Approximate theory of multiway block designs*

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ABSTRACT

Optimality properties of multiway block designs are deduced from the general results of J. Kiefer's approximate-design theory. In the model with additive effects these optimality properties solely depend on the two-dimensional marginals of the designs. Uniform designs, and designs whose two-dimensional marginals are products of the one-dimensional marginals, are shown to be optimal. Approximate Youden designs are introduced for the case when the support sets of the two-dimensional marginals are prescribed in advance. They are optimal in a relatively small class of competing designs only.

RÉSUMÉ

On se sert de la théorie des plans approximatifs de Kiefer pour déduire certaines propriétés d'optimalité des plans de blocs pluridimensionnels. Dans le cadre d'un modèle à effets additifs, ces propriétés optimales ne dépendent que des marges bidimensionnelles des plans d'expérience. On montre que les plans uniformes sont optimaux, de même que les plans dont les marges bidimensionnelles sont des produits de marges à une dimension. On introduit des plans approximatifs de Youden dans le cas où les supports des marges bidimensionnelles sont prescrits à l'avance. Ces derniers ne sont optimaux que par rapport à une classe relativement petite de plans rivaux.

1. INTRODUCTION

The approximate theory of block designs leads to structural insights which complement the optimality results from the exact theory, as has been demonstrated for a single blocking factor in recent work of Giovagnoli and Wynn (1981) and Pukelsheim (1983a). The present paper extends the approximate-theory approach to an arbitrary number of blocking factors, in models with additive effects and no interaction. It is the two-dimensional marginals of a multiway block design which determine its moment matrix, and hence its optimality properties.

In Section 2 we define various notions of product designs and identify their C-matrices. In Section 3 no restriction is placed on the set of support points. Variety-factor product designs are shown to be uniformly optimal among the designs with given variety marginals and universally optimal among all designs, for the variety contrasts (Theorem 2). Multiway product designs turn out to be simultaneously p-mean optimal among all

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designs, for a *maximal* parameter system (Theorem 3).

In Section 4 we turn to block designs with a restricted set of support points. Approximate Youden designs (AYDs) are introduced as the approximate analogue of exact Youden designs. AYDs are seen to be universally optimal for the variety contrasts (Theorem 5) and simultaneously p-mean optimal for a maximal parameter system (Theorem 6), within a rather small class of competing designs. We demonstrate that their optimality breaks down when the class of competing designs is made larger.

All our matrices are real. Transposition, generalized inversion, and Moore-Penrose inversion of a matrix A are denoted by A', A^-, and A^+, respectively. Block matrices are indicated by $[A:B]$. The orthogonal projections onto the equiangular line of $\mathbb{R}^v$ and onto its orthogonal complement are represented by J_v/v and $K_v = I_v - J_v/v$, respectively, where J_v is the $v \times v$ matrix with each entry unity and I_v is the $v \times v$ identity matrix. The equiangular line in $\mathbb{R}^v$ is $\mathbf{1}_v = (1, \ldots, 1)'$, and $\bar{\mathbf{1}}_v = \mathbf{1}_v/v$ is the stochastic vector corresponding to the uniform distribution on v points.

2. *C*-MATRICES OF PRODUCT DESIGNS

An approximate block design for v varieties in $b_1 \times \cdots \times b_m$ blocks, or simply a *multiway block design*, is a probability distribution ξ on the design space

$$\mathscr{X} = \{1, \ldots, v\} \times \{1, \ldots, b_1\} \times \cdots \times \{1, \ldots, b_m\},$$

indicating that a proportion $\xi(i, j_1, \ldots, j_m)$ of all observations is to be drawn when variety i is combined with factor levels $j_1, \ldots, j_m$. The *variety marginals* of a design ξ consist of the variety replication vector $r \in \mathbb{R}^v$ with entries $r_i = \xi(i, \cdot, \ldots, \cdot)$, the dots indicating summation. With an analogous definition factor k has *factor marginals*, or block-size vector, $s_k \in \mathbb{R}^{b_k}$. Two-dimensional marginals are identified with weight matrices, i.e. with matrices having nonnegative entries summing to unity. The *variety-factor marginals* with factor k are denoted by $W_k \in \mathbb{R}^{v \times b_k}$, and $W_{kl} \in \mathbb{R}^{b_k \times b_l}$ stands for the *factor-factor marginals* of two distinct factors k and l.

