Efficient and optimal designs
for correlated observations

A thesis submitted for the degree of Doctor of Philosophy

at

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by

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Abstract of: Efficient and optimal designs for correlated observations.

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This thesis considers some aspects of the problem of finding efficient and optimal designs when observations are correlated. The two main areas that are examined are nested row-column (NRC) designs and early generation variety trials (EGVTs).

In NRC designs, the experimental area is divided into b blocks, and each block is divided into p_1 rows and p_2 columns (blocks of size $p_1 \times p_2$). Here, optimal NRC designs, which can be constructed from semi-balanced arrays, are obtained under the assumption that within-block observations are correlated.

For a stationary reflection symmetric dependence structure, optimal NRC designs with blocks of size 2×2 are obtained for models with fixed block effects, which may also include row and/or column effects. It is shown that the efficiency of binary designs can be very low for some correlation values.

Also, optimal NRC designs for blocks of size 3×3 and $p_1 \times 2$ ($p_1 \geq 3$) are determined. The optimality region for blocks of size $p_1 \times p_2$ ($p_1, p_2 \geq 2$) under the AR(1)*AR(1) process is also specified. It is shown that optimal NRC designs are highly specific to the correlation values.

The purpose of EGVTs is to select top performing new crop varieties for further testing. Recently there has been much interest in the spatial analysis of EGVTs, but there has been little work on the design of efficient EGVTs when a spatial analysis is intended.

Several intuitively simple criteria to assess the efficiency of designs for EGVTs are examined, and simulation studies suggest that some of these criteria are well associated with probabilities of selecting the highest yielding new varieties.

Also, the efficiency and robustness of some systematic designs for EGVTs is investigated over several models and dependence structures. For the examples considered, it is shown that designs in which the plots containing control varieties are at least a knight's move apart are robust.

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1   Introduction

Efficient experimental designs are designs in which as much information as possible is gained from a given amount of experimental material. The experimental material consists of units called *plots* and each plot receives a *treatment*. In an agricultural context, treatments may be varieties of wheat or different pesticides. It is assumed here that the object of the experiment is the comparison of treatments.

There are many methods to design efficient experiments. One of the main techniques is that of *blocking*, where relatively homogeneous plots are grouped together in *blocks*. Also, the choice of treatment contrast estimator and the allocation of treatments to plots are usually very important considerations.

Prior knowledge can often be used to select an estimator and blocking structure which can lead to an efficient design. In this thesis, attention is restricted to the allocation of treatments to plots in such a way that an efficient design results, given that the blocking structure and estimator to be used in an experiment have been determined using prior information.

Before the arrival of the computer, the simplicity of the analysis of experiments was important. Therefore only standard situations with simple models, such as experiments with equal block sizes and treatments of equal status were usually considered. Under *randomisation* the treatments are allocated to the plots at random, subject to the design structure. This means that it becomes more reasonable to assume that observations are uncorrelated and follow a Normal distribution, although randomisation implies that observations are actually equally correlated within strata (blocking structures). Under these assumptions, tables of efficient or optimal experimental designs

are usually available. Examples of such tables are in Fisher & Yates (1963), John *et al.* (1972), John (1981) and Lamacroft & Hall (1982). More recently, computer algorithms to find efficient (or near-optimal) designs when observations are assumed to be uncorrelated have been given, for example, by Paterson & Patterson (1983) and John & Whittaker (1993). Also, such algorithms are used in the software package ALPHA+ (Williams & Talbot, 1993). However, rather than assuming observations to be uncorrelated, advances in computing power have made it possible to fit realistic models that take account of non-standard features, such as a postulated dependence between the observations or unequal interest in comparisons between treatments. For such situations tabulated optimal designs are usually not available.

This thesis considers the problem of finding efficient and optimal designs when observations are correlated. Recently there has been much interest in this area. Martin (1996) provides a comprehensive review, outlining various methods to find efficient designs under dependence. The two main areas that are examined in this thesis are *nested row-column* designs and *early generation variety trials*.

In nested row-column (NRC) designs, the experimental area is divided into blocks, and each block is divided into rows and columns, which may represent two blocking factors. These designs can be used to take account of possible differences in the two blocking factors within each block. John & Williams (1995, section 5.9) give an example of a NRC design for an agricultural experiment, where the rows and columns might be used to control field gradient and soil type, respectively, and the blocks represent different locations at which the experiment is carried out. If it is assumed that the experimental material consists of sets of *spatial* (i.e. two dimensional) material, the rows and columns may be taken to represent the 2 dimensions of the spatial arrangement, with the blocks being the sets (such as location or

batch) of the spatial material. An agricultural field trial is an obvious example of a spatial application. Other examples, given by Martin (1996), are sheet metal production and paper making.

There has been a great deal of work on finding optimal NRC designs when errors are assumed to be uncorrelated and treatment contrasts are estimated from comparisons made within all of blocks, rows and columns. Between block, row or column information may also be taken in to account. Morgan (1996) provides a review of optimal NRC designs when observations are assumed to be uncorrelated.

If observations are assumed to be correlated, the dependence structure can be modelled and then used to estimate the treatment contrasts. If the dependence structure is adequately modelled this approach is likely to result in treatment contrasts being estimated with greater precision. A number of recent papers have addressed the problem of obtaining optimal and efficient block designs when errors are assumed to be correlated. See, for example, Cheng (1988), Martin & Eccleston (1991, 1993), Uddin & Morgan (1997a, 1997b) and Martin (1998). Further optimality results for NRC designs with correlated errors are given in this thesis.

In addition to the results on NRC designs, early generation variety trials are also considered. Many agricultural variety trials are carried out across the world and their results are often of considerable economic importance. This includes many variety selection programmes. At the early stages of a variety selection programme there is often a large number of new varieties to be tested with insufficient seed to allow within-site replication of the new varieties. However, replicated standard varieties are included for comparative purposes. These experiments are called *early generation variety trials*. The purpose of these trials is to select top performers from the new varieties, to be further tested in later stages of the programme.

Recently there has been much interest in the spatial analysis of agricultural variety trials that take account of the inherent spatial dependence of adjoining plots; see, for example, Besag & Kempton (1986), Gleeson & Cullis (1987), Cullis & Gleeson (1989), Cullis *et al.* (1989), Cullis & Gleeson (1991), Kempton *et al.* (1994), Grondona *et al.* (1996), Gilmour *et al.* (1997), Cullis *et al.* (1998). However, little has been published on the design of efficient early generation variety trials under spatial correlation. Indeed, Cullis *et al.* (1998) recognise that this is an 'important issue requiring attention'.

There is no commonly used simple criterion to assess the efficiency of early generation variety trials. The efficacy of several intuitively simple criteria is considered in chapter 10. The experimental designs most frequently employed for early generation variety trials have had the standard varieties systematically distributed over the experimental area. The robustness of some systematic designs is investigated in chapter 11.

Chapter 2 of the thesis provides some background material for designs under dependence. Chapter 3 outlines various methods to find optimal and efficient designs. Chapters 4 to 8 consider the NRC design problem, and early generation variety trials are investigated in chapters 9 to 11. Chapter 12 brings the thesis to a close with a discussion of the main conclusions and suggestions for further research.

Glossary

The following is a list of abbreviations used in this thesis. A reference to the section in which the corresponding definition can be found is also given.

