

Choosing designs for nested blocks*

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SUMMARY

A design is said to have nested blocks if the set of experimental units (plots) is partitioned into blocks and each block is further partitioned into subblocks. A review is given of estimators and their variances when information is combined from the plots stratum and the subblocks stratum. The relative size of these two stratum variances is usually unknown but a plausible range may be suggested by previous experiments. A method of comparing designs is proposed and is illustrated for several examples. It is shown that a design may be optimal for the intrablock analysis when subblocks are ignored, and also optimal for the intra-subblock analysis when blocks are ignored, without being optimal for the combination of information. Nevertheless, some theorems are proved showing that certain designs are optimal over certain classes of design when information is combined and the subblocks stratum variance is at least as big as the plots stratum variance. Heuristic strategies are proposed for finding good designs in other situations.

KEY WORDS: combining information, nested balanced block design, nested blocks, nested regular graph design, optimal design.

1. Introduction

Let Ω be a set of N plots, or experimental units. Suppose that Ω is partitioned into b blocks of ck plots each, and that each block is partitioned into c subblocks of k plots each: thus $N = bck$. Then subblocks are said to be *nested* in blocks; alternatively, we say that the partition of Ω into subblocks is *finer* than the partition of Ω into blocks.

The structure of nested blocks is a particular one of the infinite class of structures called *simple orthogonal block structures*, introduced by Nelder (1965a). His 1965 notation for this structure was $b \rightarrow c \rightarrow k$, but this has been replaced by $b/c/k$

*Dedicated to Professor Tadeusz Caliński on his 70-th birthday.

in many statistical computing packages, for example Genstat (Payne et al., 1993). Simple orthogonal block structures have been described in detail by Speed and Bailey (1982, 1987) and Bailey (1996).

Designs for nested blocks have been given by Preece (1967), Robinson (1970), Homel and Robinson (1972, 1975), Jimbo and Kuriki (1983), Dey, Das and Banerjee (1986), Banerjee and Kageyama (1990, 1993), Gupta (1993), and Mejza and Kageyama (1995, 1998). (Note that the phrase 'nested design' has a different meaning in the work of Federer, 1972 and Longyear, 1981: see Bailey, 1985.) However, there is no general advice on choosing among such designs.

In Sections 2–5 I review the theory of nested block designs as a special case of the theory of designs for simple orthogonal block structures. This review includes covariance structure, randomization, estimation, general balance, and combination of information. Caliński (1994, 1997) has also given the theory of nested block designs, especially randomization and combination of information, although from a slightly different perspective. Morgan (1996) also reviews the covariance structure and the multi-stratum analysis, and gives many methods of constructing designs.

In the remainder of the paper I discuss the problem of choosing a good design for the nested block structure, assuming that information will be combined from two strata, the ratio of whose stratum variances may be known approximately. Mukhopadhyay (1981), Bhattacharya and Shah (1984) and Bogacka and Mejza (1994) made a similar comparison of designs. They used the structure b/k and combined information from the two strata, assuming that the ratio of stratum variances is known. Designs for the structure $(b * b)/k$ have been compared by Bailey (1993) and Leeming (1998), under the assumption that only the bottom two strata are used for estimation. A harder problem, involving three unknown stratum variances, was solved in a few cases by Morgan and Uddin (1993) and Leeming (1997, 1998, 1999): there the structure is $b/(s * k)$ and information from the three bottom strata is combined.

2. Nested blocks

We define four *relation* matrices on Ω . These are symmetric matrices R_0 , R_B , R_S and R_P in $\mathbb{R}^{\Omega \times \Omega}$ with every entry equal to 0 or 1. We put R_0 equal to the all-1 matrix J_Ω and R_P equal to the identity matrix I_Ω . For elements α and β of Ω , the (α, β) -entry of R_B is equal to 1 if α and β are in the same block, and to 0 otherwise. Similarly, the (α, β) -entry of R_S is equal to 1 if α and β are in the same subblock, and to 0 otherwise.

We also define four subspaces V_0 , V_B , V_S and V_P of the real vector space \mathbb{R}^Ω . The subspace V_0 is the one-dimensional space consisting of the constant vectors, that is, those vectors taking the same value everywhere. The subspace V_B consists of those

vectors which take the same value throughout each block; and V_S consists of those vectors which take the same value throughout each subblock. The whole space is labelled V_P . Thus we have

$$V_0 < V_B < V_S < V_P$$

and the dimensions are 1, b , bc and N respectively. The matrices of orthogonal projection onto these four spaces are $N^{-1}R_0$, $(ck)^{-1}R_B$, $k^{-1}R_S$ and R_P respectively.

Define four further subspaces W_0 , W_B , W_S and W_P as follows:

$$\begin{aligned} W_0 &= V_0; \\ W_B &= V_B \cap V_0^\perp; \\ W_S &= V_S \cap V_B^\perp; \\ W_P &= V_S^\perp. \end{aligned}$$

These subspaces are called the *mean stratum*, the *blocks stratum*, the *subblocks stratum* and the *plots stratum* respectively. Their dimensions are equal to 1, $b - 1$, $b(c - 1)$ and $bc(k - 1)$. The matrices of orthogonal projection onto the four strata are Q_0 , Q_B , Q_S and Q_P , where

$$\begin{aligned} Q_0 &= N^{-1}R_0 = N^{-1}J_\Omega; \\ Q_B &= (ck)^{-1}R_B - N^{-1}R_0; \\ Q_S &= k^{-1}R_S - (ck)^{-1}R_B; \\ Q_P &= R_P - k^{-1}R_S = I_\Omega - k^{-1}R_S. \end{aligned}$$

Given a design on this set of plots, the appropriate randomization is as follows:

- (i) randomize blocks (that is, block labels);
- (ii) within each block separately and independently, randomize subblocks;
- (iii) within each subblock separately and independently, randomize plots.

Let Y be the random vector of responses on the plots when an experiment is performed. The above randomization procedure allows us to assume that

$$\text{Cov}(Y) = \xi_P Q_P + \xi_S Q_S + \xi_B Q_B + \xi_0 Q_0, \tag{1}$$

where ξ_P , ξ_S , ξ_B and ξ_0 are all non-negative (Nelder, 1965a; Bailey, 1981, 1991; Caliński, 1994, 1997; Caliński and Kageyama, 1991, 1996). If this randomization is the *only* source of variability then $\xi_0 = 0$ (Bardin and Azaïs, 1990). The quantities ξ_P , ξ_S , ξ_B and ξ_0 are called the *stratum variances*.

An alternative justification for Equation (1) is via components of variance: see Cornfield and Tukey (1956), Speed and Bailey (1987), Speed (1987) or Morgan (1996). It is assumed that there are independent random variables for each plot, each sub-

block, each block (and possibly one for the whole experiment). If the variances are σ^2 , σ_S^2 , σ_B^2 and σ_0^2 respectively then this leads to Equation (1) with $\xi_P = \sigma^2$, $\xi_S = k\sigma_S^2 + \sigma^2$, $\xi_B = ck\sigma_B^2 + k\sigma_S^2 + \sigma^2$ and $\xi_0 = N\sigma_0^2 + ck\sigma_B^2 + k\sigma_S^2 + \sigma^2$. Thus

$$\xi_P \leq \xi_S \leq \xi_B \leq \xi_0. \quad (2)$$

If subblocks and blocks have been chosen to encapsulate the natural heterogeneity of the experimental material then Equation (2) should hold. However, one or more of the inequalities may be reversed: see Nelder (1954). If subblocks are chosen to be representative rather than internally homogeneous, or if plots within a subblock have to compete for limited resources, then we may have $\xi_S < \xi_P$. In this paper I do not always assume that (2) is true.

3. Designs for nested blocks

Let Θ be a set of n treatments. Suppose that we wish to apply these treatments to the plots in Ω and perform an experiment to compare the treatments. Once Θ and Ω have been specified, a *design* Δ is just a function from Ω to Θ : plot ω receives treatment θ if and only if $\Delta(\omega) = \theta$. We can also represent Δ by the $\Omega \times \Theta$ *design matrix* X , defined by

$$X(\omega, \theta) = \begin{cases} 1 & \text{if } \Delta(\omega) = \theta \\ 0 & \text{otherwise.} \end{cases}$$

Our second assumption about Y is that

$$E(Y) = X\tau, \quad (3)$$

where τ is a vector of treatment effects in \mathbb{R}^Θ . A vector x in \mathbb{R}^Θ is called a *treatment contrast* if its entries sum to zero. We want to estimate the linear combinations $x'\tau$ for contrasts x .

Some classes of design for nested blocks have been extensively studied. In *split-plot* designs for two treatment factors our blocks and subblocks are usually called *blocks* and *whole plots* respectively. One main effect is estimated in the subblocks stratum; the interaction and the other main effect are estimated in the plots stratum. These designs are equi-replicate with replication b .

Other factorial designs for ck treatments in nested blocks are constructed by putting each treatment once in each block and *confounding* different (parts of) interactions or main effects with subblocks in each block.

When the treatments are unstructured and $n = ck$ our blocks and subblocks are often called *replicates* and *blocks* respectively. The design is *resolvable* if each treatment occurs once per block. It seems to me to be begging the question to call

a subset of Ω a *replicate*, because our blocks exist before the design Δ is chosen. Following a suggestion of Donald Preece, I also prefer to say that a design is *resolved* if it is a design for the structure $b/c/k$ in which each treatment occurs once per block, leaving the term *resolvable* for a block design for the structure $(bc)/k$ in which the subblocks *can* be grouped into sets containing each treatment once.

4. Estimation in one stratum

Nelder (1965b) showed how to use Equations (1) and (3) to derive the best linear unbiased estimators in each stratum. Projecting onto the plots stratum gives

$$E(Q_P Y) = Q_P X \tau \quad \text{and} \quad \text{Cov}(Q_P Y) = \xi_P Q_P.$$

Put $L_P = X'Q_P X$. If there is a vector z in \mathbb{R}^Θ such that $L_P z = x$ then the best linear unbiased estimator of $x'\tau$ in this stratum is $z'X'Q_P Y$, whose variance is $z'L_P z \xi_P$. If there is no such z then $x'\tau$ is not estimable in this stratum. If $x \in \text{Im}(L_P)$ then we may take $z = L_P^- x$, so the variance is $x'L_P^- x \xi_P$.

Compare this with the situation when $\text{Cov}(Y) = I_\Omega \sigma^2$. Then the best linear unbiased estimator of $x'\tau$, using all the data, has variance $x'(X'X)^{-1}x\sigma^2$. The ratio of these variances is

$$\frac{x'(X'X)^{-1}x \sigma^2}{x'L_P^- x \xi_P},$$

so the quantity $x'(X'X)^{-1}x/x'L_P^- x$ is called the *efficiency factor* for x in the plots stratum. The efficiency factor depends on the design and the contrast but not on the variability of the experimental units.

For θ in Θ , let r_θ be the replication of θ . Let T be the $\Theta \times \Theta$ diagonal matrix whose (θ, θ) -entry is $\sqrt{r_\theta}$, so that $T^2 = X'X$. Suppose that $T^{-1}x$ is an eigenvector of the symmetric matrix $T^{-1}L_P T^{-1}$ with eigenvalue e . Then e is the efficiency factor for x in the plots stratum. Pearce, Caliński and Marshall (1974) called such contrasts x the *basic contrasts* of the design.

James and Wilkinson (1971) defined the *canonical efficiency factors* of the design to be the eigenvalues of $XT^{-2}X'Q_P XT^{-2}X'$ on vectors of the form Xy for treatment vectors y other than multiples of the all-1 vector. But $XT^{-2}X'Q_P XT^{-2}X'Xy = eXy$ if and only if $L_P y = eT^2y$. In this case put $x = T^2y$: then x is a basic contrast.

Although he did not use the same words, Nelder (1965b) defined efficiency factors and basic contrasts for *all* strata of a multi-stratum design. So I shall refer to the $n - 1$ eigenvalues of $T^{-1}L_P T^{-1}$ (excluding the eigenvector with entries $\sqrt{r_\theta}$) as the canonical efficiency factors in the plots stratum, and the corresponding contrasts x as the basic contrasts in the plots stratum.

Similarly, put $L_S = X'Q_S X$ and $L_B = X'Q_B X$. If $x \in \text{Im}(L_S)$ then $x'\tau$ can be estimated in the subblocks stratum. The variance of the best linear unbiased estimator is $x'L_S^-x\xi_S$ and the efficiency factor for x in this stratum is $x'(X'X)^{-1}x/x'L_S^-x$. Basic contrasts and canonical efficiency factors for the subblocks stratum are defined analogously to those for the plots stratum.