In the model with additive effects and no interaction (Cheng 1978, p. 1262) the *moment matrix* $M(\xi)$ of a design ξ is determined by its two-dimensional marginals W_k and W_{kl} according to

$$M(\xi) = \begin{bmatrix} \Delta_r & W_1 & W_2 & \cdots & W_m \\ W_1' & \Delta_1 & W_{12} & \cdots & W_{1m} \\ W_2' & W_{12}' & \Delta_2 & \cdots & W_{2m} \\ \vdots & \vdots & \vdots & & \vdots \\ W_m' & W_{1m}' & W_{2m}' & \cdots & \Delta_m \end{bmatrix} = \begin{bmatrix} \Delta_r & W \\ W' & E \end{bmatrix}, \quad \text{say,} \tag{1}$$

where $\Delta_r, \Delta_1, \ldots, \Delta_m$ are the diagonal matrices formed from the one-dimensional marginals $r, s_1, \ldots, s_m$ of ξ. The converse problem of constructing a design ξ from a given moment matrix M is discussed by Pukelsheim and Titterington (1986a).

Optimal designs will turn out to have product structure on their two-dimensional marginals, suggesting the following terminology. A multiway block design ξ with moment matrix $M(\xi)$ as in (1) is called a

variety-factor product design if $W_k = rs_k'$ for $k = 1, \ldots, m$,
factor-factor product design if $W_{kl} = s_k s_l'$ for $k \neq l$, $k, l = 1, \ldots, m$,

multiway product design if it is both a variety-factor and a factor-factor product design. The design $\boldsymbol{r} \otimes \boldsymbol{s}_1 \otimes \cdots \otimes \boldsymbol{s}_m$ is a very special case of a multiway product design.

Interest will be in the parameter system of symmetrized *variety contrasts* $(\alpha_1 - \overline{\alpha}., \ldots, \alpha_v - \overline{\alpha}.)' = \boldsymbol{K}_v\boldsymbol{\alpha}$, where $\boldsymbol{\alpha}$ is the v-dimensional vector of variety effects. Given a design ξ, its information matrix for $\boldsymbol{K}_v\boldsymbol{\alpha}$, called the *C-matrix*, is $\boldsymbol{C}(\xi) = ([\boldsymbol{K}_v : \boldsymbol{0}]\boldsymbol{M}(\xi)^- [\boldsymbol{K}_v : \boldsymbol{0}]')^+$ if $\boldsymbol{K}_v\boldsymbol{\alpha}$ is identifiable under ξ, and $\boldsymbol{C}(\xi) = 0$ otherwise. If $\boldsymbol{K}_v\boldsymbol{\alpha}$ is identifiable under ξ, then ξ has positive variety marginals. If ξ is a multiway product design with positive variety marginals, then $\boldsymbol{K}_v\boldsymbol{\alpha}$ is identifiable under ξ. The following theorem presents a set of useful representations for C-matrices.

THEOREM 1. *Suppose ξ is a multiway block design with moment matrix $\boldsymbol{M}(\xi)$ as in* (1) *such that the variety contrasts are identifiable. Then*

$$\boldsymbol{C}(\xi) = \boldsymbol{\Delta}_r - \boldsymbol{W}\boldsymbol{E}^-\boldsymbol{W}'. \tag{2}$$

For variety-factor product designs, (2) *specializes to*

$$\boldsymbol{C}(\xi) = \boldsymbol{\Delta}_r - \boldsymbol{r}\boldsymbol{r}', \tag{3}$$

and for factor-factor product designs, (2) *specializes to*

$$\boldsymbol{C}(\xi) = \boldsymbol{\Delta}_r - \boldsymbol{r}\boldsymbol{r}' - \sum_{k=1}^{m} (\boldsymbol{W}_k\boldsymbol{\Delta}_k^+\boldsymbol{W}_k' - \boldsymbol{r}\boldsymbol{r}'). \tag{4}$$

Proof. Define $\boldsymbol{C} = \boldsymbol{\Delta}_r - \boldsymbol{W}\boldsymbol{E}^-\boldsymbol{W}'$, which is invariant under the choice of E^- (Styan 1985, p. 45). First we show $\boldsymbol{C}(\xi) = \boldsymbol{C}$. Partition $\boldsymbol{M}(\xi)$ into

$$\boldsymbol{M}(\xi) = \begin{bmatrix} \boldsymbol{\Delta}_r & \boldsymbol{W}_1 & \boldsymbol{R} \\ \boldsymbol{W}_1' & \boldsymbol{\Delta}_1 & \boldsymbol{S} \\ \boldsymbol{R}' & \boldsymbol{S}' & \boldsymbol{T} \end{bmatrix},$$

and choose a symmetric generalized inverse $\bar{\boldsymbol{F}}$ of $\boldsymbol{F} = \boldsymbol{T} - \boldsymbol{S}'\boldsymbol{\Delta}_1^+\boldsymbol{S}$. Then a generalized inverse of $\boldsymbol{E}$ is

$$\bar{\boldsymbol{E}} = \begin{bmatrix} \boldsymbol{\Delta}_1^+ + \boldsymbol{\Delta}_1^+\boldsymbol{S}\bar{\boldsymbol{F}}\boldsymbol{S}'\boldsymbol{\Delta}_1^+ & -\boldsymbol{\Delta}_1^+\boldsymbol{S}\bar{\boldsymbol{F}} \\ -\bar{\boldsymbol{F}}\boldsymbol{S}'\boldsymbol{\Delta}_1^+ & \bar{\boldsymbol{F}} \end{bmatrix}.$$