Abbreviation		Defined in section:
AD	Augmented design.	9.1.2
AR(1)*AR(1)	Doubly geometric process.	2.3.3.1
AR(2a)	Special case of AR(2) with $\eta_1 = 2\eta$ and $\eta_2 = -\eta^2$ for $|\eta| < 1$.	5.2.5
AR(2b)	Special case of AR(2) with $\eta_1 = \eta$ and $\eta_2 = 2\eta^2$ for $|\eta| < \frac{1}{2}$.	5.2.5
AR(p)	Autoregressive process of order p, ARIMA(p,0,0).	2.3.2.2
ARIMA(p,d,q)	Autoregressive integrated moving-average process of autoregressive order p, moving average order q and differencing d.	A1.6
ARMA	Autoregressive moving-average process, ARIMA(p,0,q).	A1.6
BIB design	Balanced incomplete block design.	A1.7
BIBRC design	Balanced incomplete block row-column design.	5.1.1
BLUE	Best linear unbiased estimator.	2.4.4
BLUP	Best linear unbiased predictor.	2.4.5
BNRC design	Balanced nested row-column design.	5.1.3
CAR(1)	Conditional autoregressive process of order 1.	2.3.3.3
CAR(2)	Conditional autoregressive process of order 2.	2.3.3.3
CG(d)	Cullis-Gleeson model of order d.	2.3.2.4
EGVT	Early generation variety trial.	9.1
gls	Generalised least squares estimation.	2.4.1
HCS	Harmonic correlation structure.	2.3.2.3
LV	Linear variance model, CG(1).	2.3.2.4
MA(q)	Moving-average process of order q, ARIMA(0,0,q).	2.3.2.1
MAD	Modified augmented design	9.1.2
NN1*NN1	Separable structure with the NN1 process in both directions.	2.3.3.2
NNq	Nearest neighbour process of order q.	2.3.2.1
NRC design	Nested row-column design.	4.1
NSW	New South Wales.	9.1.2
ols	Ordinary least squares estimation.	2.4.2

REML	Residual maximum likelihood.	9.1
SBA	Semi-balanced array of strength 2.	3.1.3
SDEN design	Strongly directionally equineighboured design.	5.2.4
SEN design	Strongly equineighboured design.	5.2.4
SSDEN design	Spatial block strongly directionally equineighboured design.	5.3.1
SSEN design	Spatial block strongly equineighboured design.	5.3.1
SSENC design	Spatial block strongly equineighboured design under complete symmetry.	5.3.1
SSENR design	Spatial block strongly equineighboured design under reflection symmetry.	5.3.1

2   Background material

In this chapter, background material is provided for block designs. Definitions of optimality, efficiency and dependence are given here.

Consider the situation with t treatments to be allocated to b blocks each consisting of p_1 rows and p_2 columns. Let $k = p_1 p_2$ and let the total number of plots be $m = bk$. Treatments will be labelled $1, 2, ..., t$. Treatments are *equally replicated* in a design if each treatment occurs an equal number of times. When plots are spatially arranged, it is assumed that all plots are *congruent*, that is, all plots are of the same shape and size. Plots are said to be arranged in one-dimension when either p_1 or p_2 equal 1, and the corresponding design is called a *one-dimensional design*. For p_1 and p_2 greater than 1, plots are said to arranged in two-dimensions, and the corresponding design is called a *two-dimensional design*.

Example 2.1
Let Example 2.1 be a design which has $t = 5$ treatments, $b = 10$ blocks and $p_1 = p_2 = 2$ rows and columns.   ∎

Example 2.1 is considered throughout chapter 2 as an illustrative example. An allocation of treatments to plots for Example 2.1 is given by the following design, labelled D2.1.

$$
\begin{array}{|c|c|}\hline 1 & 2 \\\hline 3 & 4 \\\hline\end{array} ,
\begin{array}{|c|c|}\hline 1 & 4 \\\hline 2 & 5 \\\hline\end{array} ,
\begin{array}{|c|c|}\hline 2 & 3 \\\hline 4 & 5 \\\hline\end{array} ,
\begin{array}{|c|c|}\hline 2 & 5 \\\hline 3 & 1 \\\hline\end{array} ,
\begin{array}{|c|c|}\hline 3 & 1 \\\hline 4 & 2 \\\hline\end{array} ,
$$

$$
\begin{array}{|c|c|}\hline 3 & 4 \\\hline 5 & 1 \\\hline\end{array} ,
\begin{array}{|c|c|}\hline 4 & 2 \\\hline 5 & 3 \\\hline\end{array} ,
\begin{array}{|c|c|}\hline 4 & 5 \\\hline 1 & 2 \\\hline\end{array} ,
\begin{array}{|c|c|}\hline 5 & 1 \\\hline 2 & 3 \\\hline\end{array} ,
\begin{array}{|c|c|}\hline 5 & 3 \\\hline 1 & 4 \\\hline\end{array} .
\qquad \text{D2.1}
$$

2.1 Blocking

It is assumed that plots are allocated to blocks, such that the blocks comprise relatively homogeneous plots. For example, in a multi-site agricultural field trial, it would be unusual to have blocks comprised of plots from different sites, since these plots are unlikely to be homogeneous. Also, when blocks consist of plots from a single site, spatially well separated plots would not usually be in the same block.

The assumption of within-block homogeneity means that comparisons made within blocks are usually more accurate than comparisons between blocks. Hence, allocating treatments so that the treatment comparisons of interest can be made within blocks is essential, unless a *between-block* analysis is used. In a between-block analysis, the blocks are regarded as a random sample of blocks from some population, and treatment contrast estimates are made from comparisons between blocks.

In practice, as well as the need for within-block homogeneity, the blocking structure often depends on practical considerations. For example, in a field trial, long thin plots may be more manageable than square plots.

Complete block designs have each of the treatments allocated equally often to every block. When there are a large number of treatments, complete block designs are often not feasible and so *incomplete block designs* are used. For these designs, the size of the blocks is less than the number of treatments, that is $k < t$. Assume henceforth, unless otherwise stated, that $k \leq t$.

2.2 Modelling

Let y_{i,j_1,j_2} be the response from the plot in the j_1^{th} row and j_2^{th} column of block i, where $i = 1, 2, \ldots, b$, $j_1 = 1, 2, \ldots, p_1$ and $j_2 = 1, 2, \ldots, p_2$. The plots are

assumed to be ordered *lexicographically*. That is, block by block, and row by row within blocks. Let the ordered plots be numbered $1, 2, \ldots, m$. Figure 2.1 gives the plot numbering and the responses for Example 2.1.

Figure 2.1
Responses for Example 2.1. Plot numbering in parentheses

$y_{1,1,1}$	$y_{1,1,2}$		$y_{2,1,1}$	$y_{2,1,2}$		$y_{10,1,1}$	$y_{10,1,2}$
(1)	(2)		(5)	(6)		(37)	(38)
$y_{1,2,1}$	$y_{1,2,2}$	,	$y_{2,2,1}$	$y_{2,2,2}$	,$\ldots$,	$y_{10,2,1}$	$y_{10,2,2}$
(3)	(4)		(7)	(8)		(39)	(40)
Block 1			Block 2			Block 10	

Let the postulated model be

$$y = X\underline{\tau} + Z\underline{\alpha} + \underline{\varepsilon}, \tag{2.1}$$

where

$\underline{y}$ is the m-vector of observations ordered lexicographically. That is, the first p_2 observations are from the first row of the first block, observations $p_2 + 1$ to $2p_2$ are from the second row of the first block, $\ldots$, observations $p_2(p_1 - 1) + 1$ to k are from the p_1^{th} row of the first block, $\ldots$, observations $k+1$ to $k + p_2$ are from the first row of the second block, $\ldots$, the last p_2 observations are from the p_1^{th} row of block b;

$\underline{\tau} = (\tau_1, \tau_2, \ldots, \tau_t)'$ is a t-vector of fixed treatment effects;

X is the $m \times t$ treatment design matrix. The $(l, v)^{\text{th}}$ element of X is equal to 1 if plot l receives treatment v, for $l = 1, \ldots, m$ and $v = 1, \ldots, t$, and 0 otherwise;

$\underline{\alpha}$ is a q-vector of fixed nuisance effects, such as block, row or column effects;

Z is the $m \times q$ design matrix corresponding to $\underline{\alpha}$;

$\underline{\varepsilon}$ is the m-vector of errors such that $E(\underline{\varepsilon}) = \underline{0}_m$ and $var(\underline{\varepsilon}) = V\sigma^2$, for V a positive definite $m \times m$ matrix. For uncorrelated errors, V is the $m \times m$ identity matrix, I_m.