In principle, we can also obtain estimators in the blocks stratum, with variances $x'L_B^-x\xi_B$. In this paper I shall assume that ξ_B is so large that there is no value in using such estimators. This assumption includes the limiting case that $\xi_B = \infty$, which corresponds to fixed block effects and may be a reasonable assumption if blocks are used for management operations such as harvesting: for example, see Williams and Matheson (1994, Section 8.3).

Mejza and Kageyama (1995) considered only designs for which $L_B = 0$, that is, there is no information on treatment contrasts in the blocks stratum. I do not restrict designs in this way. If n does not divide ck there can be no equi-replicate design with $L_B = 0$. Even when such designs exist they may not be optimal for combining information, as Example 2 shows.

There is no information on treatment contrasts in the mean stratum, so the term $\xi_0 Q_0$ may be ignored.

Both split-plot and confounded designs are *orthogonal* in the sense that $L_P T^{-2} L_S = L_P T^{-2} L_B = L_S T^{-2} L_B = 0$. However, $L_S \neq 0$, so some contrasts are estimable only in the subblocks stratum. It follows that the design in subblocks is not connected. For the rest of this paper I consider only designs that are connected in subblocks: thus L_P has rank $n-1$. Such designs are also connected in blocks, as Mejza and Kageyama (1998) showed.

5. Combining information

In many practical situations the stratum variances ξ_P and ξ_S have the same order of magnitude, so there is worthwhile information on τ available from both the plots and subblocks strata. Yates (1939, 1940) recommended that this information be combined. Among many later papers about combining information, the most relevant to my context here are Nelder (1968), Patterson and Thompson (1971), Corsten (1985), Caliński (1996, 1997) and Caliński and Kageyama (1996).

Let $\psi = \xi_S/\xi_P$. If ψ is known then we can project the data onto $W_P + W_S$ and use generalized least squares to obtain the best linear unbiased estimator of $x'\tau$; it is

$$x'L_{PS}^-X'(Q_P + \psi^{-1}Q_S)Y \quad (4)$$

and has variance

$$x' L_{PS}^- x \xi_P, \tag{5}$$

where $L_{PS} = L_P + \psi^{-1} L_S$. Our connectivity assumption implies that $\ker(L_{PS})$ consists of only the constant vectors in \mathbb{R}^Θ , so that $x'\tau$ is estimable in $W_P + W_S$ for all treatment contrasts x .

An alternative method is available when the basic contrasts of the two strata are the same. This condition is called *general balance*: it was introduced by Nelder (1965b) and has been discussed by Houtman and Speed (1983), Speed (1983), Bailey and Rowley (1990), Mejza (1992), Payne and Tobias (1992), Caliński (1993) and Bailey (1994). A design for nested blocks is generally balanced if and only if $L_P T^{-2} L_S = L_S T^{-2} L_P$; that is, if and only if the matrices $T^{-1} L_P T^{-1}$ and $T^{-1} L_S T^{-1}$ have common eigenvectors.

Suppose that x is a basic contrast in both strata, with efficiency factors e_P and e_S respectively. If e_P and e_S are both non-zero then $x'\tau$ can be estimated in both strata: let the estimators be Z_P and Z_S respectively. These have variances in the ratio $\xi_P/e_P :: \xi_S/e_S$, so the unbiased linear combination of Z_P and Z_S with the minimum variance is

$$\frac{\psi e_P Z_P + e_S Z_S}{\psi e_P + e_S}, \tag{6}$$

whose variance is

$$\frac{\psi \xi_P x' (X' X)^{-1} x}{\psi e_P + e_S}.$$

As Houtman and Speed (1983) showed, the two methods give identical estimators of $x'\tau$ when x is a basic contrast of a generally balanced design.

However, ψ is not usually known *a priori*. In the method of restricted maximum likelihood (REML), introduced by Patterson and Thompson (1971), ξ_P and ξ_S are estimated from $(I - X T^{-2} X') Y$ under the assumption that Y is multivariate normal. This gives an estimate of ψ , which is substituted for ψ in the generalized least squares estimator (4).

In the second method ψ also has to be estimated from the data. A popular initial estimate is the ratio of the residual mean squares in the subblocks and plots strata. The method can then be iterated. Each estimate $\hat{\tau}$ of τ gives a new estimate $\hat{\psi}$ of ψ from $Y - X \hat{\tau}$. Each $\hat{\psi}$ is then substituted into (6). The iterated procedure appears to converge (Nelder, 1968; Caliński and Kageyama, 1996), in which case it gives the same estimates as REML (Houtman and Speed, 1983; Patterson and Thompson, 1975).

If the design is generally balanced then $T^{-1} L_P T^{-1}$ has the same eigenvectors as $T^{-1} L_P T^{-1}$ and $T^{-1} L_S T^{-1}$ irrespective of the value of ψ . The numerical simplicity of the second method is related to the fact that we do not need to keep calculating explicit generalized inverses of L_{PS} for different values of ψ .

If the design is equi-replicate, the canonical efficiency factors can be found from the concurrence matrices. For treatments θ and η , the *concurrence* $\lambda_B(\theta, \eta)$ of θ and η in blocks is equal to the number of ordered pairs of plots (α, β) such that α and β are in the same block, $\Delta(\alpha) = \theta$ and $\Delta(\beta) = \eta$. If the design is binary in blocks then $\lambda_B(\theta, \theta) = r_\theta$. The concurrence matrix Λ_B for blocks has entries $\lambda_B(\theta, \eta)$. The concurrence matrix Λ_S for subblocks is defined similarly.

Now, $\Lambda_B = X'R_BX$ and $\Lambda_S = X'R_SX$, so $L_P = X'X - k^{-1}\Lambda_S$ and $L_S = k^{-1}\Lambda_S - (ck)^{-1}\Lambda_B$. If the design is equi-replicate with replication r then T is a scalar matrix and $T^2 = X'X = rI_\Theta$. Thus the design is generally balanced if and only if $\Lambda_B\Lambda_S = \Lambda_S\Lambda_B$. Moreover, x is a basic contrast with efficiency factors e_P and e_S if and only if $L_Px = re_Px$ and $L_Sx = re_Sx$: this happens if and only if x is an eigenvector of both Λ_S and Λ_B with eigenvalues rkf_S and ckf_B respectively, where

$$\begin{aligned} e_P &= 1 - f_S, \\ e_S &= f_S - f_B. \end{aligned}$$

It is convenient to summarize the canonical efficiency factors of a generally balanced equi-replicate nested block design in a table. For each common eigenspace of Λ_S and Λ_B there is a column containing dimension, f_B , e_S and e_P .

Example 1. The equi-replicate design Δ in Figure 1 has nine treatments in three blocks of twelve plots. Each block is partitioned into three subblocks of four plots.

$$\Delta = \begin{array}{|c|c|c|c|} \hline 1 & 3 & 7 & 9 \\ \hline 2 & 4 & 8 & 1 \\ \hline 6 & 8 & 3 & 5 \\ \hline 3 & 5 & 9 & 2 \\ \hline 7 & 9 & 4 & 6 \\ \hline 8 & 1 & 5 & 7 \\ \hline 4 & 6 & 1 & 3 \\ \hline 5 & 7 & 2 & 4 \\ \hline 9 & 2 & 6 & 8 \\ \hline \end{array}$$

Figure 1. An equi-replicate design for nested blocks which is not generally balanced

The concurrence matrices for design Δ are

$$\Lambda_S = \begin{bmatrix} 4 & 1 & 2 & 2 & 1 & 1 & 2 & 2 & 1 \\ 1 & 4 & 1 & 2 & 2 & 1 & 1 & 2 & 2 \\ 2 & 1 & 4 & 1 & 2 & 2 & 1 & 1 & 2 \\ 2 & 2 & 1 & 4 & 1 & 2 & 2 & 1 & 1 \\ 1 & 2 & 2 & 1 & 4 & 1 & 2 & 2 & 1 \\ 1 & 1 & 2 & 2 & 1 & 4 & 1 & 2 & 2 \\ 2 & 1 & 1 & 2 & 2 & 1 & 4 & 1 & 2 \\ 2 & 2 & 1 & 1 & 2 & 2 & 1 & 4 & 1 \\ 1 & 2 & 2 & 1 & 1 & 2 & 2 & 1 & 4 \end{bmatrix} \quad \text{and} \quad \Lambda_B = \begin{bmatrix} 6 & 5 & 6 & 5 & 5 & 5 & 5 & 6 & 5 \\ 5 & 6 & 5 & 6 & 5 & 6 & 5 & 5 & 5 \\ 6 & 5 & 6 & 5 & 5 & 5 & 5 & 6 & 5 \\ 5 & 6 & 5 & 6 & 5 & 6 & 5 & 5 & 5 \\ 5 & 5 & 5 & 5 & 6 & 5 & 6 & 5 & 6 \\ 5 & 6 & 5 & 6 & 5 & 6 & 5 & 5 & 5 \\ 5 & 5 & 5 & 5 & 6 & 5 & 6 & 5 & 6 \\ 6 & 5 & 6 & 5 & 5 & 5 & 5 & 6 & 5 \\ 5 & 5 & 5 & 5 & 6 & 5 & 6 & 5 & 6 \end{bmatrix}.$$

These do not commute with each other so the design Δ is not generally balanced. This shows that the concept of general balance is not vacuous. \square

Resolved designs are generally balanced because they have $\Lambda_B = rJ_\Theta$. Bailey and Speed (1986) show Nelder's method in detail for a particular class of resolved designs called rectangular lattices, which were introduced by Harshbarger (1947, 1949).

Homel and Robinson (1972, 1975) extended the definition of partially balanced designs from incomplete-block designs to designs for nested blocks: if either the blocks or the subblocks are ignored the design should be partially balanced, and the association scheme must be the same in the two cases. Houtman and Speed (1983) showed that such designs are generally balanced.

Of course, in a nested partially balanced block design it may happen that either the design in blocks or the design in subblocks (or both) is partially balanced with respect to an association scheme formed from the original one by merging classes. Banerjee and Kageyama (1993) give some examples. Homel and Robinson (1972) conjectured that the requirement for the association scheme to be the same is unnecessary, in other words, that if the design in blocks and the design in subblocks are both partially balanced then the two association schemes are both formed by merging classes in a third association scheme, with respect to which the whole design in partially balanced. The design Δ in Figure 1 is a counter-example. It is not generally balanced, so it cannot be partially balanced. However, the design in blocks is group divisible, while the design in subblocks is cyclic.

6. Assessing designs

If combination of information is envisaged when the experiment is designed, how should the design Δ be chosen?

A treatment contrast x is *simple*, or *elementary*, if $x'\tau = \tau(\theta) - \tau(\eta)$ for some treatments θ and η . Call this contrast $x_{\theta\eta}$. We shall measure the quality of a design Δ by the size of the average variance of the estimators of simple contrasts, assuming that information is combined from the plots and subblocks strata and that ψ is known. The smaller is this average variance the better is the design. From (5), this average variance is equal to $g(\Delta, \psi)\xi_P$, where

$$g(\Delta, \psi) = \frac{1}{n(n-1)} \sum_{\theta \in \Theta} \sum_{\eta \neq \theta} x'_{\theta\eta} L_{PS}^- x_{\theta\eta}. \tag{7}$$

(Of course, L_{PS} depends on both Δ and ψ .)

THEOREM 1. For every design Δ , $g(\Delta, \psi) = 2 \text{tr } L_{PS}^- / (n - 1)$.

Proof. For each fixed θ ,

$$\begin{aligned} \sum_{\eta \neq \theta} x'_{\theta\eta} L_{PS}^- x_{\theta\eta} &= \sum_{\eta \neq \theta} (L_{PS}^-(\theta, \theta) - L_{PS}^-(\theta, \eta) - L_{PS}^-(\eta, \theta) + L_{PS}^-(\eta, \eta)) \\ &= \sum_{\eta \in \Theta} (L_{PS}^-(\theta, \theta) - L_{PS}^-(\theta, \eta) - L_{PS}^-(\eta, \theta) + L_{PS}^-(\eta, \eta)). \end{aligned}$$

The row and column sums of L_{PS}^- are equal to zero, so

$$\begin{aligned} g(\Delta, \psi) &= \frac{1}{n(n-1)} 2n \sum_{\theta \in \Theta} L_{PS}^-(\theta, \theta) \\ &= \frac{2}{n-1} \text{tr } L_{PS}^-. \quad \square \end{aligned}$$

If Δ and Γ are two designs, write $\Delta \succsim_{\psi} \Gamma$ if $g(\Delta, \psi) \leq g(\Gamma, \psi)$, meaning that Δ is at least as good as Γ for this value of ψ . Similarly, put $\Delta \equiv_{\psi} \Gamma$ if $g(\Delta, \psi) = g(\Gamma, \psi)$, meaning that Δ and Γ are equally good for this value of ψ , and $\Delta \succ_{\psi} \Gamma$ if $g(\Delta, \psi) < g(\Gamma, \psi)$, meaning that Δ is strictly better than Γ for this value of ψ .

