IMPROVING MULTI-WAY BLOCK DESIGNS AT THE COST OF NUISANCE PARAMETERS

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Abstract: For a model of multi-way elimination of heterogeneities we show that information on the parameters of interest is increased to an optimum by generating dependencies among nuisance parameters. Such designs realize more information than Youden designs and their generalizations.

1. Introduction

We consider an m-way classification, with additive fixed effects and no interaction, as given by

$$Y_{ij_1\cdots j_m l} = \alpha_i + \gamma_{j_1}^{(1)} + \cdots + \gamma_{j_m}^{(m)} = \sigma e_{ij_1\cdots j_m l}, \quad (1)$$

where α_i, for $i = 1, \ldots, v$, is the effect of level i of a treatment (or variety) factor, and $\gamma_{j_k}^{(k)}$, for $j_k = 1, \ldots, b_k$ and $k = 1, \ldots, m$, is the effect of level j_k of the k-th (out of m) blocking factor. The error terms $e_{ij_1\cdots j_m l}$ are assumed to be independent, each with mean 0 and variance 1, while $\sigma > 0$ is an unknown scaling factor. Interest is in the symmetrized treatment contrast $(\alpha_1 - \bar{\alpha}_., \ldots, \alpha_v - \bar{\alpha}_.)'$, with $\bar{\alpha}_. = \Sigma\alpha_i/v$, while the $\gamma_{j_k}^{(k)}$ effects are considered as nuisance parameters. The information matrix for the symmetrized treatment contrasts is called the C-matrix, as usual.

For such a setting Youden designs and generalizations thereof are known to be optimal (Krafft, 1978; Cheng, 1978, 1981). Here optimality refers to wide classes of criteria, in the spirit of Kiefer's (1975) concept of universal optimality. Moreover, optimality obtains only among a *subset* of all designs, namely among these designs which have uniform marginals between any two blocking factors. Delimiting a subset of competing designs is indeed essential, as demonstrated by example in Pukelsheim (1983, p. 38). That example is for two blocking factors with six levels each, and fails to indicate a general method.

In the present note we propose a general result on the optimality of block designs when the class of competing designs places *no* restriction on the marginals between any two blocking factor. The idea is simple: we choose designs with a heavy dependence structure between the levels of blocking factors. This destroys identifiability of certain nuisance parameters and thus effectively decreases their total number, while at the same time information about the parameters of interest is increased to an optimum.

In Section 2 we identify one-way block designs with null information for the treatment contrasts, producing the type of dependence to be aimed at.

In Section 3 we give the detailed result for two-way block designs, indicating the extension to the multi-way case in Section 4.

2. Simple block designs with one treatment per block

Consider a one-way classification (1), setting $b_1 = b$ and $j_1 = j$ for short. A design ξ may be identified with the $v \times b$ matrix W whose entries w_{ij} give the proportion of observations to be realized at level i of the treatment factor and at level j of the blocking factor. Let r be the v-dimensional treatment replication vector with entries $r_i = \Sigma_j w_{ij}$, and let s be the b-dimensional blocksize vector with entries $s_j = \Sigma_i w_{ij}$. Then the C-matrix is well known to have the explicit form

$$C(\xi) = \Delta_r - W\Delta_s^- W', \tag{2}$$

where Δ_r and Δ_s are diagonal matrices formed from the vectors r and s respectively, while $^-$ indicates generalized inversion and $'$ transposition.

It is intuitively clear that a design is useless for investigating treatment contrasts if each blocking level contains one single treatment level only. Formally we define a *one-treatment-per-block design* by requiring that just a single treatment level $i(j)$ appears with blocking level j, for all $j = 1, \ldots, b$. We now show that these are the designs with null information for the symmetrized treatment contrasts.

Lemma 1. *ξ is a one-treatment-per-block design if and only if $C(\xi) = 0$.*

Proof. For the direct part assume ξ to be a one-treatment-per-block design with associated weight matrix W. Letting $1\{\cdots\}$ be the indicator function with values 0 and 1,

$$w_{ij} = s_j 1\{i = i(j)\}.$$

Always $(W\Delta_s^- W')_{ik} = \Sigma_j w_{ij} s_j^- w_{kj}$. In case $i \neq k$ the latter equals

$$\Sigma_j s_j s_j^- s_j 1\{i = i(j)\} 1\{k = i(j)\} = 0,$$

and in case $i = k$ we obtain

$$\Sigma_j s_j 1\{i = i(j)\} = \Sigma_j w_{ij} = r_i.$$

In summary, $W\Delta_s^- W' = \Delta_r$, and $C(\xi) = 0$. For the converse part observe that if $C(\xi) = 0$ then $W\Delta_s^- W'$ is diagonal. The latter is impossible unless ξ is a one-treatment-per-block design. □

One-treatment-per-block designs were shown to provide maximal information in the interblock model which is associated with random block effects; see Christof and Pukelsheim (1985). At the opposite extreme Lemma 1 shows that under model (1) they provide as little information as possible, namely none at all. We now step up to two-way block designs.