For some models, including the models for NRC designs given in chapter 4,

$$Z = I_b \otimes B,$$

where 1_n is a n-vector of ones and $\otimes$ is the Kronecker product (see Appendix A1.3). For a model where $\underline{\alpha}$ is a b-vector of fixed block effects only (no row or column effects), $B = 1_k$. Then the $(l, i)^{\text{th}}$ element of Z is equal to 1 when plot l is in block i, for $l = 1,...,m$ and $i = 1,...,b$, and 0 otherwise;

The treatment design matrix for the design D2.1 is

$$X = \begin{pmatrix} X_1 \\ \hline X_2 \\ \hline \vdots \\ \hline X_b \end{pmatrix},$$

where X_i is the treatment design matrix for block i, so that

$$X_1 = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix}, \quad X_2 = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}, \quad \text{etc.}$$

2.3   Dependence structures

Usually the true dependence structure is not known and so simple structures are often modelled, at least initially. With this in mind, it is often assumed that observations between blocks are uncorrelated and that the within-block dependence structure is the same for all blocks. This means that $V = I_b \otimes \Lambda$, where $\sigma^2 \Lambda$ is a $k \times k$ covariance matrix for plots within any block. For spatially arranged plots, another simplification is to assume that the dependence structure is a second order stationary process. This means that observations have the same variance, and the correlation between observations is the same if they are the same lag apart. More formally, under stationarity,

the correlation between two observations in the same block, that are lag g_1 apart within rows and lag g_2 apart within columns, is defined as

$$\text{corr}(y_{i,j_1,j_2}, y_{i,j_1+g_2,j_2+g_1}) = \rho_{g_1,g_2}$$

where $\rho_{g_1,g_2} = \rho_{-g_1,-g_2}$ and $|\rho_{g_1,g_2}| < 1 \quad \forall \; g_1, g_2$.

If Λ is the within-block correlation matrix, then for blocks of size 2×2, as in Example 2.1,

$$\Lambda = \begin{pmatrix} 1 & \rho_{1,0} & \rho_{0,1} & \rho_{1,1} \\ \rho_{1,0} & 1 & \rho_{-1,1} & \rho_{0,1} \\ \rho_{0,1} & \rho_{-1,1} & 1 & \rho_{1,0} \\ \rho_{1,1} & \rho_{0,1} & \rho_{1,0} & 1 \end{pmatrix},$$

under these assumptions.

As will be seen in section 2.4.1, for generalised least squares estimation of the treatment contrasts, the inverse of Λ is needed. It is usually difficult to derive results on optimal designs when the postulated Λ has an inverse with a complicated structure and a large number of parameters.

2.3.1   Symmetries in the dependence structure

When plots are spatially arranged, Martin & Eccleston (1991, 1993) consider some further simplifications to the dependence structure. Often Λ is centro-symmetric (see Appendix A1.4 for a definition), which essentially means that the direction of the ordering of plots within blocks is not relevant. Usually the *plot structure* should be symmetric for centro-symmetry to be reasonable. The plot structure refers to the actual physical layout of the block and the plots within the block. Note that for a stationary process, Λ is centro-symmetric.

Some other symmetries, which are special cases of centro-symmetry, are given below. First let $(\Lambda)_{l_1 l_2} = u_{l_1 l_2}$, and for any block, let

$$f(j_1, j_2) = p_2(j_1 - 1) + j_2$$

transform the two-dimensional plot co-ordinates (j_1, j_2) to the one-dimensional plot number $f(j_1, j_2)$, given that the plots are in lexicographical order.

For illustration purposes, let the centre of each plot be represented by a node, and let the element of Λ, $u_{f(j_1,j_2),f(j_1',j_2')}$, corresponding to plots in $f(j_1, j_2)$ and $f(j_1', j_2')$, be represented by a line connecting the nodes for these two plots. If $j_1 = j_1'$ and $j_2 = j_2'$ then $u_{f(j_1,j_2),f(j_1',j_2')}$ is represented by the node for plot $f(j_1, j_2)$. For example, Figure 2.2 shows, for a block of size 5×5, the line connecting the nodes for plots $f(3,3) = 13$ and $f(4,5) = 20$.

Figure 2.2
Illustration of the line representing $u_{13,20}$ for a block of size 5×5.
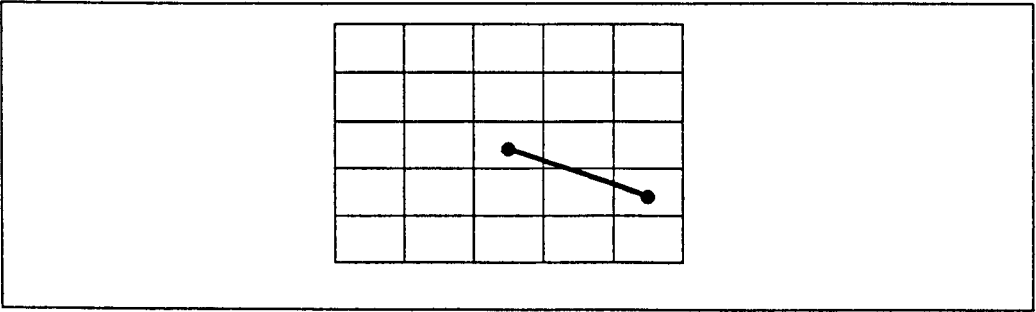
For a *reflection symmetric* dependence structure, the elements of Λ, which correspond to vertical and horizontal reflections of the line (or node) for $u_{f(j_1,j_2),f(j_1',j_2')}$, are equal. For example, Figure 2.3a illustrates that for blocks of size 5×5 under reflection symmetry, $u_{6,13} = u_{10,13} = u_{13,16} = u_{13,20}$. In general, a dependence structure is *reflection symmetric* if

$$u_{f(j_1,j_2),f(j_1',j_2')} = u_{f(p_1+1-j_1,j_2),f(p_1+1-j_1',j_2')}$$

$$= u_{f(j_1,p_2+1-j_2),f(j_1',p_2+1-j_2')}$$

$$= u_{f(p_1+1-j_1,p_2+1-j_2),f(p_1+1-j_1',p_2+1-j_2')}.$$

Under stationarity, this means that

$$\rho_{g_1,g_2} = \rho_{g_1,-g_2} = \rho_{-g_1,g_2} = \rho_{-g_1,-g_2} \quad \forall \ g_1, g_2.$$

Martin & Eccleston (1993) say that this may be a reasonable assumption if the *plot structure* is symmetric under vertical and horizontal reflections, which is true here when plots are rectangular.

Figure 2.3
Elements of Λ equal to $u_{13,20}$ for blocks of size 5×5 under:

a) reflection symmetry,　　　b) axial symmetry
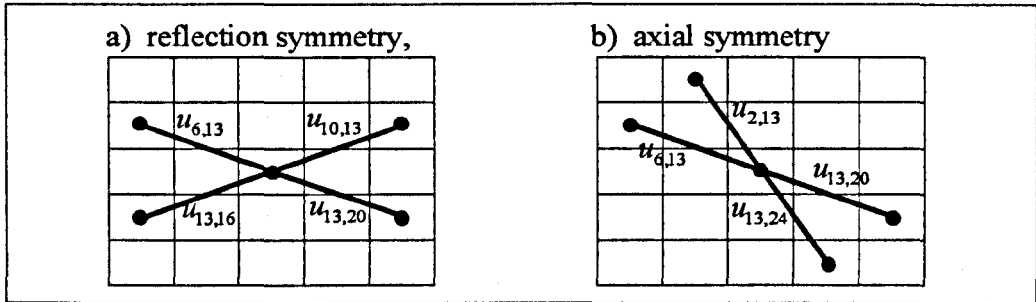
A dependence structure is *axially symmetric* if

$$u_{f(j_1,j_2),f(j_1',j_2')} = u_{f(j_2,j_1),f(j_2',j_1')}$$

$$= u_{f(p_2+1-j_2,\,p_1+1-j_1),f(p_2+1-j_2',\,p_1+1-'j_1')}$$

$$= u_{f(p_1+1-j_1,\,p_2+1-j_2),f(p_1+1-j_1',\,p_2+1-j_2')}.$$

This means that the elements of Λ, which correspond to NE-SW and NW-SE diagonal reflections of the line (or node) for $u_{f(j_1,j_2),f(j_1',j_2')}$, are equal. For the example with blocks of size 5×5, Figure 2.3b illustrates that under axial symmetry, $u_{2,13} = u_{6,13} = u_{13,20} = u_{13,24}$. Axial symmetry may be reasonable if the plot structure is symmetric about NE-SW and NW-SE diagonal reflections. Under stationarity, axial symmetry means that

$$\rho_{g_1,g_2} = \rho_{g_2,g_1} = \rho_{-g_1,-g_2} = \rho_{-g_2,-g_1} \quad \forall \ g_1, g_2.$$

If a dependence structure is both axially and reflection symmetric then it is *completely symmetric*.