With this choice direct computation yields the representation

$$\boldsymbol{C} = \boldsymbol{\Delta}_r - \boldsymbol{W}_1\boldsymbol{\Delta}_1^+\boldsymbol{W}_1' - (\boldsymbol{R} - \boldsymbol{W}_1\boldsymbol{\Delta}_1^+\boldsymbol{S})\bar{\boldsymbol{F}}(\boldsymbol{R} - \boldsymbol{W}_1\boldsymbol{\Delta}_1^+\boldsymbol{S})'. \tag{5}$$

Now $\boldsymbol{W}_1\boldsymbol{\Delta}_1^+\boldsymbol{W}_1'\boldsymbol{1}_v = \boldsymbol{r}$, and $(\boldsymbol{R} - \boldsymbol{W}_1\boldsymbol{\Delta}_1^+\boldsymbol{S})'\boldsymbol{1}_v = \boldsymbol{0}$. This gives $\boldsymbol{C}\boldsymbol{1}_v = 0$ and $\boldsymbol{C}^+\boldsymbol{1}_v = 0$. For $\boldsymbol{M}(\xi)$ choose the generalized inverse

$$\boldsymbol{G} = \begin{bmatrix} \boldsymbol{C}^+ & -\boldsymbol{C}^+\boldsymbol{W}\bar{\boldsymbol{E}} \\ -\bar{\boldsymbol{E}}\boldsymbol{W}'\boldsymbol{C}^+ & \bar{\boldsymbol{E}} + \bar{\boldsymbol{E}}\boldsymbol{W}'\boldsymbol{C}^+\boldsymbol{W}\bar{\boldsymbol{E}}' \end{bmatrix}.$$

Hence we have $\boldsymbol{C}(\xi) = ([\boldsymbol{K}_v : \boldsymbol{0}]\boldsymbol{G}([\boldsymbol{K}_v : \boldsymbol{0}]')^+ = (\boldsymbol{K}_v\boldsymbol{C}^+\boldsymbol{K}_v)^+ = \boldsymbol{C}^{++} = \boldsymbol{C}$.

When $\boldsymbol{W}_k = \boldsymbol{r}\boldsymbol{s}_k'$ for all k, then $\boldsymbol{W}_1\boldsymbol{\Delta}_1^+\boldsymbol{W}_1' = \boldsymbol{r}\boldsymbol{r}'$ and $\boldsymbol{R} = \boldsymbol{W}_1\boldsymbol{\Delta}_1^+\boldsymbol{S}$; thus (5) entails (3). When $\boldsymbol{W}_{kl} = \boldsymbol{s}_k\boldsymbol{s}_l'$ for all $k \neq l$, then $\boldsymbol{F} = \text{Blockdiag}\,[\boldsymbol{\Delta}_2 - \boldsymbol{s}_2\boldsymbol{s}_2' : \cdots : \boldsymbol{\Delta}_m - \boldsymbol{s}_m\boldsymbol{s}_m']$, and we find that (5) simplifies to (4) upon choosing $\bar{\boldsymbol{F}} = \text{Blockdiag}\,[\boldsymbol{\Delta}_2^+ : \cdots : \boldsymbol{\Delta}_m^+]$. Q.E.D.

Theorem 1 generalizes the well-known formula for simple block designs; the two-way results of Krafft (1978, p. 219), Raghavarao and Federer (1975, p. 731), and Pukelsheim (1983b, p. 36); and the multiway representation in Cheng (1978, p. 1265). Notice that a single iteration on Schur complementation in (5) suffices, independently of the number of blocking factors.

3. OPTIMALITY OF PRODUCT DESIGNS

The following theorem describes the optimality properties of variety-factor product designs. Its proof uses the inequality

$$\boldsymbol{W}_k \boldsymbol{\Delta}_k^+ \boldsymbol{W}_k' - \boldsymbol{r}\boldsymbol{r}' = (\boldsymbol{W}_k - \boldsymbol{r}\boldsymbol{s}_k')\boldsymbol{\Delta}_k^+(\boldsymbol{W}_k - \boldsymbol{r}\boldsymbol{s}_k')' \geqq \mathbf{0}, \tag{6}$$

with equality if and only if $\boldsymbol{W}_k = \boldsymbol{r}\boldsymbol{s}_k'$. This inequality also shows that (4) reflects the loss in information relative to (3) when variety-factor marginals fail to be product distributions.