3. Two-way blocks designs with a determining blocking factor

Consider a two-way classification (1), setting $b_1 = b$, $b_2 = c$, and $j_1 = j$, $j_2 = k$, for short. A design ξ now is a weight distribution on $\{1, \ldots, v\} \times \{1, \ldots, b\} \times \{1, \ldots, c\}$, and can no longer be identified by any one of its two-dimensional marginals W_1, W_2, or W_{12} between treatment factor and first blocking factor, treatment factor and second blocking factor, and first and second blocking factor, respectively. Let r, s, and t be the vectors of treatment replications and first and second blocksizes, respectively. The C-matrix then takes the form

$$C(\xi) = \Delta_r - W_1\Delta_s^- W_1' - (W_2 - W_1\Delta_s^- W_{12}) \times \bar{F}(W_2 - W_1\Delta_s^- W_{12})', \tag{3}$$

where $\bar{F}$ is a nonnegative definite generalized inverse of $F = \Delta_t - W_{12}'\Delta_s^- W_{12}$ (Pukelsheim, 1983, p. 36). We can take $\bar{F} = 0$ if $F = 0$, and this is where Lemma 1 comes in.

For a two-way block design ξ we shall say that the first blocking factor is a *determining factor* if just a single level $k(j)$ of the second blocking factor appears with level j of the first blocking factor, for all $j = 1, \ldots, b$. Our optimality result now is as follows.

Theorem 1. *Suppose ξ is a two-way block design with a determining first blocking factor and with a C-matrix of rank $v - 1$. Then ξ is uniformly optimal for the symmetrized treatment contrasts among all designs which have the same two-dimensional margi-*

nal between treatment factor and first blocking factor as ξ.

Proof. The C-matrix of ξ has maximal rank, by assumption. This shows that the symmetrized treatment contrasts are identifiable, whence the design ξ is feasible.

Let W_1 be the two-dimensional marginal of ξ between treatment factor and first blocking factor. In view of Lemma 1 we have $F=0$, so that (3) turns into $C(\xi)=\Delta_r - W_1\Delta_s^- W_1'$. As a result of (3) every competing design η has $C(\eta) = \Delta_r - W_1\Delta_s^- W_1' - G$, say, since ξ and η share W_1, and hence also r and s. Therefore the difference $C(\xi) - C(\eta)$ equals G, which itself is a nonnegative definite matrix. Hence the result. □

A two-way block design ξ with a determining first blocking factor is essentially reduced to a simple block design, rendering the effects of the second blocking factor non-identifiable. The example of Pukelsheim (1983, p. 38) illustrates that the designs of Theorem 1 are uniformly better than generalized Youden designs.

Extension to multi-way block designs is now quite feasible.

4. Multi-way block designs with a determining blocking factor

For a two-way design the roles of the first and second blocking factors are evidently interchangeable. This suggests the following definition for an m-way classification (1) with blocking factors $k=1,\ldots,m$.

Definition. A design ξ is said to have a *determining* blocking factor k if for every other blocking factor $l \neq k$ just a single level $j_l(j_k)$ appears with level j_k of factor k, for all $j_k = 1,\ldots,b_k$.

In a general m-way setting no closed form expression is available for the C-matrix of an arbitrary design ξ. However, when blocking factor k is a determining factor the essential quantities are the two-dimensional marginal W_k between treatment factor and k-th blocking factor, and its corresponding one-dimensional marginals r and s_k. These indeed prove sufficient for the computation of the C-matrix of such designs ξ.

Lemma 2. *The C-matrix of an m-way design ξ with determining blocking factor k is*

$$C(\xi) = \Delta_r - W_k\Delta_{s_k}^- W_k'.$$

Proof. The C-matrix of an arbitrary design ξ can be expressed as

$$C(\xi) = \Delta_r - W_k\Delta_{s_k}^- W_k' - \left(R - W_k\Delta_{s_k}^- S\right) \times \bar{F}\left(R - W_k\Delta_{s_k}^- S\right)', \tag{4}$$

with appropriate matrices R, S, and F; see formula (5) in Pukelsheim (1985). We do not need the explicit form of R, S, and F, except that F is nonnegative definite with blocks $\Delta_{s_l} - W_{lk}\Delta_{s_k}^- W_{lk'}$ for $l \neq k$, down the diagonal. Hence (4) generalizes (3), with $\bar{F}$ again denoting a nonnegative definite generalized inverse of F.

Thus if blocking factor k is a determining factor then F has a vanishing diagonal and, being nonnegative definite, must vanish itself. The feasible choice $\bar{F}=0$ now proves the lemma. □

The proof of Theorem 1 readily caries over to the multiway situation, giving the following general result.

Theorem 2. *Suppose ξ is an m-way block design with a determining blocking factor k and with a C-matrix of rank $v-1$. Then ξ is uniformly optimal for the symmetrized treatment contrasts among all designs which have the same two-dimensional marginals between treatment factor and k-th blocking factor as ξ.* □

Section 4 of Pukelsheim (1985) presents additional details about where optimality of generalized and pseudo Youden designs holds, and where it fails. Here we have taken a more constructive approach by explicitly giving those designs which are optimal.

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