Under stationarity, a special case of a reflection symmetric dependence structure has

$$\rho_{g_1, g_2} = \rho_{g_1, 0}\rho_{0, g_2} \quad \forall \ g_1, \ g_2,$$

This is called a *separable* process. Recall that $\rho_{g_1, 0}$ and ρ_{0, g_2} are the lag g_1 row and lag g_2 column correlations, respectively. For a separable process, $\Lambda = \Lambda_2 \otimes \Lambda_1$, where Λ_1 and Λ_2 are the correlation matrices for observations within rows and columns, respectively.

2.3.2 One-dimensional processes

For plots arranged in one dimension, simple time series processes, such as low order autoregressive moving-average (ARMA) processes (see Appendix A1.6), are often considered. Let N_g be the $k \times k$ lag g neighbour matrix, such that

$$\left(N_g\right)_{i,j} = \begin{cases} 1 & \text{if } |i - j| = g \\ 0 & \text{otherwise} \end{cases}, \quad \text{for } 0 \le g \le k-1.$$

Clearly $N_0 = I_k$ and $\sum_{g=0}^{k-1} N_g = J_k$, where $J_n = \underline{1}_n \underline{1}_n'$ is an $n \times n$ matrix of ones. For example, if $k = 4$,

$$N_1 = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}, \ N_2 = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix} \text{ and } N_3 = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}.$$

Then for any stationary process, the within-block correlation matrix is

$$\Lambda = \sum_{g=0}^{k-1} \rho_g N_g,$$

where ρ_g is the correlation of observations lag g apart, and $\rho_0 = 1$. Here Λ is a symmetric Toeplitz matrix and is therefore also centro-symmetric (see Appendix A1.4).

2.3.2.1 Nearest neighbour and moving average processes

Under the nearest neighbour process of order q, NNq, plots which are lag q apart are correlated, and plots which are greater than q lags apart are uncorrelated. That is, $\rho_q \neq 0$ and $\rho_g = 0$ for $g > q$, so the within-block correlation matrix is

$$\Lambda = \sum_{g=0}^{q} \rho_g N_g .$$

The NNq process is a finite-k version of the qth-order moving average process, MA(q), where for plot j,

$$\varepsilon_j = \xi_j + \sum_{h=1}^{q} \varphi_h \xi_{j-h} ,$$

and ε_j is the random error and $\{\xi_j\}$ are independent random variables with zero mean and constant variance $\forall\, j$.

The NN1 process has $\Lambda = I_k + \rho_1 N_1$ with $|\rho_1| < \left[2\cos\{(k+1)^{-1}\pi\}\right]^{-1}$ for Λ positive definite. Therefore $|\rho_1| < 1$ when $k = 2$, and $\left[2\cos\{(k+1)^{-1}\pi\}\right]^{-1} \to \frac{1}{2}$ as $k \to \infty$. For example, when $k = 4$,

$$\Lambda = \begin{pmatrix} 1 & \rho_1 & 0 & 0 \\ \rho_1 & 1 & \rho_1 & 0 \\ 0 & \rho_1 & 1 & \rho_1 \\ 0 & 0 & \rho_1 & 1 \end{pmatrix} \quad \text{for } |\rho_1| < \{2\cos(\tfrac{1}{5}\pi)\}^{-1} \approx 0.62 .$$

For the MA(1) process,

$$\rho_1 = \frac{\varphi_1}{(1+\varphi_1^2)}$$

and

$$\rho_g = 0 \text{ for } g > 1 .$$

Hence $|\rho_1| < \frac{1}{2}$. Therefore the MA(1) process is a special case of the NN1 process.

For the NN1 process, Λ has a very simple structure. However, the form of Λ^{-1} is fairly cumbersome, with

$$\left(\Lambda^{-1}\right)_{i,j(i\leq j)} = \frac{(1+\varphi_1^2)(-\varphi_1)^{j-i}(1-\varphi_1^{2i})(1-\varphi_1^{2(k-j+1)})}{(1-\varphi_1^2)(1-\varphi_1^{2(k+1)})}.$$

For example when $k = 4$, in terms of ρ_1,

$$\Lambda^{-1} = \frac{1}{(1-3\rho_1^2+\rho_1^4)}\begin{pmatrix} 1-2\rho_1^2 & -\rho_1(1-\rho_1^2) & \rho_1^2 & -\rho_1^3 \\ -\rho_1(1-\rho_1^2) & 1-\rho_1^2 & -\rho_1 & \rho_1^2 \\ \rho_1^2 & -\rho_1 & 1-\rho_1^2 & -\rho_1(1-\rho_1^2) \\ -\rho_1^3 & \rho_1^2 & -\rho_1(1-\rho_1^2) & 1-2\rho_1^2 \end{pmatrix}.$$

2.3.2.2   *Autoregressive processes*

For the stationary autoregressive process of order p, AR(p),

$$\varepsilon_j = \sum_{h=1}^{p} \eta_h \varepsilon_{j-h} + \xi_j,$$

where the $\{\eta_j\}$ are such that the process is stationary.

For the AR(1) process,

$$\rho_g = \eta_1^g = \rho_1^g \quad \text{for } |\eta_1| < 1 \text{ and } g \geq 0.$$

For example, when $k = 4$, the within-block correlation matrix is

$$\Lambda = \begin{pmatrix} 1 & \rho_1 & \rho_1^2 & \rho_1^3 \\ \rho_1 & 1 & \rho_1 & \rho_1^2 \\ \rho_1^2 & \rho_1 & 1 & \rho_1 \\ \rho_1^3 & \rho_1^2 & \rho_1 & 1 \end{pmatrix}.$$

For the AR(1) process Λ^{-1} has a simple form:

$$\left(1-\rho_1^2\right)\left(\Lambda^{-1}\right)_{i,j} = \begin{cases} 1 & \text{for } i = j = 1,k \\ 1+\rho_1^2 & \text{for } i = j \neq 1,k \\ -\rho_1 & \text{for } |i-j| = 1 \\ 0 & \text{otherwise} \end{cases}.$$

Hence, for the $k = 4$ example,

$$\Lambda^{-1} = \frac{1}{(1-\rho_1^2)}\begin{pmatrix} 1 & -\rho_1 & 0 & 0 \\ -\rho_1 & 1+\rho_1^2 & -\rho_1 & 0 \\ 0 & -\rho_1 & 1+\rho_1^2 & -\rho_1 \\ 0 & 0 & -\rho_1 & 1 \end{pmatrix}.$$

For the AR(2) process,

$$\rho_1 = \frac{\eta_1}{(1-\eta_2)}$$

and $\rho_g = \eta_1 \rho_{g-1} + \eta_2 \rho_{g-2}$ for $g > 1$,

where $|\eta_2| < 1$ and $|\eta_1| < 1 - \eta_2$.

2.3.2.3 Harmonic correlation structure

The harmonic correlation structure, HCS, has

$$\rho_g = \frac{\rho_1}{g} \quad \text{for } g > 0,$$

where $\rho_L \le \rho_1 \le \rho_U$, such that $\rho_L \le 0$ and $\rho_U \ge \{\ln(4)\}^{-1} \approx 0.72$ depends on k. See Martin & Eccleston (1992) for further details. The within-block correlation matrix is

$$\Lambda = I_k + \rho_1 \sum_{g=1}^{k-1} \frac{1}{g} N_g.$$

As for the MA(1) process, Λ^{-1} has a complicated structure for the HCS. For example, when $k = 4$,

$$\Lambda = \begin{pmatrix} 1 & \rho_1 & \tfrac{1}{2}\rho_1 & \tfrac{1}{3}\rho_1 \\ \rho_1 & 1 & \rho_1 & \tfrac{1}{2}\rho_1 \\ \tfrac{1}{2}\rho_1 & \rho_1 & 1 & \rho_1 \\ \tfrac{1}{3}\rho_1 & \tfrac{1}{2}\rho_1 & \rho_1 & 1 \end{pmatrix} \quad \text{and} \quad \Lambda^{-1} = \frac{1}{g(\rho_1)}\begin{pmatrix} \zeta_0 & \zeta_1 & \zeta_2 & \zeta_3 \\ \zeta_1 & \zeta_4 & \zeta_5 & \zeta_2 \\ \zeta_2 & \zeta_5 & \zeta_4 & \zeta_1 \\ \zeta_3 & \zeta_2 & \zeta_1 & \zeta_0 \end{pmatrix},$$

where $\zeta_0 = 36(2-\rho_1)(2+\rho_1-4\rho_1^2)$, $\quad \zeta_1 = -12\rho_1(12-8\rho_1-5\rho_1^2)$,

$\zeta_2 = -6\rho_1(6-13\rho_1)(2-\rho_1)$, $\quad \zeta_3 = -12(4-12\rho_1+11\rho_1^2)$,

$\zeta_4 = 4(36-49\rho_1^2+12\rho_1^3)$, $\quad \zeta_5 = -4\rho_1(36-36\rho_1+11\rho_1^2)$

and $g(\rho_1) = (12-16\rho_1+\rho_1^2)(12+16\rho_1-23\rho_1^2)$.