THEOREM 2.

(a) *Let* $\boldsymbol{r} \in \mathbb{R}^v$ *be a positive stochastic vector. Then the variety-factor product designs with variety marginals* $\boldsymbol{r}$ *are the only uniformly optimal designs for the variety contrasts among the designs with variety marginals* $\boldsymbol{r}$*; their common C-matrix is* $\boldsymbol{\Delta}_r - \boldsymbol{r}\boldsymbol{r}'$.

(b) *The variety-factor product designs with uniform variety marginals* $\bar{\mathbf{1}}_v$ *are the only universally optimal designs for the variety contrasts among all designs; their common C-matrix is* $\rho \boldsymbol{K}_v$, *with* $\rho = 1/v$.

Proof. Part (a) simply uses the explicit estimate $\boldsymbol{C}(\xi) \leqq \boldsymbol{\Delta}_r - \boldsymbol{W}_1\boldsymbol{\Delta}_1^+\boldsymbol{W}_1' \leqq \boldsymbol{\Delta}_r - \boldsymbol{r}\boldsymbol{r}'$ which follows from (5) and (6); equality forces $\boldsymbol{W}_1 = \boldsymbol{r}\boldsymbol{s}_1'$. The same argument applies to any other factor k as well. Hence $\boldsymbol{C}(\xi) \leqq \boldsymbol{\Delta}_r - \boldsymbol{r}\boldsymbol{r}'$, with equality if and only if ξ is a variety-factor product design.

For part (b) partition the set of all designs into its subsets with given variety marginals $\boldsymbol{r}$ which, due to identifiability, must be positive. Applying (a) within these subsets, we see that we need compare the matrices $\boldsymbol{\Delta}_r - \boldsymbol{r}\boldsymbol{r}'$ only. The Cauchy inequality gives $\operatorname{trace} \boldsymbol{\Delta}_r - \boldsymbol{r}\boldsymbol{r}' = \mathbf{1} - \boldsymbol{r}'\boldsymbol{r} \leqq 1 - 1/v = \operatorname{trace} \rho\boldsymbol{K}_v$, with equality if and only if $\boldsymbol{r} = \bar{\mathbf{1}}_v$. Q.E.D.

The theorem extends earlier results for one- and two-way block designs, see Pukelsheim (1983a, p. 202; 1983b, p. 37). Loewner comparability among C-matrices of the special form $\boldsymbol{\Delta}_r - \boldsymbol{r}\boldsymbol{r}'$ is discussed by Baksalary and Pukelsheim (1985). An example where a two-way product design has gone unnoticed is the design d' of Kiefer (1958, p. 690).

We now pass to maximal parameter systems. For a multiway product design ξ with positive marginals, $\boldsymbol{r}, \boldsymbol{s}_1, \ldots, \boldsymbol{s}_m$ the matrix

$$\boldsymbol{G} = \operatorname{Blockdiag}[\boldsymbol{\Delta}_r^{-1} : \boldsymbol{\Delta}_1^{-1} - \boldsymbol{J}_{b_1} : \cdots : \boldsymbol{\Delta}_m^{-1} - \boldsymbol{J}_{b_m}]$$

is a reflexive generalized inverse of the moment matrix $\boldsymbol{M}$ of ξ, i.e., $\boldsymbol{MGM} = \boldsymbol{M}$ and $\boldsymbol{GMG} = \boldsymbol{G}$. Verification uses the idempotent matrix

$$\boldsymbol{MG} = \begin{bmatrix} \boldsymbol{I}_v & \mathbf{0} & \cdots & \mathbf{0} \\ \boldsymbol{s}_1\mathbf{1}_v' & \boldsymbol{I}_{b_1} - \boldsymbol{s}_1\mathbf{1}_{b_1}' & \cdots & \mathbf{0} \\ \vdots & \vdots & & \vdots \\ \boldsymbol{s}_m\mathbf{1}_v' & \mathbf{0} & \cdots & \boldsymbol{I}_{b_m} - \boldsymbol{s}_m\mathbf{1}_{b_m}' \end{bmatrix} = \boldsymbol{K}(\boldsymbol{s}), \quad \text{say}, \tag{7}$$

with $s = [s_1' : \cdots : s_m']'$; cf. Cheng (1978, p. 1264), Pukelsheim (1983a, p. 202). Hence $\boldsymbol{M}$ has maximal rank $v + \Sigma_{k=1}^m (b_k - 1)$ among all moment matrices. We consider the maximal parameter system $\boldsymbol{K}(s)'\boldsymbol{\beta}$, where $\boldsymbol{\beta}$ is the $(v + \Sigma b_k)$-dimensional vector of variety effects and factor-level effects. Recall that Kiefer's Φ_p-optimality is the same as maximizing the p-mean of the information matrices for the parameters of interest; cf. Pukelsheim (1983a).