Although we expect ψ to be in $[1, \infty]$, in fact ψ could be any non-negative number. However, the values $\psi = 1$ and $\psi = \infty$ are special. When $\psi = 1$ we have $\xi_S = \xi_P$ and so the subblocks have no role and the strata W_P and W_S can be collapsed into a single stratum. Let Δ_B be the quotient block design for the structure $b/(ck)$ obtained from Δ by ignoring the subblocks. Then $g(\Delta, 1)\xi_P$ is the average variance of the estimators of simple contrasts in Δ_B using only intrablock information.

Let \succsim be the partial order on block designs such that \succ means "has a smaller value of the average variance of the intrablock estimators of simple contrasts than". Then $\Delta \succsim_1 \Gamma$ if and only if $\Delta_B \succsim \Gamma_B$. At the other extreme, if $\psi = \infty$ then $\xi_S = \infty$. As Williams and Matheson (1994, Section 8.3) explain, this forces all estimation to be done in the plots stratum, as if the subblock effects were fixed, making an extra contribution to (3). In practice, this is also done if ψ is finite but large. Let Δ_S be the quotient block design for the structure $(bc)/k$ obtained from Δ by ignoring the blocks. Then $\Delta \succsim_{\infty} \Gamma$ if and only if $\Delta_S \succsim \Gamma_S$.

When Δ is equi-replicate and generally balanced we can calculate $g(\Delta, \psi)$ directly from the canonical efficiency factors, as the following theorem shows.

THEOREM 2. *Let Δ be an equi-replicate generally balanced design for n treatments with replication r in nested blocks. Suppose that the basic contrasts are x_1, \dots, x_{n-1} , and that the canonical efficiency factors for x_i are e_{P_i} and e_{S_i} in the plots and*

subblocks strata, for $i = 1, \dots, n - 1$. Then

$$g(\Delta, \psi) = \frac{2}{rA(\Delta, \psi)},$$

where $A(\Delta, \psi)$ is the harmonic mean of the values $e_{P_i} + \psi^{-1}e_{S_i}$.

Proof. Since Δ is generally balanced with replication r , the eigenvalues of L_{PS} are 0 and $re_{P_i} + r\psi^{-1}e_{S_i}$ for $i = 1, \dots, n - 1$. Thus

$$\text{tr } L_{PS}^- = \sum_{i=1}^{n-1} \frac{1}{re_{P_i} + r\psi^{-1}e_{S_i}} = \frac{n-1}{rA(\Delta, \psi)}.$$

From Theorem 1, $g(\Delta, \psi) = 2/(rA(\Delta, \psi))$. \square

The quantity $A(\Delta, \infty)$ is the harmonic mean of the e_{P_i} . It is the A -criterion of the block design Δ_S . Similarly, $A(\Delta, 1)$ is the harmonic mean of the $e_{P_i} + e_{S_i}$, which is the A -criterion of the block design Δ_B . Theorem 2 for $\psi = \infty$ and $\psi = 1$ give Equation (2.9) of John (1987) for the block designs Δ_S and Δ_B .

Usually ψ is unknown *a priori* and must be estimated from the data. Let $h(\Delta, \psi)$ be the average variance of simple contrasts, divided by ξ_P , when design Δ is used and ψ is estimated. When ψ is estimated the estimators of treatment contrasts are no longer linear, so this variance depends heavily on the distribution of $Y - E(Y)$. Caliński (1996) and Caliński and Kageyama (1996) investigated the behaviour of the function analogous to h for ordinary block designs. Following Kackar and Harville (1984), they showed that $h(\Delta, \psi) \geq g(\Delta, \psi)$ but remarked that otherwise the behaviour of $h(\Delta, \psi)$ appears to be intractable, and that the approximation suggested by Kackar and Harville (1984) is unlikely to be useful unless Y has a multivariate normal distribution and $N - n$ is very large. In particular, there appears to be no analogue of Equation (7) or Theorem 2 for $h(\Delta, \psi)$. Caliński (1997) made a similar investigation for nested blocks, but under different assumptions from those in this paper: he assumed that either $L_B = 0$ or information from the blocks stratum is combined with information from the plots and subblocks strata. He reached similar conclusions about the intractability of h .

Programs such as the `reml` directive in Genstat print estimates of variance as if ψ had not been estimated, even though variances are increased when ψ is estimated (see also Kenward and Roger, 1997). For large values of ψ , this increase in variance nullifies the decrease in variance from combining information. Thus many statisticians revert to the inter-subblock analysis if $\hat{\psi}$ is large.

Write $\Delta \sqsupseteq_{\psi} \Gamma$ if $h(\Delta, \psi) \leq h(\Gamma, \psi)$. In the absence of precise knowledge of ψ and of \sqsupseteq_{ψ} , it is reasonable to hope that if ψ' is close to ψ then the partial order $\succ_{\psi'}$ is close to the partial order \sqsupseteq_{ψ} . Previous experiments on similar experimental units

may suggest an interval Ψ of plausible values for ψ . Although the best choice of Δ may depend on the value of ψ , there may exist a design which is near-optimal under \succsim_ψ for all ψ in Ψ .

7. Comparing designs

Suppose that Δ and Γ are two designs for nested blocks. If $\Delta \succsim_\psi \Gamma$ and we use Γ rather than Δ , then the relative increase in variance is $g(\Gamma, \psi)/g(\Delta, \psi) - 1$. Since Δ may be better than Γ for some values of ψ and worse for others, it is sensible to compare Δ and Γ across a range of values by plotting $g(\Gamma, \psi)$ and $g(\Delta, \psi)$ on a log scale against ψ . Lower values of g correspond to the better design. The use of the log scale on the vertical axis implies that vertical distances between the plotted curves have a consistent interpretation as relative decrease in variance. Moreover, there is some merit in showing ψ on a log scale too, because ψ is also a ratio. This graphical approach remains possible when there are three or more designs to be compared.

If Δ is not equi-replicate and generally balanced then $g(\Delta, \psi)$ must be evaluated from (7) by numerical inversion of L_{PS} or from Theorem 1 by numerical evaluation of the eigenvalues of L_{PS} . However, if Δ is equi-replicate and generally balanced then $g(\Delta, \psi)$ is a rational function of ψ . In fact, if Δ and Γ are both equi-replicate and generally balanced then

$$\begin{aligned} \Delta \succsim_\psi \Gamma &\iff A(\Delta, \psi) \geq A(\Gamma, \psi) \\ &\iff \sum_i \frac{1}{e_{P_i}^\Delta + \psi^{-1} e_{S_i}^\Delta} \leq \sum_i \frac{1}{e_{P_i}^\Gamma + \psi^{-1} e_{S_i}^\Gamma}, \end{aligned} \tag{8}$$

where the superscripts show which design the canonical efficiency factors refer to. Inequality (8) is equivalent to a polynomial inequality for ψ .

Example 2. Suppose that there are 12 treatments to be applied to 36 plots, and that the set of plots is partitioned into three blocks of three subblocks of four plots each. Three candidate designs are shown in Figure 2. The design Δ was chosen because Δ_S is optimal, being the dual of a balanced incomplete-block design. However, it is not resolved, so Δ_B is not as good as it might be. The other two designs Γ and Φ are both resolved, so Γ_B and Φ_B are both optimal. In fact, Γ , which is constructed by extending the idea of rectangular lattices by the method of Bose and Nair (1962), is the best design that I know among resolved designs, while Φ has optimal Φ_S among doubly resolved designs (Bailey, 1992) and is partially balanced with respect to the extended group divisible association scheme 2/3/2.

$$\Delta = \begin{array}{|c|c|c|c|} \hline 1 & 4 & 7 & 10 \\ \hline 2 & 4 & 9 & 11 \\ \hline 3 & 4 & 8 & 12 \\ \hline \end{array} \parallel \begin{array}{|c|c|c|c|} \hline 1 & 5 & 8 & 11 \\ \hline 2 & 5 & 7 & 12 \\ \hline 3 & 5 & 9 & 10 \\ \hline \end{array} \parallel \begin{array}{|c|c|c|c|} \hline 1 & 6 & 9 & 12 \\ \hline 2 & 6 & 8 & 10 \\ \hline 3 & 6 & 7 & 11 \\ \hline \end{array}$$

dim	2	3	6
f_B	$\frac{1}{4}$	0	0
e_S	0	0	$\frac{1}{4}$
e_P	$\frac{3}{4}$	1	$\frac{3}{4}$

$$\Gamma = \begin{array}{|c|c|c|c|} \hline 1 & 2 & 3 & 4 \\ \hline 1 & 2 & 7 & 11 \\ \hline 1 & 2 & 8 & 12 \\ \hline \end{array} \parallel \begin{array}{|c|c|c|c|} \hline 5 & 6 & 7 & 8 \\ \hline 5 & 6 & 4 & 12 \\ \hline 5 & 6 & 3 & 11 \\ \hline \end{array} \parallel \begin{array}{|c|c|c|c|} \hline 9 & 10 & 11 & 12 \\ \hline 9 & 10 & 3 & 8 \\ \hline 9 & 10 & 4 & 7 \\ \hline \end{array}$$

dim	5	4	2
f_B	0	0	0
e_S	0	$\frac{1}{4}$	$\frac{1}{2}$
e_P	1	$\frac{3}{4}$	$\frac{1}{2}$

$$\Phi = \begin{array}{|c|c|c|c|} \hline 1 & 2 & 3 & 4 \\ \hline 7 & 8 & 9 & 10 \\ \hline 5 & 6 & 11 & 12 \\ \hline \end{array} \parallel \begin{array}{|c|c|c|c|} \hline 5 & 6 & 7 & 8 \\ \hline 1 & 2 & 11 & 12 \\ \hline 3 & 4 & 9 & 10 \\ \hline \end{array} \parallel \begin{array}{|c|c|c|c|} \hline 9 & 10 & 11 & 12 \\ \hline 3 & 4 & 5 & 6 \\ \hline 1 & 2 & 7 & 8 \\ \hline \end{array}$$

dim	7	4
f_B	0	0
e_S	0	$\frac{1}{2}$
e_P	1	$\frac{1}{2}$

Figure 2. Three generally balanced designs for twelve treatments in three blocks of three subblocks of four plots, with their tables of canonical efficiency factors

Figure 2 also includes the table of canonical efficiency factors for each design. Hence we find that

$$\frac{33}{2}g(\Delta, \psi) = \frac{17}{3} + \frac{24\psi}{3\psi + 1},$$

$$\frac{33}{2}g(\Gamma, \psi) = 5 + \frac{16\psi}{3\psi + 1} + \frac{4\psi}{\psi + 1},$$

and

$$\frac{33}{2}g(\Phi, \psi) = 7 + \frac{8\psi}{\psi + 1}.$$

The functions $g(\psi)$ are plotted against ψ on a log-log scale in Figure 3.

