Optimal Block Designs with Autocorrelation

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Introduction

Block designs, where the experimental runs are partitioned into homogenous groups, are ubiquitous in many areas of science and industry. The assumption that the blocks constitute a random sample from a population leads naturally to a mixed model for the data analysis and the ability to predict the response from unobserved blocks.

Here, we consider an extension to the usual exchangeable correlation structure and assume that the ordering of units within a block may have an influence on the response. This effect is modelled by assuming an autoregressive process of order 1 for the intra-block effects.

Such models are appropriate for a variety of situations, for example in agricultural and clinical science. Our motivation is factorial experiments to understand the impact of manufacturing process variables on the fabrication of optical fibres, which is important in next generation communication and internet applications. Fibres are manufactured through a drawing process which naturally gives rise to blocks and potential ordering effects within a block.

Linear Mixed Models

An appropriate mixed model for a block design for f factors, each having l levels, with n runs in b blocks of size k and random block effects is

$$\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \mathbf{Z}\boldsymbol{\gamma} + \boldsymbol{\epsilon}, \tag{1}$$

where, as in the standard regression model, $\mathbf{Y}$ is the $n \times 1$ vector of responses, $\mathbf{X}$ is the $n \times p$ model matrix and $\boldsymbol{\beta}$ is the $p \times 1$ vector of parameters which are of primary interest. Also,

- $\mathbf{Z}$ is the $n \times b$ matrix representing the allocation of runs to blocks (the (i,j)th entry of $\mathbf{Z}$ is 1 if the ith run is in the jth block),
- $\boldsymbol{\gamma} \sim N(\mathbf{0}, \sigma^2_\gamma \mathbf{I}_b)$ is the $b \times 1$ vector of random block effects, which are not of interest here (σ^2_γ accounts for the variation between blocks),
- $\boldsymbol{\epsilon} \sim N(\mathbf{0}, \sigma^2_\epsilon \mathbf{R})$ is the $n \times 1$ vector of within block errors (σ^2_ϵ accounts for the variation between runs within a block). $\boldsymbol{\epsilon}$ and $\boldsymbol{\gamma}$ are independent.
- $\mathbf{V} = \text{var}(\mathbf{Y}) = \sigma^2_\gamma \mathbf{Z}\mathbf{Z}^T + \sigma^2_\epsilon \mathbf{R}$ where the structure of $\mathbf{R}$ depends on the correlation structure assumed for the errors within blocks.

Autoregressive Correlation Structure

When the error for the hth run in the jth block follows a stationary autoregressive process of order 1,

$$\epsilon_{jh} = \rho \epsilon_{j,h-1} + e_{jh}, \tag{2}$$

where $|\rho| < 1$ is the autoregressive parameter, e_{jh} are independent and identically distributed (iid) $N(0, \sigma^2_\epsilon)$ and $\epsilon_{j,1}$ are iid $N(0, \sigma^2_\epsilon/(1-\rho^2))$ [2]. It is assumed that ϵ_{jh} from different blocks are independent.

If (2) holds, then $\mathbf{V}$ is a block diagonal matrix with diagonal submatrices given by

$$\sigma^2_\epsilon \left(\frac{1}{1-\rho^2} \begin{pmatrix} 1 & \rho & \dots & \rho^{k-1} \\ \rho & 1 & \dots & \rho^{k-2} \\ \vdots & \vdots & \ddots & \vdots \\ \rho^{k-1} & \rho^{k-2} & \dots & 1 \end{pmatrix} + \eta \mathbf{J}_k \right), \tag{3}$$

where $\mathbf{J}_k$ is the $k \times k$ matrix of 1's and $\eta = \sigma^2_\gamma / \sigma^2_\epsilon$ is the relative magnitude of the variance components [6]. The exchangeable structure is a special case of (3) with $\rho = 0$.

The correlation between the two responses within a block, $r, s \leqslant k$, is

$$\tau_{rs} = \frac{(1-\rho^2)\eta + \rho^{|r-s|}}{(1-\rho^2)\eta + 1}. \tag{4}$$

D-Optimality

A D-optimal block design maximises

$$\phi_D = |\mathbf{X}^T \mathbf{V}^{-1} \mathbf{X}|, \tag{5}$$

and hence provides parameter estimators with the joint confidence ellipsoid of smallest volume [1, 4].

The relative D-efficiency of two designs for a given ρ and η is

$$\text{eff}(\mathbf{X}_1 \mathbf{X}_2, \rho, \eta) = \frac{n_2}{n_1} \times \left(\frac{|\mathbf{X}_1^T \mathbf{V}^{-1}_{\rho,\eta} \mathbf{X}_1|}{|\mathbf{X}_2^T \mathbf{V}^{-1}_{\rho,\eta} \mathbf{X}_2|} \right)^{\frac{1}{p}} \times 100, \tag{6}$$

where $\mathbf{V}_{\rho,\eta}$ is the $\mathbf{V}$ matrix for ρ and η, $\mathbf{X}_1$ is the model matrix for design 1 with n_1 runs and $\mathbf{X}_2$ is the model matrix for design 2 with n_2 runs.

Comparative Study

A comparative study found D-optimal designs for four experiments:

- $f = 3, l = 2, n = 8, b = 2, k = 4, p = 8$ (full interaction model),
- $f = 3, l = 2, n = 16, b = 4, k = 4, p = 8$ (full interaction model),
- $f = 4, l = 2, n = 12, b = 4, k = 3, p = 5$ (main effects model),
- $f = 4, l = 2, n = 12, b = 4, k = 3, p = 11$ (two-factor interaction model).