THEOREM 3. *The multiway product designs with marginals* $\boldsymbol{r}, s_1, \ldots, s_m$ *are the only designs which are p-mean optimal for the maximal parameter system* $\boldsymbol{K}(s)'\boldsymbol{\beta}$, *simultaneously for all* $p \in [-\infty, +1]$, *among the designs* η *such that the one-dimensional marginals coincide with the corresponding member from* $\boldsymbol{r}, s_1, \ldots, s_m$, *unless this member is uniform, in which case the corresponding marginals of* η *is unrestricted.*

The proof parallels the proof of Theorem 5 in Pukelsheim (1983a) and is omitted. We next turn to incomplete block designs.

4. APPROXIMATE YOUDEN DESIGNS

Youden's (Youden 1937) rectangles, Kiefer's (Kiefer 1975) generalized Youden designs, and Cheng's (Cheng 1981) pseudo-Youden designs correspond to approximate designs with two-dimensional marginals which are uniform on restricted support sets. To be precise, associate with a fixed *variety-factor support set* $S_k \subset \mathscr{X}_k = \{1, \ldots, v\} \times \{1, \ldots, b_k\}$

the $v \times b_k$ indicator matrix $\boldsymbol{N}_k$ with (i, j_k) entry equal to unity or zero according as (i, j_k) lies in S_k or not,

the number of points $n_k = \mathbf{1}_v'\boldsymbol{N}_k\mathbf{1}_{b_k}$ in S_k, and

the weight matrix $\bar{\boldsymbol{N}}_k = \boldsymbol{N}_k/n_k$ of the uniform distribution on S_k.

A multiway block design ξ with moment matrix (1) is called an *approximate Youden design* (AYD) if it satisfies the following three properties:

(A) ξ has variety-factor marginals which are uniform distributions on support sets $S_k \subset \mathscr{X}_k$, i.e., $\boldsymbol{W}_k = \bar{\boldsymbol{N}}_k$ for all $k = 1, \ldots, m$.

(B) ξ is a factor-factor product design.

(C) ξ is balanced for the variety contrasts, i.e., $\boldsymbol{C}(\xi) = \rho\boldsymbol{K}_v$ for some $\rho > 0$.

An AYD with uniform factor marginals has uniform variety marginals, as follows from the following transcription of property (C).

THEOREM 4. *Suppose* ξ *is a multiway block design with uniform factor marginals which satisfies properties* (A) *and* (B); *let* $a = \Pi_{k=1}^m n_k^2$. *Then* (C) *holds true if and only if*

(C′) $a\Sigma_{k=1}^m b_k\bar{\boldsymbol{N}}_k\bar{\boldsymbol{N}}_k' = (\mu - \lambda)\boldsymbol{I}_v + \lambda\boldsymbol{J}_v$ *for some scalars* v, λ;

and in this case

(D) $\boldsymbol{r} = \bar{\mathbf{1}}_v$,

(E) $\lambda = (a/v)(m - \Sigma_{k=1}^m b_k/n_k)/(v - 1)$ *and* $v = (a/v)\Sigma_{k=1}^m b_k/n_k$ *are positive integers*,

(F) $\rho = 1/v - \Sigma_{k=1}^m (b_k/n_k - 1/v)/(v - 1) < 1/v$,

(G) $\operatorname{rank}[\boldsymbol{N}_1 : \cdots : \boldsymbol{N}_m] = v \leqq \Sigma_{k=1}^m b_k$.

The proof follows standard lines and is omitted. Formula (C′) requires $\Sigma_{k=1}^m \boldsymbol{N}_k\boldsymbol{N}_k'$ to be completely symmetric in case $b_1 = \cdots = b_m$ and $n_1 = \cdots = n_m$ as in Cheng (1981).

Hence AYDs are more general than Cheng's pseudo-Youden designs, in the approximate theory. The inequality $\rho < 1/v$ in (F) exhibits the loss of information relative to the designs which appear in Theorem 2(b). The rank condition in (G) is an extension of Fisher's inequality on BIBDs. We now turn to the optimality properties of AYDs.