The formulae for g show that

$$\Gamma \succ_{\psi} \Phi \iff (\psi - 1)^2 \geq 0.$$

So Γ is at least as good as Φ for all values of ψ , so there is no point in considering Φ

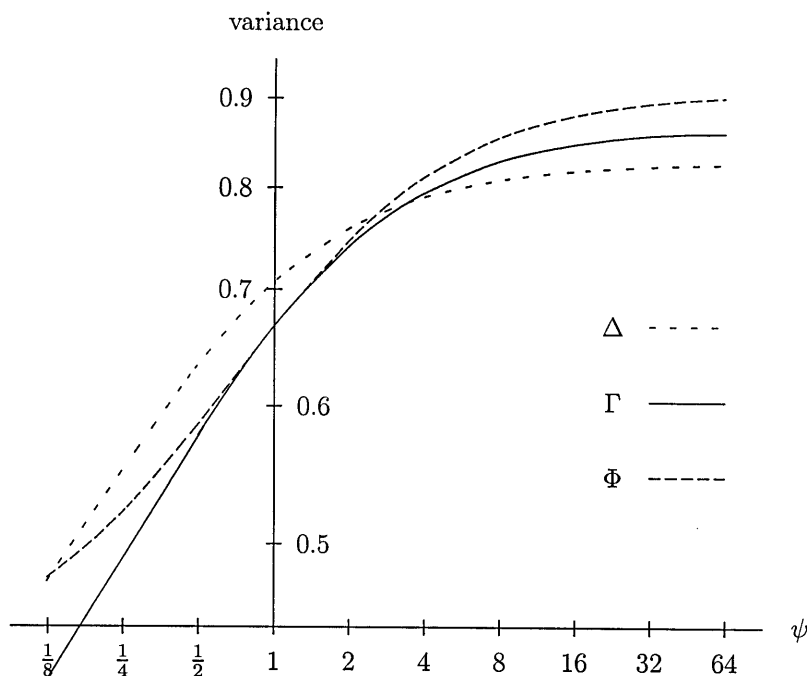


Figure 3. Average pairwise variance for each of the designs in Figure 2

further. On the other hand,

$$\Gamma \succ_{\psi} \Delta \iff 3\psi^2 - 10\psi - 1 \leq 0 \iff \psi \leq \frac{5 + 2\sqrt{7}}{3} \approx 3.43.$$

The value 3.43 is well within the range of plausible values of ψ in many practical examples. If you think that ψ will surely be larger than 5 then choose Δ . If you think that ψ will probably be between 1 and 2 then choose Γ . What should you do if you think that ψ lies in $[2.5, 4.5]$? The worst relative loss by choosing Γ is at $\psi = 4.5$, where $g(\Gamma, 4.5)$ is 0.9% more than $g(\Delta, 4.5)$, while the worst relative loss by choosing Δ is at $\psi = 2.5$, where $g(\Delta, 2.5)$ is 1.3% more than $g(\Gamma, 2.5)$. So a minimax strategy chooses Γ . In fact one could choose either design if $\psi \in [2.5, 4.5]$ because the relative increase in variance for the wrong choice is almost negligible. However, if ψ really is unknown then the loss from the wrong choice could be as high as 6%, or more if $\psi < 1$. \square

Consider the $2(n - 1)$ ordered pairs (e_P, e_S) which occur as canonical efficiency factors for the same basic contrast in either of the two designs. Those with $e_S = 0$ contribute constant terms to (8); those with $e_S \neq 0$ but with a given value u of the ratio e_P/e_S contribute the multiple e_S^{-1} of the same rational function $\psi/(u\psi + 1)$ of ψ to (8). For positive real numbers u , let $m_{\Delta}(u) = \sum_i 1/e_{S_i}^{\Delta}$, the sum being taken over those i for which $e_{S_i}^{\Delta} \neq 0$ and $e_{P_i}^{\Delta}/e_{S_i}^{\Delta} = u$; if there are no such i then $m_{\Delta}(u) = 0$. Define $m_{\Gamma}(u)$ similarly. Let

$$d(\Delta, \Gamma) = |\{u \in \mathbb{R}^+ : m_{\Delta}(u) \neq m_{\Gamma}(u)\}|.$$

Then the inequality (8) is equivalent to an integer polynomial inequality in ψ of degree $d(\Delta, \Gamma)$. For small values of $d(\Delta, \Gamma)$, the explicit solution of (8) may be as useful as the plotted graphs of $g(\Delta, \psi)$ and $g(\Gamma, \psi)$.

All three pairwise comparisons in Example 2 had $d = 2$, which led to quadratic inequalities and clear conclusions. The next example also has $d = 2$.

Example 3. Again suppose that there are 12 treatments, but that now there are 72 plots, arranged in six blocks of two subblocks of six plots. Figure 4 shows two possible designs. The design Δ is affine-resolved, so Δ_B is optimal and Δ_S is optimal among resolved designs (Bailey, Monod and Morgan, 1995). The design Γ is partially balanced with respect to the extended group divisible association scheme 3/2/2. It is not resolvable, so $\Gamma_B \prec \Delta_B$. However, Γ_S is group divisible for three groups of four, with between-group concurrence equal to one more than the within-group concurrence. It is semi-regular, so Theorem 2.2 of Cheng and Bailey (1991) shows that Γ_S is optimal.

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Figure 4. Two generally balanced designs for twelve treatments in six blocks of two subblocks of six plots, with their tables of canonical efficiency factors

From the canonical efficiency factors we calculate

$$\frac{66}{2}g(\Delta, \psi) = 5 + \frac{36\psi}{5\psi + 1}$$

and

$$\frac{66}{2}g(\Gamma, \psi) = \frac{43}{8} + \frac{54\psi}{8\psi + 1}.$$

Thus

$$\Delta \succ_{\psi} \Gamma \iff 8\psi^2 - 61\psi - 1 \leq 0 \iff \psi \leq \frac{61 + 3\sqrt{417}}{16} \approx 7.64.$$

Table 1 shows some values of $g(\Delta, \psi)$ and $g(\Gamma, \psi)$. The curves are plotted in Figure 5. For $\psi \in [1, \infty]$ the worst relative loss by choosing Γ is at $\psi = 1$, where it is 3.4%, while the worst relative loss by choosing Δ is at $\psi = \infty$, where it is 0.6%. Since subblock information is unlikely to be recovered if ψ is much bigger than 8, we

Table 1. Average variances of simple contrasts for the designs in Figure 4

ψ	2^{-3}	2^{-2}	2^{-1}	1	2	4	8	16	∞
$g(\Delta, \psi)$	0.2354	0.2727	0.3074	0.3333	0.3499	0.3593	0.3644	0.3670	0.3697
$g(\Gamma, \psi)$	0.2652	0.2992	0.3265	0.3447	0.3554	0.3612	0.3643	0.3658	0.3674

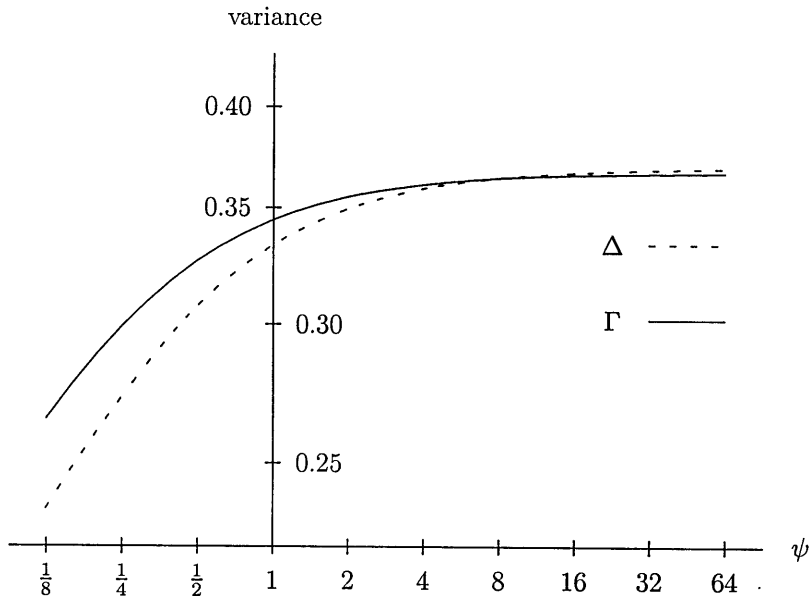


Figure 5. Average pairwise variance for each of the designs in Figure 4

can make a clear recommendation in this case: use Δ unless you are absolutely sure that subblock information will not be recovered, in which case use Γ . \square

We can expect more complicated behaviour when $d > 2$, for the graphs of $g(\Delta, \psi)$ and $g(\Gamma, \psi)$ may cross up to $d(\Delta, \Gamma)$ times. But both functions are monotonic increasing and differentiable, so $|\log g(\Gamma, \psi) - \log g(\Delta, \psi)|$ cannot be very large between the crossing points.

In Example 3 the clear recommendation is to use the design which is better for $\psi = 1$. Sometimes the opposite is the case.

Example 4. Figure 6 shows two designs for nine treatments in nine blocks of two subblocks of size two. Design Ξ is cyclic; it was chosen because, according to John and Mitchell (1977), Ξ_B is optimal. Design Π is partially balanced with respect to a Hamming association scheme $H(2, 3)$, and Π_B is only slightly worse than Ξ_B .

$$\Xi = \begin{array}{|c|c|c|c|} \hline 1 & 2 & 4 & 8 \\ \hline 3 & 4 & 6 & 1 \\ \hline 5 & 6 & 8 & 3 \\ \hline 7 & 8 & 1 & 5 \\ \hline 9 & 1 & 3 & 7 \\ \hline \end{array} \quad \begin{array}{|c|c|c|c|} \hline 2 & 3 & 5 & 9 \\ \hline 4 & 5 & 7 & 2 \\ \hline 6 & 7 & 9 & 4 \\ \hline 8 & 9 & 2 & 6 \\ \hline \end{array}$$

$$\Pi = \begin{array}{|c|c|c|c|} \hline 2 & 3 & 4 & 7 \\ \hline 1 & 2 & 6 & 9 \\ \hline 4 & 6 & 2 & 8 \\ \hline 8 & 9 & 1 & 4 \\ \hline 7 & 8 & 3 & 6 \\ \hline \end{array} \quad \begin{array}{|c|c|c|c|} \hline 1 & 3 & 5 & 8 \\ \hline 5 & 6 & 1 & 7 \\ \hline 4 & 5 & 3 & 9 \\ \hline 7 & 9 & 2 & 5 \\ \hline \end{array}$$

dim	2	2	2	2
f_B	$\frac{1}{4}$	$\frac{2+x}{16}$	$\frac{2+y}{16}$	$\frac{2+z}{16}$
e_S	0	$\frac{6-3x}{16}$	$\frac{6-3y}{16}$	$\frac{6-3z}{16}$
e_P	$\frac{3}{4}$	$\frac{4+x}{8}$	$\frac{4+y}{8}$	$\frac{4+z}{8}$

Here $x = \epsilon + \epsilon^8$, $y = \epsilon^2 + \epsilon^7$, and $z = \epsilon^4 + \epsilon^5$, where ϵ is a primitive ninth root of unity.

dim	4	4
f_B	$\frac{1}{16}$	$\frac{1}{4}$
e_S	$\frac{9}{16}$	0
e_P	$\frac{3}{8}$	$\frac{3}{4}$

Figure 6. Two generally balanced designs for nine treatments in nine blocks of two subblocks of two plots, with their tables of canonical efficiency factors

Graphs of $g(\psi)$ are shown in Figure 7, which should be contrasted with Figure 5. Although $d(\Xi, \Pi) = 4$, the graphs cross only at $\psi = 3/2$, where the polynomial equation $\Xi \equiv_{\psi} \Pi$ has a triple root. Thus $\Xi \succ_{\psi} \Pi$ if and only if $\psi \leq 1.5$. The difference between $g(\Xi, 1)$ and $g(\Pi, 1)$ is negligible, but Ξ is 5% worse than Π at $\psi = \infty$. So it seems safe to recommend choosing Π rather than Ξ . \square

The contrast between the conclusions in Examples 3 and 4 shows that it is not wise to choose a design solely on its behaviour at $\psi = 1$ (that is, ignoring subblocks) or on its behaviour at $\psi = \infty$ (that is, ignoring blocks).

I have deliberately plotted the graphs over a much wider range of ψ than seems necessary for practical purposes at first sight. Although we expect ψ to be greater than 1, it may happen that $\psi < 1$. Figures 3 and 7 demonstrate that variance curves which are close for $\psi \in [1, 8]$ may diverge sharply for smaller values of ψ . If possible,

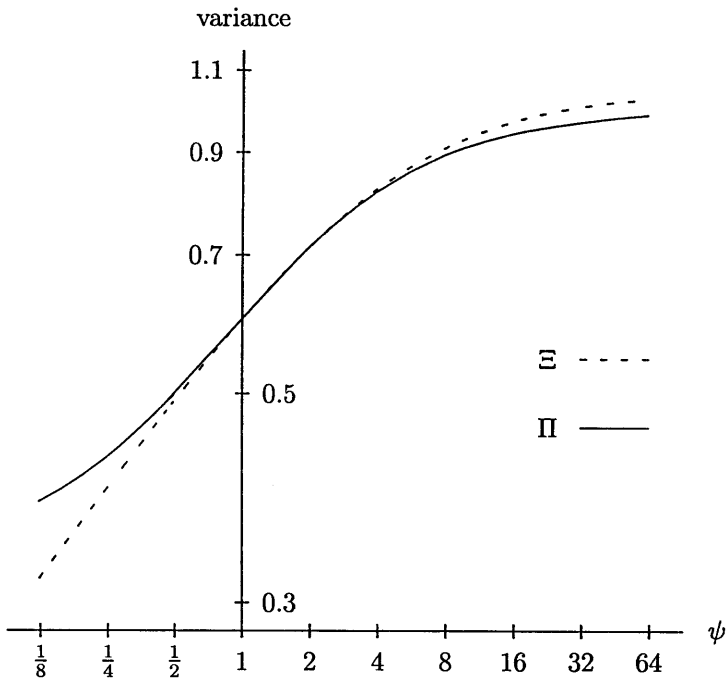


Figure 7. Average pairwise variance for each of the designs in Figure 6

we want to avoid choosing a design which is much worse than a competitor if ψ turns out to be a little smaller than it was expected to be. At the other end of the range, most statisticians would revert to the inter-subblock analysis if $\hat{\psi} > 8$ (some would do this even at $\hat{\psi} > 4$). But this is exactly the analysis for $\psi = \infty$. So if the graphs are curtailed at, say, $\psi = 8$, then they should be augmented by the values at $\psi = \infty$. If the information is given in tabular form, as in Table 1, then the value $\psi = \infty$ should always be included.