2.3.2.4   The Cullis-Gleeson model

Recall that for model (2.1), $\text{var}(\underline{y}) = V\sigma^2$, where V is positive definite. An extension to this variance model is when the data are differenced so that the variance of the differenced data is finite, as in the Cullis-Gleeson model of order d, CG(d), which is now defined. For this model the variance of the within-block d-differenced data,

$$\text{var}\{(I_b \otimes \nabla_d)\underline{y}\} = I_b \otimes (\psi I_{k-d} + \nabla_d \nabla_d')\sigma^2,$$

where ∇_d is the $(k-d) \times k$ within-block d-difference matrix (see Appendix A1.6) and $\psi \geq 0$ for $0 < d < k$.

The CG(d) process is a special case of an autoregressive integrated moving average process of dth level differencing, autoregressive order 0 and moving-average order d, i.e. an ARIMA(0, d, d) process (see Appendix A1.6). The CG(1) model is also known as the linear variance, LV, model.

2.3.3   Some two-dimensional processes

Some simple two-dimensional processes are considered in section 2.3.3.

2.3.3.1   The AR(1)*AR(1) process

The separable process (see section 2.3.1) with AR(1) in both directions is the AR(1)*AR(1) process. This is also known as the *doubly geometric process*.
Here $\rho_{g_1,0} = \rho_{1,0}^{g_1}$ and $\rho_{0,g_2} = \rho_{0,1}^{g_2}$.

Hence from the definition of the AR(1) process in section 2.3.2.2, it follows that for the AR(1)*AR(1) process,

$$\Lambda_1 = \begin{pmatrix} 1 & \rho_{1,0} & \rho_{1,0}^2 & \cdots & \rho_{1,0}^{p_2-1} \\ \rho_{1,0} & 1 & \rho_{1,0} & \cdots & \rho_{1,0}^{p_2-2} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \rho_{1,0}^{p_2-1} & \rho_{1,0}^{p_2-2} & \rho_{1,0}^{p_2-3} & \cdots & 1 \end{pmatrix}$$

and $\Lambda_2 = \begin{pmatrix} 1 & \rho_{0,1} & \rho_{0,1}^2 & \cdots & \rho_{0,1}^{P_1-1} \\ \rho_{0,1} & 1 & \rho_{0,1} & \cdots & \rho_{0,1}^{P_1-2} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \rho_{0,1}^{P_1-1} & \rho_{0,1}^{P_1-2} & \rho_{0,1}^{P_1-3} & \cdots & 1 \end{pmatrix}$

with $|\rho_{1,0}|, |\rho_{0,1}| < 1$. For blocks of size 2×2 as in Example 2.1,

$$\Lambda = \begin{pmatrix} 1 & \rho_{0,1} \\ \rho_{0,1} & 1 \end{pmatrix} \otimes \begin{pmatrix} 1 & \rho_{1,0} \\ \rho_{1,0} & 1 \end{pmatrix},$$

and by (A1.11) (in Appendix A1.3) and the inverse of the within-block correlation matrix for an AR(1) process (in section 2.3.2.2),

$$\Lambda^{-1} = \frac{1}{(1-\rho_{0,1}^2)(1-\rho_{1,0}^2)} \begin{pmatrix} 1 & -\rho_{0,1} \\ -\rho_{0,1} & 1 \end{pmatrix} \otimes \begin{pmatrix} 1 & -\rho_{1,0} \\ -\rho_{1,0} & 1 \end{pmatrix}.$$

2.3.3.2 The NN1*NN1 process

The separable dependence structure with the NN1 process in both directions, NN1*NN1, has

$$\rho_{g_1,0} = \begin{cases} \rho_{1,0} & \text{if } g_1 = 1 \\ 0 & \text{if } g_1 > 1 \end{cases} \quad \text{and} \quad \rho_{0,g_2} = \begin{cases} \rho_{0,1} & \text{if } g_2 = 1 \\ 0 & \text{if } g_2 > 1 \end{cases}.$$

Note that for Example 2.1, where blocks are of size 2×2, the AR(1)*AR(1) and NN1*NN1 processes are equivalent, with $|\rho_{1,0}|, |\rho_{0,1}| < 1$.

2.3.3.3 Conditional autoregressive processes

Dependence structures are sometimes defined in terms of the conditional mean and variance of the error at each plot given the errors at the other plots within a block. In order to ease the notation slightly, since within-block dependence is considered, the subscript i in ε_{i,j_1,j_2} is omitted in this section.

Consider the process with

$$\mathrm{E}\left(\varepsilon_{j_1,j_2} \middle| \varepsilon_{j_1',j_2'}, \text{s.t.} (j_1, j_2) \neq (j_1', j_2')\right) = \sum \zeta_{g_1,g_2} \varepsilon_{j_1-g_2, j_2-g_1},$$

where the summation is over all lags $(g_1, g_2) \neq (0, 0)$, $\zeta_{g_1,g_2} = \zeta_{-g_1,-g_2}$ for all

g_1, g_2, and $\sum \zeta_{g_1,g_2} < 1$.

Also,

$$\mathrm{var}\left(\varepsilon_{j_1,j_2} \middle| \varepsilon_{j_1',j_2'}, \text{s.t.} (j_1, j_2) \neq (j_1', j_2')\right) = \sigma_\eta^2,$$

say, is constant.

For the second order conditional autoregressive process, CAR(2), $\zeta_{g_1,g_2} = 0$

for all (g_1, g_2) except $(g_1, g_2) = (0, 1), (1, 0), (1, 1)$ and $(-1, 1)$. Therefore,

$$\mathrm{E}\left(\varepsilon_{j_1,j_2} \middle| \varepsilon_{j_1',j_2'}, \text{s.t.} (j_1, j_2) \neq (j_1', j_2')\right) =$$

$$\zeta_{0,1}\left(\varepsilon_{j_1-1,j_2} + \varepsilon_{j_1+1,j_2}\right) + \zeta_{1,0}\left(\varepsilon_{j_1,j_2-1} + \varepsilon_{j_1,j_2+1}\right)$$

$$+ \zeta_{1,1}\left(\varepsilon_{j_1+1,j_2+1} + \varepsilon_{j_1-1,j_2-1}\right) + \zeta_{-1,1}\left(\varepsilon_{j_1-1,j_2+1} + \varepsilon_{j_1+1,j_2-1}\right),$$

for $\zeta_{0,1} + \zeta_{1,0} + \zeta_{1,1} + \zeta_{-1,1} < 1$.

Within any block, a plot with plot co-ordinates (j_1, j_2) is said to be an
external plot if

     j_1 is 1 or p_1,

or j_2 is 1 or p_2.

The off-diagonal element of Λ^{-1} for a pair of distinct plots that are both not
external plots and are lag (g_1, g_2) apart, is given by $-\zeta_{g_1,g_2}$. The diagonal
element of Λ^{-1} for a plot that is not an external plot is 1. When
$\zeta_{1,1} = \zeta_{-1,1} = -\zeta_{0,1}\zeta_{1,0}$, the CAR(2) process is equivalent to the AR(1)*AR(1)
process (see Martin, 1982). The CAR(2) process with $\zeta_{1,1} = \zeta_{-1,1} = 0$ is called
the first order conditional autoregressive, CAR(1), process.