THEOREM 5. *An AYD ξ, with variety-factor support sets $S_1, \ldots, S_m$ and positive one-dimensional marginals $\boldsymbol{r}, \boldsymbol{s}_1, \ldots, \boldsymbol{s}_m$, is universally optimal for the variety contrasts among the factor-factor product designs η whose variety-factor support sets are contained in $S_1, \ldots, S_k$ and whose one-dimensional marginals coincide with the corresponding member from $\boldsymbol{r}, \boldsymbol{s}_1, \ldots, \boldsymbol{s}_m$, unless r is uniform, in which case the variety marginals of η are unrestricted.*

Proof. Property (C) ascertains that ξ has a completely symmetric C-matrix. It remains to show that the C-matrix has maximal trace, and this will follow solely from properties (A) and (B). Thus merely assume that ξ satisfies properties (A) and (B) such that the treatment contrasts are identifiable, and denote its C-matrix by $\boldsymbol{C}$. Since trace $\bar{\boldsymbol{N}}_k \boldsymbol{\Delta}_k^{-1} \bar{\boldsymbol{N}}_k'$ equals b_k/n_k, the formula (4) yields

$$\operatorname{trace} \boldsymbol{C} = 1 + (m-1)\boldsymbol{r}'\boldsymbol{r} - \sum_{k=1}^{m} \frac{b_k}{n_k}. \tag{8}$$

In order to show that this is maximal we apply the necessary and sufficient condition (3) of Pukelsheim (1983a).

Identifiability entails $\boldsymbol{C}^+\boldsymbol{C} = \boldsymbol{K}_v$. For $\boldsymbol{M}(\xi)$ choose the generalized inverse

$$\boldsymbol{G} = \begin{bmatrix} \boldsymbol{C}^+ & -\boldsymbol{C}^+\bar{\boldsymbol{N}}_1\boldsymbol{\Delta}_1^{-1} & \boldsymbol{G}_2 & \cdots & \boldsymbol{G}_m \\ -\boldsymbol{\Delta}_1^{-1}\bar{\boldsymbol{N}}_1'\boldsymbol{C}^+ & \boldsymbol{\Delta}_1^{-1} + \boldsymbol{\Delta}_1^{-1}\bar{\boldsymbol{N}}_1'\boldsymbol{C}^+\bar{\boldsymbol{N}}_1\boldsymbol{\Delta}_1^{-1} & \boldsymbol{G}_{12} & \cdots & \boldsymbol{G}_{1m} \\ \boldsymbol{G}_2' & \boldsymbol{G}_{12}' & \boldsymbol{G}_{22} & \cdots & \boldsymbol{G}_{2m} \\ \vdots & \vdots & \vdots & & \vdots \\ \boldsymbol{G}_m' & \boldsymbol{G}_{1m}' & \boldsymbol{G}_{2m}' & \cdots & \boldsymbol{G}_{mm} \end{bmatrix}, \tag{9}$$

where for $k \neq l$, $k, l = 2, \ldots, m$,

$$\begin{aligned} \boldsymbol{G}_k &= -\boldsymbol{C}^+\bar{\boldsymbol{N}}_k(\boldsymbol{\Delta}_k^{-1} - \boldsymbol{J}_{b_k}), \\ \boldsymbol{G}_{1k} &= \boldsymbol{\Delta}_1^{-1}\bar{\boldsymbol{N}}_1'\boldsymbol{C}^+\bar{\boldsymbol{N}}_k(\boldsymbol{\Delta}_k^{-1} - \boldsymbol{J}_{b_k}), \\ \boldsymbol{G}_{kk} &= \boldsymbol{\Delta}_k^{-1} - \boldsymbol{J}_{b_k} + (\boldsymbol{\Delta}_k^{-1} - \boldsymbol{J}_{b_k})\bar{\boldsymbol{N}}_k'\boldsymbol{C}^+\bar{\boldsymbol{N}}_k(\boldsymbol{\Delta}_k^{-1} - \boldsymbol{J}_{b_k}), \\ \boldsymbol{G}_{kl} &= (\boldsymbol{\Delta}_k^{-1} - \boldsymbol{J}_{b_k})\bar{\boldsymbol{N}}_k'\boldsymbol{C}^+\bar{\boldsymbol{N}}_l(\boldsymbol{\Delta}_l^{-1} - \boldsymbol{J}_{b_l}). \end{aligned}$$

We then obtain $\boldsymbol{C}[\boldsymbol{K}_v : \boldsymbol{0}]\boldsymbol{G} = \boldsymbol{K}_v[\boldsymbol{I}_v : \boldsymbol{V}_1 : \cdots : \boldsymbol{V}_m] = \boldsymbol{K}_v[\boldsymbol{I}_v : \boldsymbol{V}]$, say, with $\boldsymbol{V}_1 = -\bar{\boldsymbol{N}}_1\boldsymbol{\Delta}_1^{-1}$ and with $\boldsymbol{V}_k = \boldsymbol{r}\boldsymbol{1}_{b_k}' - \bar{\boldsymbol{N}}_k\boldsymbol{\Delta}_k^{-1}$ for $k \geqq 2$. Now for every competing design η with moment matrix

