 2* sequence has index unity. A question naturally arises that if a type 2* sequence be repeated $m\,(>1)$ times, then whether such a sequence will also be universally optimal, both for direct and residual effects, within the class $\mathcal{C}(mv(v-1))$ of sequences of length $mv(v-1)$. The answer to the above question will, however, be in the negative as the following example illustrates.

Example 5.1 : With $v = 3$, $m = 3$, consider the two sequences

$$
\begin{array}{llcll}
S_1 : & 0\ 1\ 2 & \qquad\qquad & S_v : & 0\ 1\ 2 \\
 & 1\ 0\ 2 & & & 2\ 0\ 1 \\
 & 0\ 1\ 2\ , & & & 1\ 2\ 0\ . \\
 & 1\ 0\ 2 & & & 0\ 2\ 1 \\
 & 0\ 1\ 2 & & & 1\ 0\ 2 \\
 & 1\ 0\ 2 & & & 2\ 1\ 0
\end{array}
$$

S_1 is obtained by repeating a type 2* sequence thrice, while S_2 is a type 1 sequence (Sampford, 1957). Both S_1 and S_2 belong to $\mathcal{C}(18)$. By direct computation it can be shown that S_1 is inferior to S_2 from the point of view of D-optimality for estimating any complete set of orthonormal contrasts of direct effects. Hence S_1 cannot be universally optimal in $\mathcal{C}(18)$ for direct effects.

The above phenomenon is expected since if a type 2* sequence be repeated $m\,(>1)$ times then the direct effect versus residual effect incidence matrix no longer remains that of an SBIB design and the technique of Lemma 3.3 fails.

Before concluding, it may be remarked that the universal optimality results proved in this paper hold even if in the model (2.1) the random disturbances e_{ij} have a (known) intraclass correlation structure, instead of being uncorrelated. It may be pointed out that "class" in the intraclass correlation structure refers to a block. Since in this kind of experimentation all the observations relate to the same experimental unit, the study of optimality properties in the presence of correlation of this kind sometimes becomes relevant. The proof of this robustness property of the optimality results is lengthy but straightforward and, for the interested reader, reference may be made to Mukerjee and Sen (1983) for the details.

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