For the CAR(2), the lag (g_1, g_2) correlation is specified by the integral

$$\frac{\sigma_\eta^2}{4\pi^2\sigma^2}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi}\frac{\cos(g_1\vartheta_1)\cos(g_2\vartheta_2)}{1-2\zeta_{1,0}\cos(\vartheta_1)-2\zeta_{0,1}\cos(\vartheta_2)-2\zeta_{1,1}\cos(\vartheta_1+\vartheta_2)-2\zeta_{-1,1}\cos(\vartheta_1-\vartheta_2)}d\vartheta_1 d\vartheta_2 \cdot$$

The elements of Λ^{-1} for a pair of external plots can usually only be obtained numerically. To avoid this, non-stationary versions of the CAR(2) process are sometimes used. One such process takes the off-diagonal elements of Λ^{-1}, for all plots that are lag (g_1, g_2) apart to be $-\zeta_{g_1,g_2}$, and the diagonal elements of Λ^{-1} to be 1. That is,

$$\begin{aligned}
\Lambda^{-1} = I_{p_1 p_2} &- \zeta_{1,0}(I_{p_1}\otimes N_{p_2}) - \zeta_{0,1}(N_{p_1}\otimes I_{p_2}) \\
&- \zeta_{1,1}(N_{p_1}^L\otimes N_{p_2}^L + N_{p_1}^U\otimes N_{p_2}^U) \\
&- \zeta_{-1,1}(N_{p_1}^L\otimes N_{p_2}^U + N_{p_1}^U\otimes N_{p_2}^L),
\end{aligned} \tag{2.2}$$

for $\zeta_{0,1} + \zeta_{1,0} + \zeta_{1,1} + \zeta_{-1,1} < 1$, where N_n^L, N_n^U and N_n are $n\times n$ matrices such that

$$\left(N_n^L\right)_{i,j} = \begin{cases} 1 & \text{if } i-j=1 \\ 0 & \text{otherwise} \end{cases},$$

$$\left(N_n^U\right)_{i,j} = \begin{cases} 1 & \text{if } i-j=-1 \\ 0 & \text{otherwise} \end{cases} \quad \text{and}$$

$$N_n = N_n^L + N_n^U.$$

Such a non-stationary version of the CAR(1) and CAR(2) processes, for blocks of size 2×2, as in Example 2.1, where all pairs of plots are external plots, has Λ^{-1} equal to

$$\begin{pmatrix} 1 & -\zeta_{1,0} & -\zeta_{0,1} & 0 \\ -\zeta_{1,0} & 1 & 0 & -\zeta_{0,1} \\ -\zeta_{0,1} & 0 & 1 & -\zeta_{1,0} \\ 0 & -\zeta_{0,1} & -\zeta_{1,0} & 1 \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} 1 & -\zeta_{1,0} & -\zeta_{0,1} & -\zeta_{1,1} \\ -\zeta_{1,0} & 1 & -\zeta_{-1,1} & -\zeta_{0,1} \\ -\zeta_{0,1} & -\zeta_{-1,1} & 1 & -\zeta_{1,0} \\ -\zeta_{1,1} & -\zeta_{0,1} & -\zeta_{1,0} & 1 \end{pmatrix},$$

respectively.

A special case of (2.2), which will be called the *3-parameter CAR(2)* in this thesis, has $\zeta_{1,1} = \zeta_{-1,1}$. Therefore (2.2) simplifies to

$$\Lambda^{-1} = I_{p_1 p_2} - \zeta_{1,0}(I_{p_1} \otimes N_{p_2}) - \zeta_{0,1}(N_{p_1} \otimes I_{p_2}) - \zeta_{1,1}(N_{p_1} \otimes N_{p_2}),$$

for $\zeta_{0,1} + \zeta_{1,0} + 2\zeta_{1,1} < \frac{1}{2}$, where Λ^{-1} is positive definite if

$$2\zeta_{1,0}\cos\left(\frac{\pi}{(p_2 + 1)}\right) + 2\zeta_{0,1}\cos\left(\frac{\pi}{(p_1 + 1)}\right)$$

$$+ 4\zeta_{1,1}\cos\left(\frac{\pi}{(p_1 + 1)}\right)\cos\left(\frac{\pi}{(p_2 + 1)}\right) < 1.$$

(2.3)

Note that $\zeta_{0,1}, \zeta_{1,0}, \zeta_{1,1} \geq 0$, such that $\zeta_{0,1} + \zeta_{1,0} + 2\zeta_{1,1} < \frac{1}{2}$, implies that the condition in (2.3) is satisfied.

For a two-dimensional block, the left and right edges or the top and bottom edges may be joined, giving a *cylindrical* block. It is assumed here that the rows are circular for cylindrical blocks (i.e. left and right edges are joined). A cylinder version of the CAR(2) process has Λ^{-1} as given by (2.2), but $N_{p_2}^L$ and $N_{p_2}^U$ are defined as

$$\left(N_{p_2}^L\right)_{i,j} = \begin{cases} 1 & \text{if } i - j = 1 \pmod{p_2} \quad \text{for } p_2 > 2 \\ 0 & \text{otherwise} \end{cases}$$

and

$$\left(N_{p_2}^U\right)_{i,j} = \begin{cases} 1 & \text{if } i - j = -1 \pmod{p_2} \quad \text{for } p_2 > 2 \\ 0 & \text{otherwise} \end{cases}.$$

If both left and right edges and top and bottom edges of a two-dimensional block are joined then the block forms a *torus*. The CAR(2) process for a torus is a stationary process, which has Λ^{-1} as given by (2.2) with $N_{p_2}^L$ and $N_{p_2}^U$ as given for the cylinder version of the CAR(2) process, and $N_{p_1}^L$ and $N_{p_1}^U$ defined as

$$\left(N^{L}_{p_1}\right)_{i,j} = \begin{cases} 1 & \text{if } i - j = 1 \,(\text{mod } p_1) \quad \text{for } p_1 > 2 \\ 0 & \text{otherwise} \end{cases}$$

and

$$\left(N^{U}_{p_1}\right)_{i,j} = \begin{cases} 1 & \text{if } i - j = -1 \,(\text{mod } p_1) \quad \text{for } p_1 > 2 \\ 0 & \text{otherwise} \end{cases}.$$

2.4   Treatment effect estimation

The design implications of analyses that take the correlation structure into account have been investigated by, for example, Martin (1982), Gill & Shukla (1985b) and Martin (1986). In particular, Martin (1986) considered designs with $b = 1$ under model (2.1). Note that when $b = 1$, $Z = \underline{1}_b$ and $\underline{\alpha}$ is a scalar, so $Z\underline{\alpha}$ is a constant term in model (2.1). Martin (1986) concluded that a reasonable approach for field trials is generalised least squares estimation (see section 2.4.1) with the correlation specified by a small number of parameters, and that the estimated treatment contrasts are likely to be reasonably robust to the exact form of the dependence process chosen.

2.4.1   Generalised least squares estimation

Assume that V is known and used to find $\hat{\underline{\tau}}$, the generalised least squares (gls) estimate of treatment effects. To find $\hat{\underline{\tau}}$, it is necessary to solve equations (2.4) and (2.5),

$$(X'V^{-1}X)\hat{\underline{\tau}} + (X'V^{-1}Z)\hat{\underline{\alpha}} = X'V^{-1}\underline{y} \tag{2.4}$$

and $(Z'V^{-1}X)\hat{\underline{\tau}} + (Z'V^{-1}Z)\hat{\underline{\alpha}} = Z'V^{-1}\underline{y}.$ $\qquad\qquad$ (2.5)

Note that in practice V is not usually known exactly. However, if a prior estimate of V is used, the design implications will be approximately correct if the prior estimate is close to V (Martin, 1986). For design purposes, V is assumed to be known.

Solving (2.5) for $\underline{\hat{\alpha}}$ in terms of $\underline{\hat{\tau}}$, gives

$$\underline{\hat{\alpha}} = (Z'V^{-1}Z)^+ Z'V^{-1}(\underline{y} - X\underline{\hat{\tau}}) \qquad (2.6)$$

where for a matrix T, T^+ is its Moore-Penrose generalised inverse (see Appendix A1.2).