8. Combinatorial considerations

Preece (1967) defined a nested design Δ to be a *nested balanced incomplete-block design* if both Δ_B and Δ_S are balanced incomplete-block designs. Such a design must be equi-replicate with $ck < n$; moreover, $\lambda_S(\theta, \eta) = r(k - 1)/(n - 1)$ and $\lambda_B(\theta, \eta) = r(ck - 1)/(n - 1)$ whenever $\theta \neq \eta$. All contrasts in a nested balanced incomplete-block

design are basic contrasts, with

$$\begin{aligned} f_B &= \frac{n - ck}{(n - 1)ck}, \\ e_S &= \frac{n}{(n - 1)} \frac{(c - 1)}{ck}, \\ e_P &= \frac{n}{(n - 1)} \frac{(k - 1)}{k}. \end{aligned}$$

Example 5. An example Δ with $n = b = 9$, $c = 2$ and $k = 4$ can be constructed by writing the treatments in a 3×3 square array. For each treatment there is a corresponding block which contains all the other treatments. These treatments are allocated to the two subblocks in this block in the manner shown in Figure 8. The figure shows the block which omits the treatment in the empty cell. The treatments labelled * are in one subblock, those labelled \circ in the other.

	*	*
*	\circ	\circ
*	\circ	\circ

Figure 8. One block of a nested balanced incomplete-block design for nine treatments: see Example 5

This design has $f_B = 1/64$, $e_S = 9/64$ and $e_P = 27/32$ for all contrasts. Thus $A(\Delta, \psi) = (54 + 9\psi^{-1})/64$ and so Theorem 2 shows that $g(\Delta, \psi) = 16\psi/(54\psi + 9)$. \square

Morgan (1996) gives a table of known nested balanced incomplete-block designs with $n \leq 14$ and $r \leq 30$.

Following Kiefer's (1958) definition of balanced block design, we may generalize Preece's definition to *nested balanced block designs*. A nested design Δ is a nested balanced block design if

- (i) it is equi-replicate;
- (ii) each pair of entries in $X'R_S$ differ by at most one (these entries show how often a treatment occurs in a subblock);
- (iii) all off-diagonal elements in Λ_S are equal;
- (iv) each pair of entries in $X'R_B$ differ by at most one;
- (v) all off-diagonal elements in Λ_B are equal.

For example, if Δ_S is a complete-block design, or if Δ is a resolved balanced incomplete-block design, then Δ is a nested balanced block design.

Caliński (1971) commented on the importance of block designs in which all non-1 canonical efficiency factors in the plots stratum are equal. In such a design the treatments subspace of \mathbb{R}^Ω is an orthogonal direct sum of two parts, one of which is orthogonal to the blocks subspace and the other of which has first order balance with respect to the blocks subspace, in the terminology of James and Wilkinson (1971). Mejza and Kageyama (1998) conjectured that if Δ_S has this property then so has Δ_B . The design Δ in Figure 9 provides a counterexample.

If a block design is the dual of a balanced incomplete-block design but is not itself balanced then it has Caliński's property. Such designs are optimal, as we noted in Example 2. Cheng and Bailey (1991) proved that strongly regular graph designs are optimal if they have Caliński's property: hence the optimality of Γ_S in Example 3. (Regular graph designs are block designs whose concurrences take only two values, differing by one. Strongly regular graph designs are regular graph designs which are partially balanced with two associate classes.)

Block designs with Caliński's property are often very efficient. Other examples include the affine-resolvable designs, such as Δ_S in Figure 4, and various others, such as Δ_B and Φ_S in Figure 2, Γ_B in Figure 4, and Γ_B and Φ_B in Figure 13.

We also need the concept of isomorphic designs.

Designs Γ and Δ for nested blocks are *isomorphic* (written $\Gamma \cong \Delta$) if there is a permutation π_1 of the plot set Ω and a permutation π_2 of the treatment set Θ such that

(i) $\pi_2(\Gamma(\omega)) = \Delta(\pi_1(\omega))$ for all $\omega \in \Omega$;

(ii) α and β are in the same block if and only if $\pi_1(\alpha)$ and $\pi_1(\beta)$ are in the same block, for all α and β in Ω ;

(iii) α and β are in the same subblock if and only if $\pi_1(\alpha)$ and $\pi_1(\beta)$ are in the same subblock, for all α and β in Ω .

Isomorphism of block designs is defined similarly, but omitting one of conditions (ii) and (iii). Thus $\Delta_B \cong \Gamma_B$ if and only if (i) and (ii) are satisfied, while $\Delta_S \cong \Gamma_S$ if and only if (i) and (iii) are satisfied. If $\Delta \cong \Gamma$ then $\Delta_B \cong \Gamma_B$ and $\Delta_S \cong \Gamma_S$ but it is possible to have $\Delta_B \cong \Gamma_B$ and $\Delta_S \cong \Gamma_S$ without $\Delta \cong \Gamma$.

Example 6. Suppose that there are eight treatments to be applied to 32 plots arranged in eight blocks of two subblocks of two plots. Figure 9 shows three possible designs. They are all cyclic. John and Mitchell (1977) report that Γ_B is optimal. But $\Phi_B = \Gamma_B$, so $\Gamma \equiv_1 \Phi$ and Φ_B is also optimal, while Δ_B is only slightly worse. On the other hand, Δ_S is group divisible for two groups of four, with between-group concurrence equal to one more than the within-group concurrence, so the corollary to Theorem 3.1 of Cheng (1978) shows that Δ_S is optimal, while Γ_S and Φ_S are worse. In fact, $\Gamma_S \cong \Phi_S$, so $\Gamma \equiv_\infty \Phi$. Note, however, that Γ cannot be isomorphic to Φ , because the canonical efficiency factors e_S^Γ and e_S^Φ are different.

$$\Delta = \begin{array}{|c|c|c|c|} \hline 1 & 2 & 3 & 6 \\ \hline 3 & 4 & 5 & 8 \\ \hline 5 & 6 & 7 & 2 \\ \hline 7 & 8 & 1 & 4 \\ \hline \end{array} \quad \begin{array}{|c|c|c|c|} \hline 2 & 3 & 4 & 7 \\ \hline 4 & 5 & 6 & 1 \\ \hline 6 & 7 & 8 & 3 \\ \hline 8 & 1 & 2 & 5 \\ \hline \end{array}$$

dim	1	2	4
f_B	0	$\frac{1}{4}$	$\frac{1}{8}$
e_S	0	$\frac{1}{4}$	$\frac{3}{8}$
e_P	1	$\frac{1}{2}$	$\frac{1}{2}$

$$\Gamma = \begin{array}{|c|c|c|c|} \hline 1 & 2 & 5 & 7 \\ \hline 3 & 4 & 7 & 1 \\ \hline 5 & 6 & 1 & 3 \\ \hline 7 & 8 & 3 & 5 \\ \hline \end{array} \quad \begin{array}{|c|c|c|c|} \hline 2 & 3 & 6 & 8 \\ \hline 4 & 5 & 8 & 2 \\ \hline 6 & 7 & 2 & 4 \\ \hline 8 & 1 & 4 & 6 \\ \hline \end{array}$$

dim	1	2	2	2
f_B	$\frac{1}{4}$	$\frac{1}{8}$	$\frac{2-\sqrt{2}}{16}$	$\frac{2+\sqrt{2}}{16}$
e_S	$\frac{1}{4}$	$\frac{1}{8}$	$\frac{6+3\sqrt{2}}{16}$	$\frac{6-3\sqrt{2}}{16}$
e_P	$\frac{1}{2}$	$\frac{3}{4}$	$\frac{4-\sqrt{2}}{8}$	$\frac{4+\sqrt{2}}{8}$

$$\Phi = \begin{array}{|c|c|c|c|} \hline 1 & 7 & 2 & 5 \\ \hline 3 & 1 & 4 & 7 \\ \hline 5 & 3 & 6 & 1 \\ \hline 7 & 5 & 8 & 3 \\ \hline \end{array} \quad \begin{array}{|c|c|c|c|} \hline 2 & 8 & 3 & 6 \\ \hline 4 & 2 & 5 & 8 \\ \hline 6 & 4 & 7 & 2 \\ \hline 8 & 6 & 1 & 4 \\ \hline \end{array}$$

dim	1	2	2	2
f_B	$\frac{1}{4}$	$\frac{1}{8}$	$\frac{2-\sqrt{2}}{16}$	$\frac{2+\sqrt{2}}{16}$
e_S	$\frac{1}{4}$	$\frac{1}{8}$	$\frac{6-\sqrt{2}}{16}$	$\frac{6+\sqrt{2}}{16}$
e_P	$\frac{1}{2}$	$\frac{3}{4}$	$\frac{4+\sqrt{2}}{8}$	$\frac{4-\sqrt{2}}{8}$

Figure 9. Three cyclic designs for eight treatments in eight blocks of two subblocks of two plots, with their tables of canonical efficiency factors

The graphs $g(\psi)$ are plotted in Figure 10. The curves for Δ and Γ cross twice, and are very close between those crossing points. As in Example 4, design Δ can safely be recommended in preference to Γ . More surprising, perhaps, is that although $\Gamma \equiv_1 \Phi$ and $\Gamma \equiv_\infty \Phi$, $\Gamma \succ_\psi \Phi$ for all ψ in $(1, \infty)$. \square

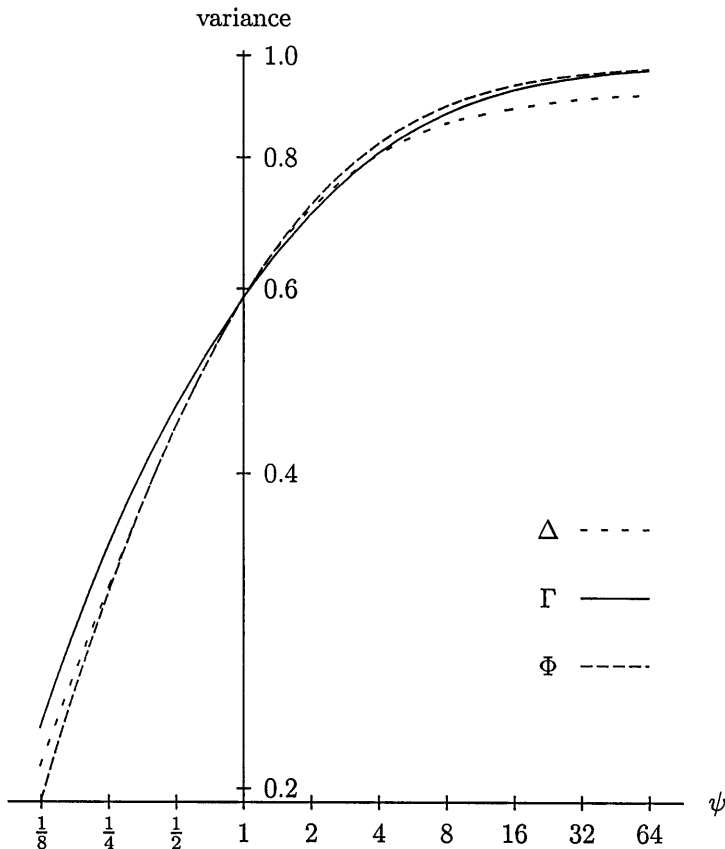


Figure 10. Average pairwise variance for each of the designs in Figure 9

9. Strategies for choosing designs

In the literature, strategies for choosing designs for nested blocks seem more implicit than explicit. It is generally assumed that we should seek designs Δ such that Δ_B and Δ_S are optimal block designs for the structures $b/(ck)$ and $(bc)/k$ respectively.

The knowledge that balanced block designs are optimal among equi-replicate block designs suggests the first strategy.

Strategy 1 If the design must be equi-replicate, choose Δ to be a nested balanced block design.

Nested balanced block designs are optimal when $\psi = 1$ and when $\psi = \infty$. Do they remain optimal for intermediate values of ψ ?

Strategy 1 is impossible for most quartets of values of n , b , c and k .

Strategy 2 If there are no nested balanced block designs, choose Δ so that both Δ_B and Δ_S are optimal block designs.