$$\boldsymbol{A} = \begin{bmatrix} \boldsymbol{\Delta}_t & \boldsymbol{W} \\ \boldsymbol{W}' & \boldsymbol{E} \end{bmatrix}$$

we must evaluate, with $\boldsymbol{K} = [\boldsymbol{K}_v : \boldsymbol{0}]'$,

$$\operatorname{trace} \boldsymbol{C}\boldsymbol{K}'\boldsymbol{G}\boldsymbol{A}\boldsymbol{G}\boldsymbol{K}\boldsymbol{C} = 1 + 2\operatorname{trace} \boldsymbol{V}\boldsymbol{W}' + \operatorname{trace} \boldsymbol{V}\boldsymbol{E}\boldsymbol{V}';$$

see (3) in Pukelsheim (1983a). If η has variety-factor marginals $\boldsymbol{W}_k$ whose support is contained in S_k, block marginals equal to $\boldsymbol{s}_k$, and variety marginals $\boldsymbol{t}$, then lengthy but straightforward computation leads to $2\,\mathrm{trace}\, \boldsymbol{VW}' = 2(m-1)\boldsymbol{r}'\boldsymbol{t} - 2\sum b_k/n_k$, and $\mathrm{trace}\, \boldsymbol{VEV}' = (\mathrm{trace}\, \boldsymbol{\Sigma}) - (m-1)\boldsymbol{r}'\boldsymbol{r} + \sum b_k/n_k$, where

$$\boldsymbol{\Sigma} = \sum_{k \neq l} (\boldsymbol{r}\boldsymbol{1}'_{b_k} - \bar{\boldsymbol{N}}_k \boldsymbol{\Delta}_k^{-1}) \boldsymbol{W}_{kl} (\boldsymbol{r}\boldsymbol{1}'_{b_l} - \bar{\boldsymbol{N}}_l \boldsymbol{\Delta}_l^{-1})'. \tag{10}$$

Now if $\boldsymbol{t} = \boldsymbol{r}$ or $\boldsymbol{r} = \boldsymbol{\bar{1}}_v$, then $\boldsymbol{r}'\boldsymbol{t} = \boldsymbol{r}'\boldsymbol{r}$, and in view of (8) we obtain

$$\mathrm{trace}\, \boldsymbol{CK}'\boldsymbol{GAGKC} = \mathrm{trace}\, \boldsymbol{C} + \mathrm{trace}\, \boldsymbol{\Sigma}.$$

Finally, if η has factor-factor marginals $\boldsymbol{W}_{kl} = \boldsymbol{s}_k\boldsymbol{s}'_l$, then $\mathrm{trace}\,\boldsymbol{\Sigma}$ vanishes because $(\boldsymbol{r}\boldsymbol{1}'_{b_k} - \bar{\boldsymbol{N}}_k\boldsymbol{\Delta}_k^{-1})\boldsymbol{s}_k = \boldsymbol{0}$. The necessary and sufficient condition for trace optimality thus is verified. Q.E.D.

As in one-way settings (Pukelsheim 1983a, p. 207) an AYD ξ with uniform factor marginals will be seen to be optimal even for a certain maximal parameter system. Indeed, the matrix $\boldsymbol{G}$ from (9) is a symmetric and reflexive generalized inverse of the moment matrix $\boldsymbol{M}$ of ξ, and the rank of $\boldsymbol{M}$ is maximal. Define the matrix $\boldsymbol{K}(\xi) = \boldsymbol{MGD}$, with $\boldsymbol{D} = \mathrm{Blockdiag}[\boldsymbol{I}_v : b_1^{-1/2}\boldsymbol{I}_{b_1} : \cdots : b_m^{-1/2}\boldsymbol{I}_{b_m}]$. Then $\boldsymbol{K}(\xi)'\boldsymbol{\beta}$ is a maximal parameter system for which we have the following optimality result.

THEOREM 6. *An AYD ξ with variety-factor support sets $S_1, \ldots, S_m$ and uniform factor marginals is p-mean optimal for the maximal parameter system $\boldsymbol{K}(\xi)'\boldsymbol{\beta}$, simultaneously for all $p \in [-\infty, +1]$, among the designs η whose variety-factor support sets are contained in $S_1, \ldots, S_m$ and whose factor-factor marginals are uniform.*