Pre-multiplying (2.6) by Z and substituting in to (2.4) gives

$$C\underline{\hat{\tau}} = \underline{q}, \qquad (2.7)$$

where

$$C = X'Q_{ZV}X, \qquad (2.8)$$

$$\underline{q} = X'Q_{ZV}\underline{y}, \qquad (2.9)$$

$$\text{and} \quad Q_{ZV} = V^{-1} - V^{-1}Z(Z'V^{-1}Z)^+ Z'V^{-1}. \qquad (2.10)$$

Note that no unique solution to equation (2.7) exists since C is not of full rank (the rows and columns of C sum to zero). All solutions to equation (2.7) can be given by

$$\underline{\hat{\tau}} = C^- \underline{q}, \qquad (2.11)$$

where for a matrix T, T^- is any generalised inverse (see Appendix A1.2). One choice of the matrix C^- in (2.11) is given by C^+, which is the unique Moore-Penrose generalised inverse of C. It is assumed henceforth, unless otherwise stated, that $\underline{\hat{\tau}}$ is obtained from (2.11) with C^- given by C^+. That is, $\underline{\hat{\tau}}$ is obtained from

$$\underline{\hat{\tau}} = C^+ \underline{q}. \qquad (2.12)$$

2.4.2 Ordinary least squares estimation

Under ordinary least squares (ols) estimation, V, in the expression for Q_{ZV} in (2.10), is replaced by I_m so

$$Q_{ZI} = I_m - Z(Z'Z)^+ Z'.$$

Kiefer & Wynn (1981) justify the use of the ols estimator by showing that it is quite robust against small perturbations in V from the uncorrelated case when $V = I_m$. However, Martin (1986) notes that a prior estimate of V can usually be chosen that is 'considerably closer' to the true V than I_m is.

2.4.3   Expectation and Variance of $\hat{\underline{\tau}}$

In order to find the expected value and variance of $\hat{\underline{\tau}}$, it is first simpler to find the expected value and variance of $\underline{q}$.

Consider the expectation of $\underline{q}$.

$$
\begin{aligned}
E(\underline{q}) &= X'Q_{ZV}E(\underline{y}) \\
&= X'Q_{ZV}X\underline{\tau} + X'Q_{ZV}Z\underline{\alpha} \\
&= C\underline{\tau}
\end{aligned}
\tag{2.13}
$$

since $Q_{ZV}Z = 0$.

Then by (2.13)

$$
E(\hat{\underline{\tau}}) = C^+ E(\underline{q}) = C^+ C\underline{\tau}.
\tag{2.14}
$$

Using $\hat{\underline{\tau}}$ obtained from (2.11),

$$
E(\hat{\underline{\tau}}) = C^- E(\underline{q}) = C^- C\underline{\tau}.
\tag{2.15}
$$

2.4.3.1   *Variance of $\hat{\underline{\tau}}$ under gls*

Note that

$$
Q_{ZV}VQ_{ZV} = Q_{ZV}.
\tag{2.16}
$$

Then,

$$
\begin{aligned}
\text{var}(\underline{q}) &= X'Q_{ZV}\,\text{var}(\underline{y})Q_{ZV}X \\
&= X'Q_{ZV}VQ_{ZV}X\sigma^2 \\
&= X'Q_{ZV}X\sigma^2 \quad \text{(by the equation in (2.16))}
\end{aligned}
$$

$$= C\sigma^2 \tag{2.17}$$

and by (2.17)

$$\mathrm{Var}(\hat{\underline{\tau}}) = C^+ \mathrm{var}(\underline{q})\, C^+ = C^+ \sigma^2. \tag{2.18}$$

2.4.3.2 *Variance of $\hat{\underline{\tau}}$ under ols*

Under ols,

$$\mathrm{var}(\underline{q}) = X'Q_{Z_J}\mathrm{var}(\underline{y})Q_{Z_J}X$$

$$= X'Q_{Z_J}VQ_{Z_J}X\sigma^2,$$

hence

$$\mathrm{var}(\hat{\underline{\tau}}) = C^+ \mathrm{var}(\underline{q})\, C^+$$

$$= C^+ X'Q_{Z_J}VQ_{Z_J}XC^+\sigma^2. \tag{2.19}$$

2.4.4 Estimability and connectedness

A linear function of the treatment effects, $\underline{c}'\underline{\tau}$, is *estimable* if

$$\mathrm{E}(\underline{c}'\hat{\underline{\tau}}) = \underline{c}'\underline{\tau}.$$

Using $\hat{\underline{\tau}}$ obtained from (2.11), it can be seen from (2.15) that if $\underline{c}' = \underline{c}'C^-C$ then $\underline{c}'\underline{\tau}$ is estimable. In fact $\underline{c}' = \underline{c}'C^-C$ is a necessary and sufficient condition for $\underline{c}'\underline{\tau}$ to be estimable, as noted in John & Williams (1995, section 1.5).

Definition 2.1
Let $D^+\sigma^2$ denote $\mathrm{var}(\hat{\underline{\tau}})$. ∎

Under gls, $D = C$ can be used. If $\underline{c}'\underline{\tau}$ is estimable then $\underline{c}'\hat{\underline{\tau}}$ is an unbiased estimator of $\underline{c}'\underline{\tau}$, and $\underline{c}'\hat{\underline{\tau}}$ is known as the *best linear unbiased estimator* (BLUE) of $\underline{c}'\underline{\tau}$. Also, $\underline{c}'\hat{\underline{\tau}}$ is invariant to all solutions of equation (2.7), and

$$\mathrm{var}(\underline{c}'\hat{\underline{\tau}}) = \underline{c}'D^+\underline{c}\sigma^2 = \underline{c}'D^-\underline{c}\sigma^2.$$

When $\underline{c}'\underline{\tau}$ is estimable, $\underline{c}'\underline{1}_t = 0$, so $\underline{c}'\underline{\tau}$ is a *contrast* of the treatment effects. For Example 2.1, $\underline{c}' = (0, 1, 0, 0, -1)$ compares treatments 2 and 5 so that $\underline{c}'\underline{\tau} = \tau_2 - \tau_5$. A contrast comparing two treatments is a *pairwise* contrast.

A design is said to be *connected* if and only if rank(C) = $t-1$. Then every treatment contrast is estimable from within-block comparisons (see John & Williams, 1995, section 1.8). It is assumed henceforth, unless otherwise stated, that all designs considered are connected.

2.4.5   Estimation and prediction under a mixed effects model

If $\underline{\tau}$ in model (2.1) is a vector of random effects, such that $(\underline{\tau}', \underline{\varepsilon}')'$ has zero mean and variance matrix

$$\begin{pmatrix} G\sigma_\tau^2 & 0 \\ 0 & V\sigma^2 \end{pmatrix},$$

where G is a $t \times t$ positive definite matrix, then

$$\mathrm{E}(\underline{y}) = Z\underline{\alpha}$$

and $\mathrm{var}(\underline{y}) = X \, \mathrm{var}(\tau) X' + \mathrm{var}(\varepsilon)$

$$= XGX'\sigma_\tau^2 + V\sigma^2 = V_*.$$

This model is called a *mixed effects model* since it includes both fixed and random effects (excluding the errors). Note that the rank of the $m \times q$ matrix Z is q.

The BLUE of the contrast $\underline{c}_q'\underline{\alpha}$ is $\underline{c}_q'\hat{\underline{\alpha}}$, where $\hat{\underline{\alpha}}$ is the gls estimator of $\underline{\alpha}$,

i.e. $\hat{\underline{\alpha}} = \left(Z'V_*^{-1}Z\right)^{-1}Z'V_*^{-1}\underline{y}$.

The best linear unbiased predictor (BLUP) of the contrast $\underline{c}_t'\underline{\tau}$ is $\underline{c}_t'\widetilde{\underline{\tau}}$, where

$$\widetilde{\underline{\tau}} = \sigma_\tau^2 GX'V_*^{-1}(\underline{y} - Z\hat{\underline{\alpha}}).$$

This form of the BLUP is given by Searle *et al.* (1992, section 7.4).

Mixed effects models are considered in this thesis (for example, in chapters 9 to 11), but the fixed effect model (2.1) is assumed unless otherwise stated.

2.5 Optimality and efficiency

An efficient design estimates the treatment contrasts of interest as well as possible. The accuracy of the estimation is usually measured by some combination of the variances of estimated contrasts, which when compared to a bound gives the *efficiency*.