For example, if the design must be equi-replicate and $ck = n$ then Δ must be a resolved design and Δ_S must be optimal even over non-resolvable block designs. Examples include square lattice designs, which were introduced by Yates (1936) and shown to be optimal by Cheng and Bailey (1991).

Again, are they optimal for intermediate values of ψ ?

Strategy 3 Choose a block design Φ optimal for treatment-set Θ in b blocks of size ck . Choose Δ by partitioning the blocks of Φ into subblocks of size k (which ensures that

(i) $\Delta_B = \Phi$;

in such a way that

(ii) Δ is generally balanced, and

(iii) Δ_S is optimal subject to (i) and (ii).

This is the strategy recommended by Yates (1939), Bose and Nair (1962) and John and Williams (1995, Chapter 4) when the design must be equi-replicate and $n = ck$: choose an incomplete-block design that is optimal subject to being resolved. An example is the affine-resolved design Δ in Figure 4, which is optimal over resolved designs but not as good as the non-resolvable design Γ in Figure 4 when $\psi > 8$. The strategy also seems to be implicit in Mejza and Kageyama (1995). Similar advice for complicated block structures, that is, optimize for the larger blocks first, is given by Nguyen and Williams (1993) and Williams and John (1996).

Does this strategy give very poor designs for large values of ψ ?

We can consider the opposite strategy.

Strategy 4 Choose a block design Φ optimal for treatment-set Θ in bc subblocks of size k . Choose Δ by grouping the subblocks of Φ into blocks of size ck (which ensures that

(i) $\Delta_S = \Phi$;

in such a way that

(ii) Δ is generally balanced, and

(iii) Δ_B is optimal subject to (i) and (ii).

Does this strategy give poor designs for small values of ψ ?

Strategy 4 is effectively recommended by Gupta (1993), because he does not use the information in the subblocks stratum.

In both Strategies 3 and 4, one might want to ignore condition (ii).

Even if the first choice in Strategies 3 and 4 is easy because optimal block designs have been tabulated, the second choice may involve a search over an unreasonably large number of permutations. A practical alternative is to generate a few thousand permutations randomly and choose the best. The `randomize` directive in Genstat provides a particularly easy way to generate such constrained permutations randomly.

Strategy 5 If Strategy 2 is impossible, choose Δ by Strategy 3 and Γ by Strategy 4. Compare the behaviour of $g(\Delta, \psi)$ and $g(\Gamma, \psi)$ for ψ in Ψ . If $g(\Delta, \psi) \leq g(\Gamma, \psi)$ for all ψ in Ψ then choose Δ ; if $g(\Gamma, \psi) \leq g(\Delta, \psi)$ for all ψ in Ψ then choose Γ . Otherwise, minimize the risk of a bad choice by choosing the design with the smaller value of the maximum relative increase in variance, the maximum being taken over ψ in Ψ .

This strategy assumes that no design is better than both Γ and Δ for any ψ in Ψ . Even if $\Psi \subset [1, \infty]$, is this true?

10. Positive results

If we restrict attention to equi-replicate designs (and later to designs which are binary in blocks) we can prove some definite results about optimal designs. Denote by $\mathcal{D}_{n;b,c,k}$ the class of equi-replicate designs for n treatments in b blocks of c subblocks of k plots, and by $\bar{\mathcal{D}}_{n;b,c,k}$ the subclass of $\mathcal{D}_{n;b,c,k}$ whose designs are binary in blocks (that is, no treatment occurs more than once in any block) and therefore necessarily binary in subblocks also.

THEOREM 3. *If Δ is a nested balanced block design in $\mathcal{D}_{n;b,c,k}$ then $\Delta \succ_{\psi} \Gamma$ for all Γ in $\mathcal{D}_{n;b,c,k}$ and all ψ in $[1, \infty]$.*

Proof. Since $L_P = rI - k^{-1}\Lambda_S$, the trace of L_P is maximized when $\text{tr}(\Lambda_S)$ is minimized. Since Δ_S is a balanced block design, $\text{tr}(L_P^\Delta)$ is maximal in $\mathcal{D}_{n;b,c,k}$. Similarly, since $L_P + L_S = rI - (ck)^{-1}\Lambda_B$ and Δ_B is a balanced block design, $\text{tr}(L_P^\Delta + L_S^\Delta)$ is

maximal in $\mathcal{D}_{n;b,c,k}$. Thus if $\Gamma \in \mathcal{D}_{n;b,c,k}$ and $\psi \geq 1$ then

$$\begin{aligned} \text{tr}(L_{PS}^\Delta) &= \text{tr}\left(L_P^\Delta + \frac{1}{\psi}L_S^\Delta\right) \\ &= \frac{(\psi-1)}{\psi}\text{tr}(L_P^\Delta) + \frac{1}{\psi}\text{tr}(L_P^\Delta + L_S^\Delta) \\ &\geq \frac{(\psi-1)}{\psi}\text{tr}(L_P^\Gamma) + \frac{1}{\psi}\text{tr}(L_P^\Gamma + L_S^\Gamma) \\ &= \text{tr}(L_{PS}^\Gamma) \end{aligned}$$

so L_{PS}^Δ has maximal trace in $\mathcal{D}_{n;b,c,k}$.

Because Δ_S and Δ_B are both balanced block designs, the matrix L_{PS}^Δ is completely symmetric for all ψ . Keifer's (1975) theorem on universal optimality shows that $\Delta \succ_\psi \Gamma$ for all Γ in $\mathcal{D}_{n;b,c,k}$ if $\psi \geq 1$. \square

Theorem 3 is analogous to Corollary 3 of Bogacka and Mejza (1994), for designs with two strata, and to the result in Section 2.3 of Morgan (1996), who combines information from all three strata. It is similar to the results of Markiewicz (1997, 1999) except that his two sets of nuisance parameters are not nested. It is not the same as Gupta's (1993) Theorem 4.1.

THEOREM 4. *Let $b \leq n < bc$. If Δ is a design in $\bar{\mathcal{D}}_{n;b,c,k}$ such that Δ_S is balanced and Δ_B is the dual of a balanced incomplete-block design then $\Delta \succ_\psi \Gamma$ for all Γ in $\bar{\mathcal{D}}_{n;b,c,k}$ and all ψ in $[1, \infty]$.*

Proof. The canonical efficiency factors of Δ are

dim	$n-b$	$b-1$
f_B	0	f
e_S	$1-e$	$1-e-f$
e_P	e	e

where $e = n(k-1)/[(n-1)k]$ and $f = (b-r)/[(b-1)r]$. Thus the eigenvalues of $r^{-1}L_{PS}^\Delta$ on contrasts are, in descending order,

$$\underbrace{\frac{(\psi-1)}{\psi}e + \frac{1}{\psi}}_{n-b \text{ times}}, \quad \underbrace{\frac{(\psi-1)}{\psi}e + \frac{(1-f)}{\psi}}_{b-1 \text{ times}}.$$

For $1 \leq i \leq n - 1$, let $T_i(\Gamma)$ be the sum of the first i largest eigenvalues of $r^{-1}L_{PS}^\Gamma$ on contrasts. Thus $T_i(\Gamma)$ is the maximal value of

$$\sum_{x \in \mathcal{X}} \frac{1}{r} \left[\frac{(\psi - 1)}{\psi} x' L_P^\Gamma x + \frac{1}{\psi} x' (L_P^\Gamma + L_S^\Gamma) x \right]$$

for orthonormal bases \mathcal{X} of i -dimensional spaces of contrasts. But

$$\sum_{x \in \mathcal{X}} \frac{1}{r} x' L_P^\Gamma x \geq ie$$

because $\text{tr}(L_P^\Gamma) = r(n - 1)e = N - bc$. The rank of L_B^Γ is at most $b - 1$, so

$$\max_{\mathcal{X}} \sum_{x \in \mathcal{X}} \frac{1}{r} x' (L_P^\Gamma + L_S^\Gamma) x = i$$

for $1 \leq i \leq n - b$; and $\text{tr}(L_P^\Gamma + L_S^\Gamma) = r[n - 1 - (b - 1)f] = N - b$ so

$$\max_{\mathcal{X}} \sum_{x \in \mathcal{X}} \frac{1}{r} x' (L_P^\Gamma + L_S^\Gamma) x \geq (n - b) + (i - n + b)(1 - f)$$

for $n - b \leq i \leq n - 1$.

Hence $T_i(\Delta) \leq T_i(\Gamma)$ for $i = 1, \dots, n - 1$. The argument of the proof of Theorem 3.3 of Bailey, Monod and Morgan (1995) shows that $\Delta \succ_{\psi} \Gamma$. \square

A similar argument proves the next theorem.

THEOREM 5. *Let $b \leq n = ck$. If Δ is an affine-resolved design then $\Delta \succ_{\psi} \Gamma$ for all Γ in $\bar{\mathcal{D}}_{n;b,c,k}$ and all ψ in $[1, \infty]$.*

Apart from balanced incomplete-block designs and their duals, optimality theorems for block designs are typically restricted to classes \mathcal{D} of designs for which $\text{tr}(L_P)$ is constant and where a design which minimizes $\text{tr}(L_P^2)$ also has other good properties. If we restrict ourselves to $\bar{\mathcal{D}}_{n;b,c,k}$ then, for each value of ψ , $\text{tr}(L_{PS})$ is constant over the class. Unfortunately, minimality of $\text{tr}(L_P^2)$ and $\text{tr}((L_P + L_S)^2)$ does not guarantee minimality of $\text{tr}((L_P + \psi^{-1}L_S)^2)$ for all ψ in $[1, \infty]$. In Example 6 the designs Φ and Γ have the same value of $\text{tr}(L_P^2)$ and of $\text{tr}((L_P + L_S)^2)$ but

$$\text{tr} \left(\left(L_P^\Phi + \frac{1}{\psi} L_S^\Phi \right)^2 \right) > \text{tr} \left(\left(L_P^\Gamma + \frac{1}{\psi} L_S^\Gamma \right)^2 \right)$$

for all ψ in $(1, \infty)$. So there seems little hope of proving the optimality of any non-balanced design for all ψ in $[1, \infty]$.

THEOREM 6. Let \mathcal{D} be a subclass of $\bar{\mathcal{D}}_{n,b,c,k}$. Suppose that Δ is a design in \mathcal{D} satisfying either of the following conditions:

- (i) Δ is partially balanced with two associate classes and one canonical efficiency factor e_P^Δ equal to 1;
(ii) Δ is generally balanced with a basic contrast x_1 such that

$$e_{P_1} \geq e_{P_2} = e_{P_3} = \cdots = e_{P_{n-1}}$$

and

$$e_{P_1} + e_{S_1} \geq e_{P_2} + e_{S_2} = \cdots = e_{P_{n-1}} + e_{S_{n-1}}.$$

Let $\psi \in [1, \infty]$. If Δ minimizes $\text{tr}((L_P + \psi^{-1}L_S)^2)$ over \mathcal{D} then $\Delta \succ_{\psi} \Gamma$ for all Γ in \mathcal{D} .

Proof. Since $\text{tr}(L_{PS})$ is constant over \mathcal{D} for each ψ and Δ minimizes $\text{tr}(L_{PS}^2)$ over \mathcal{D} , all we have to do is mimic the proofs of the analogous optimality results for block designs.

(i) If Δ is partially balanced with two associate classes then L_P^Δ and L_S^Δ have just two common eigenspaces on contrasts with corresponding canonical efficiency factors e_{P_1} , e_{S_1} and e_{P_2} , e_{S_2} . By assumption $e_{P_1} = 1$, and $e_{P_1} + e_{S_1} \leq 1$, so $e_{S_1} = 0$. Thus $r^{-1}(L_P^\Delta + \psi^{-1}L_S^\Delta)$ has two eigenvalues, 1 and $e_{P_2} + \psi^{-1}e_{S_2}$. Note that $e_{P_2} + \psi^{-1}e_{S_2} \leq e_{P_2} + e_{S_2} \leq 1$.

For Γ in \mathcal{D} , $x' L_P^\Gamma x \leq r x' x$ and $x' (L_P^\Gamma + L_S^\Gamma) x \leq r x' x$ for all contrasts x . Since $\psi \geq 1$ and

$$L_{PS}^\Gamma = \frac{(\psi - 1)}{\psi} L_P^\Gamma + \frac{1}{\psi} (L_P^\Gamma + L_S^\Gamma),$$

the maximum eigenvalue of $r^{-1}L_{PS}^\Gamma$ is at most 1.

Applying Theorem 2.1 of Cheng and Bailey (1991) to the eigenvalues of $r^{-1}L_{PS}$, and using Theorem 1 shows that $g(\Delta, \psi) \leq g(\Gamma, \psi)$.