A treatment is a combination of factor levels for the f factors in the experiment. In this study:

- a coordinate exchange algorithm [5] was used to find the optimal treatments and treatment allocation to blocks,
- an interchange algorithm [1] was used to allocate the runs from an optimal unblocked treatment design to blocks.

Saturated Designs

1. Saturated designs provide less information per run. When $n = p$, $\phi_D = |\mathbf{V}^{-1}||\mathbf{X}^T\mathbf{X}|$. If we assume $\mathbf{Z}$ is fixed from the experiment, every allocation to blocks of the optimal unblocked treatment design is equally efficient [3]. However, from (5) we can see that, for $n > p$, the D-optimal design takes account of both the allocation of treatments to blocks and the order of treatments within a block. This leads to non-saturated designs having a higher (per run) efficiency than saturated designs when $\rho, \eta \neq 0$; this is evidenced by the low relative D-efficiencies in Table 1 for $n_1 = 8$ and $n_2 = 16$.

η \ ρ	0	0.25	0.5	0.75
0	100.00	97.67	90.68	78.79
2.5	85.26	82.11	77.83	71.09
5	79.31	76.43	72.71	67.33
7.5	75.78	73.04	69.60	64.65
10	73.30	70.66	67.38	63.22

Table 1: Relative D-efficiencies (%, 2 dp) of D-optimal designs for $n_1 = 8$, $n_2 = 16$.

2. The relative D-efficiencies for the designs found using the interchange algorithm increase as the designs compared get closer to the saturated case (p gets closer to n). As p increased from 5 to 11 when $n = 12$, the relative D-efficiencies increased. The relative D-efficiencies for the D-optimal designs for the experiment with $p = 5$ and $n = 12$ varied from 91.72% to 100% (2 dp) whereas the relative D-efficiencies for the D-optimal designs for the experiment with $p = 11$ and $n = 12$ varied from 99.34% to 100% (2 dp).

Robustness to Misspecification of ρ and η

1. Design performance is robust to misspecification of ρ and η. The efficiency, (6), is close to 1 when calculated for an optimal design for one set of values of ρ and η with respect to an optimal design for a second set of ρ and η values. That is, D-optimal designs for model (1) are robust to the value of ρ and η. The minimum relative D-efficiency of two D-optimal designs found in this study is 91.72% (2 dp). This robustness may depend on the range of the intra-block correlation, (4), which was greater than 0.78 (2dp) for $\rho, \eta \neq 0$ and, for fixed η, had a maximum difference of 17% (2 sf) in this study.
2. Designs with the same value of ϕ_D, (5), do not necessarily have the same treatments (when $n = 12$) or the same treatments allocation to blocks (when $n = 8, 16$). The designs found using the coordinate exchange algorithm when $n = 12$, $\eta = 2.5, 5, 7.5$ and $\rho = 0.25, 0.5, 0.75$ have the same value of (5) but do not always have the same treatments or treatment allocation to blocks, as shown in Figure 1 for $\eta = 5$ and $\rho = 0.5, 0.75$. The designs found using the coordinate exchange algorithm when $n = 16$, $\eta = 5, 7.5, 10$ and $\rho = 0.25, 0.5$ also have the same value of (5) but do not have the same treatment allocation to blocks, see Figure 2 for $\eta = 5$. The treatment labels in Figures 1 and 2 follow the standard order for $f = 4$, $l = 2$ and $f = 3$, $l = 2$, respectively.

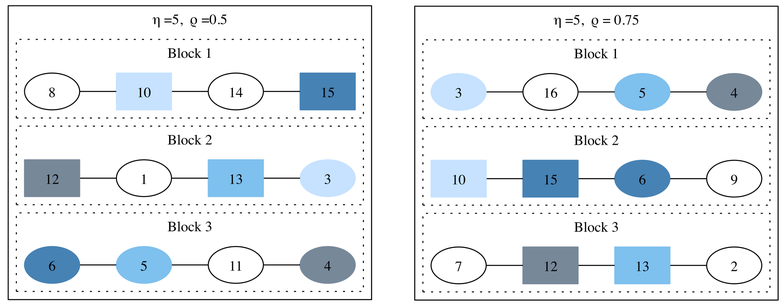

Figure 1: Treatment allocation to blocks for the designs where $n = 12$, $b = 4$, $k = 3$, $\rho = 0.5, 0.75$ and $\eta = 5$. White nodes represent the treatments that differ between the two designs.

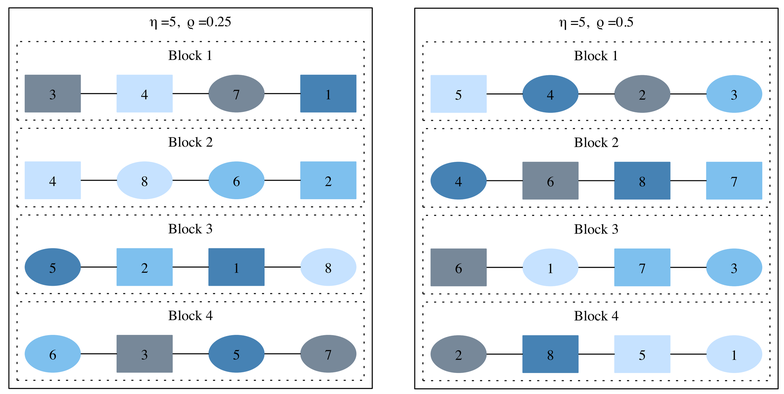

Figure 2: Treatment allocation to blocks for the designs where $n = 16$, $b = 4$, $k = 4$, $\rho = 0.25, 0.5$ and $\eta = 5$.

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