Proof. Evidently $\boldsymbol{K}(\xi)'\boldsymbol{M}^-\boldsymbol{K}(\xi) = \boldsymbol{DGD} = \boldsymbol{B}$, say, and $\boldsymbol{B}$ has a representation $\boldsymbol{V}_1 + \boldsymbol{V}_2 + \rho\boldsymbol{V}_3 + \boldsymbol{V}_4$, where

$$\boldsymbol{V}_1 = \begin{bmatrix} \boldsymbol{K}_v & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{0} \end{bmatrix}, \quad \boldsymbol{V}_2 = \begin{bmatrix} \boldsymbol{0} & -\boldsymbol{K}_v\boldsymbol{Z} \\ -\boldsymbol{Z}'\boldsymbol{K}_v & \boldsymbol{0} \end{bmatrix}, \quad \boldsymbol{V}_3 = \begin{bmatrix} \boldsymbol{0} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{U} \end{bmatrix}, \quad \boldsymbol{V}_4 = \begin{bmatrix} \boldsymbol{0} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{Z}'\boldsymbol{K}_v\boldsymbol{Z} \end{bmatrix}$$

with $\boldsymbol{Z} = [b_1^{1/2}\bar{\boldsymbol{N}}_1 : \cdots : b_m^{1/2}\bar{\boldsymbol{N}}_m]$ and $\boldsymbol{U} = \mathrm{Blockidag}[\boldsymbol{I}_{b_1} : \boldsymbol{K}_{b_2} : \cdots : \boldsymbol{K}_{b_m}]$. Since $\boldsymbol{V}_1, \ldots, \boldsymbol{V}_4$ span a four-dimensional quadratic subspace of symmetric matrices, we may argue as in the proof of Theorem 7 of Pukelsheim (1983a). Fix $t > 0$. For every competing design η we must verify $\mathrm{trace}\, \boldsymbol{M}(\eta)\boldsymbol{D}^{-1}\boldsymbol{B}^{t+1}\boldsymbol{D}^{-1} \leqq \mathrm{trace}\, \rho\boldsymbol{B}^t$. But η has variety-factor support sets contained in S_k, whence for some $d_{t+1} > 0$ we obtain

$$\mathrm{trace}\, \boldsymbol{M}(\eta)\boldsymbol{D}^{-1}\boldsymbol{B}^{t+1}\boldsymbol{D}^{-1} = \rho\, \mathrm{trace}\, \boldsymbol{B}^t + d_{t+1}\, \mathrm{trace}\, \boldsymbol{\Sigma}.$$

Since η has uniform factor-factor marginals, we obtain $\mathrm{trace}\, \boldsymbol{\Sigma} = \boldsymbol{0}$, and the proof is complete. Q.E.D.

The question arises whether we can do away with demanding uniform factor-factor marginals. The answer is in the negative: Let ξ be an AYD with uniform factor marginals. We may use its variety-factor marginals $\bar{\boldsymbol{N}}_1, \ldots, \bar{\boldsymbol{N}}_m$ to construct a feasible competitor η according to

$$\eta(i, j_1, \ldots, j_m) = r_i \prod_{k=1}^{m} \frac{\bar{N}_k(i, j_k)}{r_i}.$$

The factor-factor marginals of η are $\boldsymbol{W}_{kl} = v\bar{\boldsymbol{N}}'_k\bar{\boldsymbol{N}}_l$. The necessary and sufficient condition for optimality of ξ will be violated when the trace of $\boldsymbol{\Sigma}$ from (10) is positive. But

$$\boldsymbol{\Sigma} = v \sum_{k \neq l} \boldsymbol{H}_k \boldsymbol{H}_l, \qquad \text{with} \quad \boldsymbol{H}_k = \bar{\boldsymbol{N}}_k \boldsymbol{\Delta}_k^{-1} \bar{\boldsymbol{N}}_k' - \bar{\mathbf{1}}_v \bar{\mathbf{1}}_v'.$$

Here $\boldsymbol{H}_k \geqq 0$, by (6), and so trace $\boldsymbol{H}_k \boldsymbol{H}_l \geqq 0$. This shows that trace $\boldsymbol{\Sigma} \geqq 0$ and that trace $\boldsymbol{\Sigma}$ vanishes if and only if $\boldsymbol{H}_k \boldsymbol{H}_l = 0$ for all $k \neq l$. But $\boldsymbol{H}_k \boldsymbol{H}_l = 0$ is equivalent to $\bar{\boldsymbol{N}}_k \boldsymbol{\Delta}_k^{-1} \bar{\boldsymbol{N}}_k' \bar{\boldsymbol{N}}_l \boldsymbol{\Delta}_l^{-1} \bar{\boldsymbol{N}}_l' = \boldsymbol{J}_v / v^3$, and taking ranks, this entails $v = 1$. Thus with the trivial exception of a single variety, an AYD ξ with uniform factor marginals fails to be trace-optimal for the variety contrasts, among the designs whose variety-factor support sets are contained in those of ξ.

Which design is optimal if not an AYD? This question is resolved in Pukelsheim and Titterington (1986b). The point is to move towards a maximal dependence structure between factor-factor marginals, thereby increasing information on the parameters of interest at the cost of having fewer nuisance parameters identifiable.

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