(ii) Since $\psi \geq 1$,

$$\begin{aligned} e_{P_1} + \frac{1}{\psi} e_{S_1} &= \frac{(\psi - 1)}{\psi} e_{P_1} + \frac{1}{\psi} (e_{P_1} + e_{S_1}) \\ &\geq \frac{(\psi - 1)}{\psi} e_{P_2} + \frac{1}{\psi} (e_{P_2} + e_{S_2}) \\ &= e_{P_2} + \frac{1}{\psi} e_{S_2} \end{aligned}$$

and $e_{P_2} + \psi^{-1}e_{S_2} = e_{P_i} + \psi^{-1}e_{S_i}$ for $i = 3, \dots, n - 1$. Now Theorem 3.1 of Cheng (1978) shows that $g(\Delta, \psi) \leq g(\Gamma, \psi)$. \square

COROLLARY 6.1. *Let \mathcal{D} be a subclass of $\bar{\mathcal{D}}_{n;b,c,k}$ in which Γ_S is balanced for all Γ in \mathcal{D} . Let Δ be a design in \mathcal{D} . If Δ_B is a regular graph design and Δ satisfies either of the conditions in Theorem 6 then $\Delta \succ_{\psi} \Gamma$ for all Γ in \mathcal{D} and all ψ in $[1, \infty]$.*

Proof. All designs Γ in \mathcal{D} have the same single canonical efficiency factor e in the plots stratum. Since Δ_B is a regular graph design, $\text{tr}(\Lambda_B^2)$ is minimal, and therefore

$$\sum_i (e + e_{Si}^{\Delta})^2 \leq \sum_i (e + e_{Si}^{\Gamma})^2$$

for all Γ in \mathcal{D} . But $\sum_i e_{Si}^{\Gamma}$ has a constant value for Γ in \mathcal{D} , and so

$$\sum_i \left(e + \frac{1}{\psi} e_{Si}^{\Delta} \right)^2 \leq \sum_i \left(e + \frac{1}{\psi} e_{Si}^{\Gamma} \right)^2$$

for all Γ in \mathcal{D} and all ψ . In other words, Δ minimizes $\text{tr}(L_{PS}^2)$ for all ψ , and so Theorem 6 applies. \square

COROLLARY 6.2. *Let \mathcal{D} be a subclass of $\bar{\mathcal{D}}_{n;b,c,k}$ in which Γ_B is balanced (or complete) for all Γ in \mathcal{D} . Let Δ be a design in \mathcal{D} . If Δ_S is a regular graph design and Δ satisfies either of the conditions in Theorem 6 then $\Delta \succ_{\psi} \Gamma$ for all Γ in \mathcal{D} and all ψ in $[1, \infty]$.*

Proof. All designs Γ in \mathcal{D} have the same single canonical efficiency factor f in the blocks stratum. Since Δ_S is a regular graph design,

$$\sum_i (e_{Pi}^{\Delta})^2 \leq \sum_i (e_{Pi}^{\Gamma})^2$$

for all Γ in \mathcal{D} . But

$$\text{tr} \left((L_{PS}^{\Gamma})^2 \right) = \sum_i \left(\frac{(\psi - 1)}{\psi} e_{Pi}^{\Gamma} + \frac{1}{\psi} (1 - f) \right)^2$$

and $\sum_i e_{Pi}^{\Gamma}$ is constant for Γ in \mathcal{D} , so Δ minimizes $\text{tr}(L_{PS}^2)$ for all ψ . Thus Theorem 6 applies. \square

For example, when $b = c = k + 1$ and $n = ck$ then rectangular lattice designs are regular graph designs which satisfy condition (i) of Theorem 6. Hence they are optimal over resolved designs.

The results given in Section 3 of Mejza and Kageyama (1995) are comparable to Corollary 6.2. Those authors cover a wider range of optimality criteria than $g(\psi)$ but for subclasses of $\mathcal{D}_{n;b,c,k}$ for which $L_B = 0$.

Of course, if Δ_B is balanced but treatments are not orthogonal to blocks in Δ then Δ_S cannot satisfy condition (i) of Theorem 6. However, the methods of proof of Theorem 6 and Corollary 6.2 also prove the following.

THEOREM 7. *Suppose that $ck < n$. Let \mathcal{D} be a subclass of $\bar{\mathcal{D}}_{n;b,c,k}$ in which Γ_B is balanced with canonical efficiency factor e for all Γ in \mathcal{D} . If Δ is a design in \mathcal{D} such that Δ_S is a strongly regular graph design with one canonical efficiency factor equal to e then $\Delta \succ_{\psi} \Gamma$ for all Γ in \mathcal{D} and all ψ in $[1, \infty]$.*

Example 7. Let \mathcal{D} be the subclass of $\bar{\mathcal{D}}_{16;16,2,3}$ consisting of designs Γ such that Γ_B is balanced. Then $f_B^{\Gamma} = 1/9$ for all Γ in \mathcal{D} .

Figure 11 shows a design Δ in \mathcal{D} for which Δ_S is group divisible with four groups of four. The between-group concurrence of Δ_S is one more than the within-group concurrence, and the between-group canonical efficiency factor is equal to $8/9$. Hence Δ is optimal in \mathcal{D} for all ψ in $[1, \infty]$.

$$\Delta =$$

A	E	J	D	G	I
A	I	O	B	L	M
B	G	N	D	F	M
E	L	O	F	J	N
C	K	M	D	J	O
B	E	K	C	G	L
G	J	M	H	L	P
B	H	O	D	E	P

A	H	M	C	E	N
E	I	M	F	K	P
B	F	I	C	H	J
A	K	N	B	J	P
G	K	O	H	I	N
A	G	P	C	F	O
C	I	P	D	L	N
A	F	L	D	H	K

Figure 11. Optimal design for sixteen treatments in sixteen blocks of two subblocks of three plots

Banerjee and Kageyama (1993) also give a design in \mathcal{D} . Its quotient design in subblocks is also partially balanced with two associate classes, and it has one canonical efficiency factor equal to $8/9$, as shown in Table 2. However, its concurrences differ by two. It can readily be checked from the two tables of canonical efficiency factors that their design is inferior to Δ whenever $\psi \neq 1$. \square

Table 2. Tables of canonical efficiency factors for the design in Figure 11 (left) and the design given by Banerjee and Kageyama (1993) (right)

dim	3	12
f_B	$\frac{1}{9}$	$\frac{1}{9}$
e_s	0	$\frac{2}{9}$
e_P	$\frac{8}{9}$	$\frac{2}{3}$

dim	6	9
f_B	$\frac{1}{9}$	$\frac{1}{9}$
e_s	$\frac{4}{9}$	0
e_P	$\frac{4}{9}$	$\frac{8}{9}$

11. Nested regular graph designs

Suppose that Δ_S is a regular graph design, with concurrences λ and $\lambda + 1$. Let $m_1 = r(k-1) - (n-1)\lambda$, so that, for each treatment θ , there are m_1 treatments η with $\lambda_S(\theta, \eta) = \lambda + 1$. Suppose that Δ_B is also a regular graph design, with concurrences μ and $\mu + 1$, and let $m_2 = r(ck - 1) - (n - 1)\mu$. If there are $t(\theta)$ treatments η such that $\lambda_S(\theta, \eta) = \lambda + 1$ and $\lambda_B(\theta, \eta) = \mu + 1$ then the $n - 1$ treatments η other than θ fall into the following four categories.

$\lambda_S(\theta, \eta)$	$\lambda_B(\theta, \eta)$	number of treatments
λ	μ	$n - 1 - m_1 - m_2 + t(\theta)$
λ	$\mu + 1$	$m_2 - t(\theta)$
$\lambda + 1$	μ	$m_1 - t(\theta)$
$\lambda + 1$	$\mu + 1$	$t(\theta)$

Define Δ to be a *nested regular graph design* if Δ_S and Δ_B are both regular graph designs and $t(\theta) = \min\{0, m_1 + m_2 - n + 1\}$ for all θ .

LEMMA 1. *Suppose that $ck \leq n$. Let \mathcal{D} be any subclass of $\bar{\mathcal{D}}_{n;b,c,k}$ for which both Γ_S and Γ_B are regular graph designs for all Γ in \mathcal{D} . If a design Δ in \mathcal{D} is a nested regular graph design then Δ minimizes $\text{tr}(L_{PS}^2)$ over \mathcal{D} for all ψ in $[1, \infty)$.*

Proof.

$$\begin{aligned} L_{PS} &= L_P + \frac{1}{\psi}L_S = \left(rI - \frac{1}{k}\Lambda_S\right) + \frac{1}{\psi}\left(\frac{1}{k}\Lambda_S - \frac{1}{ck}\Lambda_B\right) \\ &= rI - \frac{1}{\psi ck}[c(\psi - 1)\Lambda_S + \Lambda_B]. \end{aligned}$$

Since Λ_S and Λ_B have constant trace over \mathcal{D} , $\text{tr}(L_{PS}^2)$ is a positive linear function of q , where

$$q = \sum_{\theta} \sum_{\eta \neq \theta} [c(\psi - 1)\lambda_S(\theta, \eta) + \lambda_B(\theta, \eta)]^2,$$

which is itself a positive linear function of

$$\begin{aligned} &\sum_{\theta} t(\theta)[c(\psi - 1)\lambda + \mu]^2 - \sum_{\theta} t(\theta)[c(\psi - 1)\lambda + \mu + 1]^2 \\ &\quad - \sum_{\theta} t(\theta)[c(\psi - 1)(\lambda + 1) + \mu]^2 + \sum_{\theta} t(\theta)[c(\psi - 1)(\lambda + 1) + \mu + 1]^2. \end{aligned}$$

But this is equal to $2c(\psi - 1) \sum_{\theta} t(\theta)$, which is minimized when $t(\theta)$ is minimized for all θ , because $\psi \geq 1$. \square

Both designs in Figure 6 are nested regular graph designs. However, neither of them satisfies either of the conditions in Theorem 6.

In fact, it is possible to show that nested regular graph designs minimize $\text{tr}(L_{PS}^2)$ over the whole of $\bar{D}_{9,9,2,2}$. However, the analogous result is not true in general.

Example 8. The design Γ in Figure 9 is a nested regular graph design with concurrences shown in Table 3. Thus

$$\begin{aligned} q^\Gamma &= 24 \times 4 + 16[2(\psi - 1) + 1]^2 + 16[2(\psi - 1) + 2]^2 \\ &= 16[8(\psi - 1)^2 + 12(\psi - 1) + 11]. \end{aligned}$$

The design Ξ in Figure 12 is partially balanced with respect to the association scheme $2 * (2/2)$, which has five associate classes. The concurrences given in Table 3 show that Ξ_B is not a regular graph design. Moreover,

$$\begin{aligned} q^\Xi &= 16 \times 4 + 8 \times 9 + 24[2(\psi - 1) + 1]^2 + 8[2(\psi - 1) + 2]^2 \\ &= 16[8(\psi - 1)^2 + 10(\psi - 1) + 12] \end{aligned}$$

so $q^\Gamma > q^\Xi$ whenever $\psi > 3/2$. This suggests that design Ξ might be better than Γ for some values of ψ .

$\Xi =$	<table border="1" style="border-collapse: collapse; text-align: center;"> <tr><td>1</td><td>4</td><td>2</td><td>3</td></tr> <tr><td>1</td><td>6</td><td>2</td><td>5</td></tr> <tr><td>1</td><td>8</td><td>2</td><td>7</td></tr> <tr><td>1</td><td>3</td><td>5</td><td>7</td></tr> </table>	1	4	2	3	1	6	2	5	1	8	2	7	1	3	5	7	<table border="1" style="border-collapse: collapse; text-align: center;"> <tr><td>5</td><td>8</td><td>6</td><td>7</td></tr> <tr><td>3</td><td>8</td><td>4</td><td>7</td></tr> <tr><td>3</td><td>6</td><td>4</td><td>5</td></tr> <tr><td>2</td><td>4</td><td>6</td><td>8</td></tr> </table>	5	8	6	7	3	8	4	7	3	6	4	5	2	4	6	8		dim	2	1	3	1
1	4	2	3																																					
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Figure 12. A fourth design for eight treatments in eight blocks of two subblocks of two plots

Table 4 shows the variances of the four designs in Figures 9 and 12 for various values of ψ . The design Ξ is the best of the four designs for ψ in $[1.5, 4.3]$. This is a very likely range for ψ if information is to be combined. However, one would have to be very sure that $\psi \in [1, 8]$ before recommending Ξ over Δ , because the relative loss from Ξ increases to 11% at $\psi = \frac{1}{2}$ and to 8% at $\psi = \infty$ while the relative loss from Δ is never more than 2%. □

Table 3. Pattern of concurrences in two designs for eight treatments in eight blocks of two subblocks of two plots

design Γ in Figure 9			design Ξ in Figure 12		
λ_S	λ_B	number of pairs	λ_S	λ_B	number of pairs
0	2	24	0	2	16
1	1	16	0	3	8
1	2	16	1	1	24
			1	2	8

Table 4. Average variances of simple contrasts for the designs in Figures 9 and 12

ψ	2^{-2}	2^{-1}	1	1.5	2	4	6	8	∞
$g(\Delta, \psi)$	0.3095	0.4429	0.5884	0.6667	0.7156	0.8066	0.8431	0.8628	0.9286
$g(\Gamma, \psi)$	0.3394	0.4627	0.5884	0.6595	0.7074	0.8083	0.8550	0.8822	0.9864
$g(\Phi, \psi)$	0.3059	0.4429	0.5884	0.6692	0.7217	0.8261	0.8711	0.8963	0.9864
$g(\Xi, \psi)$	0.4125	0.4932	0.5952	0.6595	0.7048	0.8045	0.8530	0.8819	1.0000

12. Discussion

Although Theorem 3 shows that Strategy 1 is good, the other results in Sections 10–11 give little hope of finding simple recipes for designs which are optimal for all ψ when there is no nested balanced block design.

The next example shows that even Strategy 2 can fail.

Example 9. Suppose again that there are 36 plots arranged in three blocks of three subblocks of four plots each, but that now there are only nine treatments. There are three candidate designs in Figures 1 and 13. Design Γ was chosen because, according to John and Mitchell (1977), Γ_S is optimal; Γ is a cyclic design. Design Φ was chosen because Φ_B is optimal; Φ is partially balanced with respect to the rectangular association scheme $3 * 3$. Design Δ was constructed by putting $\Delta_S = \Gamma_S$ and then rearranging subblocks in blocks so that $\Delta_B \cong \Phi_B$. Thus Δ_S and Δ_B are both optimal.

As already observed, Δ is not generally balanced, so comparisons with the other two designs must be made numerically. The functions $g(\psi)$ are plotted in Figure 14, and some specific values are shown in Table 5. We find that $\Phi \succ_{\psi} \Gamma$ unless $\psi > 100$, while the difference between the two designs is negligible for large ψ . There can be no reason to prefer Γ if information is to be combined. The design Δ is very slightly worse than Φ for $\psi \in (1, 8.5]$ and otherwise slightly better. Although there is no practical difference between Δ and Φ , this example is a blow for Strategy 2: although Δ_B and Δ_S are both optimal, Δ is not optimal for all ψ in $[1, \infty]$. \square

$$\Gamma = \begin{array}{|c|c|c|c|c|c|c|c|c|c|} \hline 1 & 3 & 7 & 9 & 4 & 6 & 1 & 3 & 7 & 9 & 4 & 6 \\ \hline 2 & 4 & 8 & 1 & 5 & 7 & 2 & 4 & 8 & 1 & 5 & 7 \\ \hline 3 & 5 & 9 & 2 & 6 & 8 & 3 & 5 & 9 & 2 & 6 & 8 \\ \hline \end{array}$$

dim	2	2	2	2
f_B	$\frac{1}{4}$	0	0	0
e_S	0	$\frac{2+x}{16}$	$\frac{2+y}{16}$	$\frac{2+z}{16}$
e_P	$\frac{3}{4}$	$\frac{14-x}{16}$	$\frac{14-y}{16}$	$\frac{14-z}{16}$

Here $x = \epsilon + \epsilon^8$, $y = \epsilon^2 + \epsilon^7$, and $z = \epsilon^4 + \epsilon^5$, where ϵ is a primitive ninth root of unity.

$$\Phi = \begin{array}{|c|c|c|c|c|c|c|c|c|c|} \hline 2 & 3 & 4 & 7 & 1 & 3 & 5 & 8 & 1 & 2 & 6 & 9 \\ \hline 1 & 7 & 5 & 6 & 2 & 8 & 4 & 6 & 3 & 9 & 4 & 5 \\ \hline 1 & 4 & 8 & 9 & 2 & 5 & 7 & 9 & 3 & 6 & 7 & 8 \\ \hline \end{array}$$

dim	2	2	4
f_B	$\frac{1}{16}$	0	0
e_S	0	$\frac{1}{16}$	$\frac{1}{4}$
e_P	$\frac{15}{16}$	$\frac{15}{16}$	$\frac{3}{4}$

Figure 13. Two generally balanced designs for nine treatments in three blocks of three subblocks of four plots, with their tables of canonical efficiency factors

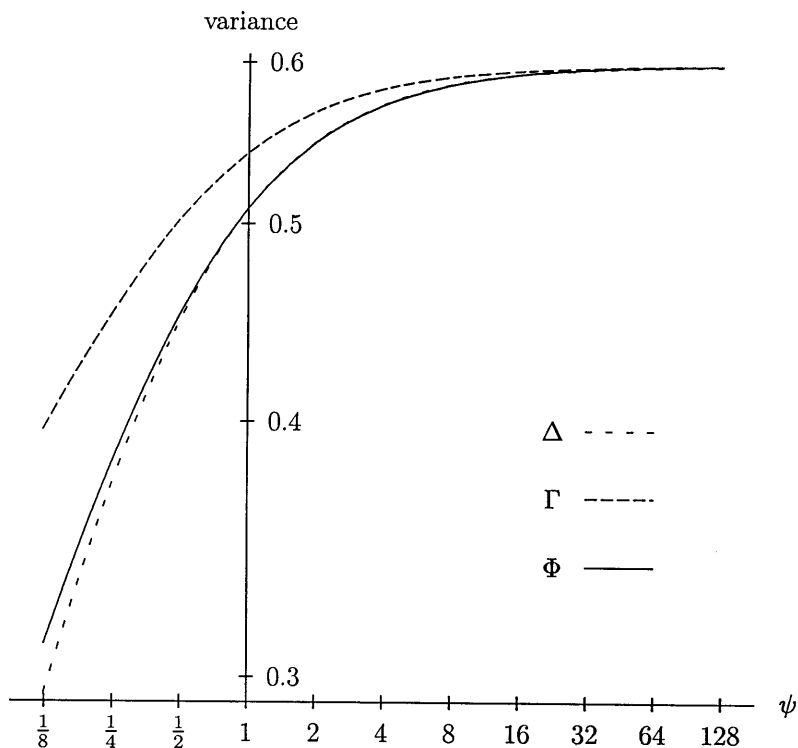


Figure 14. Average pairwise variance for each of the designs in Figures 1 and 13

Table 5. Average variances of simple contrasts for the designs in Figures 1 and 13

ψ	2^{-3}	2^{-2}	2^{-1}	1	2	4	8	16	∞
$g(\Gamma, \psi)$	0.3962	0.4509	0.5021	0.5417	0.5676	0.5826	0.5908	0.5951	0.5995
$g(\Phi, \psi)$	0.3112	0.3815	0.4510	0.5083	0.5481	0.5722	0.5856	0.5927	0.6000
$g(\Delta, \psi)$	0.2942	0.3720	0.4480	0.5083	0.5487	0.5725	0.5856	0.5925	0.5995

Thus it appears that optimality of Δ_B and Δ_S cannot, in general, ensure that Δ is optimal.

Although Strategy 3 has some support in the literature, Examples 3 and 4 show that neither Strategy 3 nor Strategy 4 can be recommended.

The final example shows Strategy 5 in action.

Example 10. Figure 15 shows two further designs for nine treatments in nine blocks of two subblocks of size two, for comparison with the designs Ξ and Π in Figure 6. Neither is generally balanced.

$\Delta =$	2 9 3 5	9 3 1 7		7 5 4 9	1 8 4 5
	4 7 5 2	4 3 1 6		4 7 2 6	7 2 8 3
	6 4 7 9	4 2 1 8	$\Gamma =$	5 3 7 1	8 2 1 6
	6 9 8 2	8 3 6 5		5 6 9 2	9 1 6 3
	5 1 7 8			9 3 4 8	

Figure 15. Two further designs for nine treatments in nine blocks of two subblocks of two plots

We know that Ξ_B is optimal for nine blocks of size four. Design Δ was obtained by starting with these nine blocks and randomly splitting each block into two subblocks of size two. This was done 9000 times. Design Δ gives the optimal Δ_S among the designs created in this way.

John and Mitchell (1977) quote a design from Mitchell and John (1976) as optimal for eighteen subblocks of size two. These were randomly grouped into nine blocks of size four, 9000 times. Design Γ gives the optimal Γ_B which was found.

In fact $\Delta_S \cong \Gamma_S$ so Δ_S is indeed optimal for the given Δ_B . But $\Gamma_B \prec \Delta_B$, so the random permutations did not generate the best Γ for the given Γ_S . This discrepancy is not so surprising: there are only 19,683 ways of splitting up the blocks of Ξ_B but there are 34,459,425 ways of grouping the subblocks of Γ_S .

Although Δ is optimal for both $\psi = 1$ and $\psi = \infty$, once again it is not optimal for all intermediate values of ψ . Table 6 shows the relative variances of the four designs. In order to show the relative loss more clearly, the variances for each value of ψ have been divided by the minimum of the four variances. Thus

$$g^*(\Delta, \psi) = \frac{g(\Delta, \psi)}{\min \{g(\Delta, \psi), g(\Gamma, \psi), g(\Pi, \psi), g(\Xi, \psi)\}}.$$

Design Δ is never more than 2% worse than the best of these four designs, but design Π is actually best for the most important values of ψ , and performs well for all $\psi \geq 1$.

□

Table 6. Relative variances for the four designs in Figures 6 and 15

ψ	2^{-2}	2^{-1}	1	2	4	8	16	∞
$g^*(\Pi, \psi)$	1.3	1.09	1.001	1	1	1	1.01	1.02
$g^*(\Xi, \psi)$	1.2	1.07	1	1.0002	1.0006	1.02	1.04	1.07
$g^*(\Delta, \psi)$	1.004	1	1	1.02	1.01	1.0002	1	1
$g^*(\Gamma, \psi)$	1	1	1.003	1.02	1.02	1.0002	1.001	1

It seems that, in general, the only clear recommendation that can be given is that $g(\Delta, \psi)$ should be tabulated and compared for a range of designs Δ for ψ in Ψ . How should the candidate designs be chosen? Certainly, designs Δ for which either Δ_S or Δ_B is optimal should be included. From the examples and results in this paper, it would be wise to include nested regular graph designs, partially balanced nested block designs, designs such that at least one of Δ_S and Δ_B has Caliński's property, and designs, like the one in Figure 12, which minimize the sum of the squares of the differences of $c(\psi - 1)\lambda_S + \lambda_B$ from their mean, for ψ in Ψ . It may also be a good idea to try to improve some of these designs by using one of the two types of random permutations described in Section 9.

This *ad hoc* approach has the advantage that it can be tailored to the experimenter's requirements. For example, the average variance of simple contrasts could be replaced by the analogue of the D-criterion or the E-criterion. As Pearce (1983, Chapter 9) has noted, it is rare for all contrasts to have equal importance. In a factorial experiment different weights could be given to main effects and to interactions; in an experiment to compare new treatments with controls the average can be restricted to those pairs (θ, η) for which θ is a control and η is a new treatment: see Leeming (1997, 1998).

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Wybór układu dla bloków zagnieżdżonych

STRESZCZENIE

Układ o zagnieżdżonych blokach to układ o jednostkach doświadczalnych pogrupowanych w bloki, w ramach których wyróżniono podbloki. Podany jest przegląd estymatorów i ich wariancji w sytuacji gdy następuje łączenie informacji z warstwy poletkowej i warstwy podbloków. Względna wielkość wariancji związanych z tymi dwiema warstwami jest zwykle nieznana, jednak rząd tej wielkości jest często określony poprzez poprzednie eksperymenty.

Zaproponowana metoda porównywania układów jest zilustrowana wieloma przykładami. Pokazano, że układ może być optymalny dla analizy wewnątrzblokowej gdy podbloki są ignorowane oraz optymalny dla analizy wewnątrzpodblokowej gdy ignorowane są bloki, nie będąc optymalny dla kombinowania informacji. Podane są twierdzenia pokazujące iż pewne układy są optymalne w pewnych klasach układów gdy następuje łączenie informacji i gdy wariancja związana z warstwą podbloków jest co najmniej tak duża jak wariancja warstwy poletkowej. Podane są heurystyczne strategie znajdowania dobrych układów doświadczalnych w innych sytuacjach.

SŁOWA KLUCZOWE: kombinowanie informacji, zagnieżdżone zrównoważone układy blokowe, bloki zagnieżdżone, zagnieżdżone układy grafu regularnego, układy optymalne.