2.5.1 The Φ_p-value

When all contrasts are of equal interest the Φ_p-value can be used to measure efficiency. If $\zeta_1, \zeta_2, \dots, \zeta_{t-1}$ are the non-zero eigenvalues of D ($t-1$ eigenvalues of D are non-zero when $\text{rank}(D) = t-1$) then

$$
\Phi_p\text{-value} = \begin{cases}
\left(\dfrac{1}{(t-1)} \sum_{i=1}^{t-1} \dfrac{1}{\zeta_i^p} \right)^{\frac{1}{p}} & \text{for } 0 < p < \infty \\[4mm]
\left(\prod_{i=1}^{t-1} \dfrac{1}{\zeta_i} \right)^{\frac{1}{(t-1)}} & \text{for } p = 0 \qquad \text{(Kiefer, 1975).} \\[4mm]
\max \dfrac{1}{\zeta_i} & \text{for } p = \infty
\end{cases}
$$

Definition 2.2
Let $\mathcal{D}$ be the set of all connected designs with t treatments and b blocks of size $p_1 \times p_2$. ∎

Let $\mathcal{D}^* \subseteq \mathcal{D}$ be the set of competing designs. For example, if interest is in binary designs only then $\mathcal{D}^*$ would be the set of binary designs in $\mathcal{D}$. A design $d^* \in \mathcal{D}^*$ is then Φ_p-*optimal* among designs in $\mathcal{D}^*$ if d^* has the smallest Φ_p-value over all designs in $\mathcal{D}^*$. Three commonly used measures of

efficiency are the A-, D- and E-values, which correspond to the Φ_p-value with $p = 1$, 0 and ∞, respectively.

2.5.2 The A-value

When $p = 1$, the Φ_p-value, which is also known as the A-value, is $1/(2\sigma^2)$ times the average variance of all pairwise contrasts. For example, for a design with 3 treatments the average variance of the pairwise contrasts is

$$\tfrac{1}{3}\{\mathrm{var}(\hat{\tau}_1 - \hat{\tau}_2) + \mathrm{var}(\hat{\tau}_1 - \hat{\tau}_3) + \mathrm{var}(\hat{\tau}_2 - \hat{\tau}_3)\}.$$

In general the average variance of all pairwise contrasts is

$$\frac{2}{t(t-1)}\sum_{i=1}^{t-1}\sum_{j=i+1}^{t}\mathrm{var}(\hat{\tau}_i - \hat{\tau}_j), \qquad (2.20)$$

which simplifies to

$$\frac{2}{t(t-1)}\left\{(t-1)\sum_{i=1}^{t}\mathrm{var}(\hat{\tau}_i) - \sum_{i=1}^{t-1}\sum_{j=i+1}^{t}2\mathrm{cov}(\hat{\tau}_i,\hat{\tau}_j)\right\}.$$

Note that

$$\sum_{i=1}^{t}\mathrm{var}(\hat{\tau}_i) = \mathrm{tr}(D^+)\sigma^2$$

and

$$\sum_{i=1}^{t-1}\sum_{j=i+1}^{t}2\mathrm{cov}(\hat{\tau}_i,\hat{\tau}_j) = \left\{1_t'D^+1_t - \mathrm{tr}(D^+)\right\}\sigma^2 = -\mathrm{tr}(D^+)\,\sigma^2,$$

since $1_t'D^+1_t = 0$ by (A1.6) in Appendix A1.2.

Therefore (2.20) is equal to

$$\frac{2\mathrm{tr}(D^+)\sigma^2}{(t-1)}.$$

In terms of any generalised inverse of D, (2.20) is equal to

$$\frac{2}{(t-1)}\left\{\mathrm{tr}(D^-) - \frac{1}{t}1_t'D^-1_t\right\}\sigma^2. \qquad (2.21)$$

2.5.3 The D- and E-values

The D-value is related to the volume of the confidence ellipsoid for $\hat{\underline{\tau}}$ under normality, and the E-value is

$$\max\left\{\frac{\text{var}(\underline{c}'\hat{\underline{\tau}})}{\underline{c}'\underline{c}\sigma^2}\right\} = \max\left\{\frac{\underline{c}'D^+\underline{c}}{\underline{c}'\underline{c}}\right\},$$

the maximum variance of an estimated standardised contrast.

2.5.4 Universal optimality

Kiefer (1975) considered *universal optimality*. This requires the minimisation of $\Phi(D)$ for all non-increasing, convex and orthogonally invariant Φ.

Under gls, if a design $d^* \in \mathcal{D}^*$ has

(i) *completely symmetric* C-matrix and

(ii) maximum trace of C over designs in $\mathcal{D}^*$

it is *universally optimal* over the set of designs $\mathcal{D}^*$ (Kiefer, 1975). Note that a $n \times n$ matrix with zero row and column sums is completely symmetric if it is of the form aE_n, where a is a scalar constant and $E_n = I_n - n^{-1}J_n$; that is, if all the diagonal elements are equal and all the off-diagonal elements are equal. The term 'completely symmetric' unfortunately has two different meanings: the one defined here and the one describing a dependence structure as defined in section 2.3.

A design is called *variance balanced* if the variances of all estimated pairwise contrasts are the same. This is true when D^+ is completely symmetric. Note that $E_t = Q_{1,J_t}$ is symmetric and idempotent. This means that if a design has $D = aE_t$ then, by (A1.7) in Appendix A1.2, $D^+ = a^{-1}E_t$. Therefore the design is variance balanced with the variance of all estimated pairwise contrasts equal to $2a^{-1}\sigma^2$.

Universal optimality includes Φ_p-optimality for all $p \geq 0$. Therefore a universally optimal design is A-, D- and E-optimal. If no universally optimal design exists, then the Φ_p-optimal design may differ from the $\Phi_{p'}$-optimal design for $p \neq p'$.

Let $\mathcal{D}_1 \subseteq \mathcal{D}$ be the set of designs for which C and $\text{var}(\underline{q})$ are completely symmetric. Let

$$C = a_1 E_t \quad \text{and} \quad \text{var}(\underline{q}) = a_2 E_t \sigma^2,$$

then

$$D^+ = \frac{a_2}{a_1^2} E_t \tag{2.22}$$

is completely symmetric. The non-zero eigenvalues of E_t are all equal to 1, hence the non-zero eigenvalues of $D = (a_1^2 / a_2) E_t$ are

$\zeta_1 = \zeta_2 = ... = \zeta_{t-1} = a_1^2 / a_2$, and so for a design in $\mathcal{D}_1$

$$\Phi_p\text{-value} = \frac{a_2}{a_1^2} \quad \text{for all } p \geq 0.$$

This means that over designs in $\mathcal{D}_1$, the Φ_p-criterion for all $p \geq 0$, simplifies to finding the minimum of a set of scalars. It follows that

$$\Phi(D) = \frac{a_2}{a_1^2}, \tag{2.23}$$

since universal optimality includes Φ_p-optimality for all $p \geq 0$. Therefore, a design that is Φ_p-optimal over $\mathcal{D}_1$ is also universally optimal over $\mathcal{D}_1$, under both ols and gls.

Note that for designs in $\mathcal{D}_1$, minimising $\text{tr}(D^+) = a_2(t-1)/a_1^2$, is equivalent to minimising the Φ_p-value. When comparing two designs d_1 and d_2, which belong to $\mathcal{D}_1$, d_1 is defined to be *universally better* than d_2 if $\text{tr}(D^+)$ for d_1 is less than or equal to $\text{tr}(D^+)$ for d_2. In fact, when $\text{tr}(D^+)$ is the same for d_1

and d_2, the designs are equivalent. However, for convenience, the definition of universally better includes the cases where designs are equivalent.

2.5.5 Weak universal optimality

Under ols, Kiefer & Wynn (1981) introduced *weak universal optimality*, which is a weaker notion of optimality than universal optimality since it includes Φ_p-optimality for $p \geq 1$ but does not generally include $0 \leq p < 1$. Hence weak universal optimality may exclude D-optimality.

Let $\mathcal{D}^* \subseteq \mathcal{D}$ be the set of designs which have, under ols, C-matrix completely symmetric. A design $d^* \in \mathcal{D}^*$, that has under ols, D^+ completely symmetric and minimal $\text{tr}(D^+)$ over $\mathcal{D}^*$, is weakly universally optimal among designs in $\mathcal{D}^*$ (Kiefer & Wynn, 1981).

It is clear that $d^* \in \mathcal{D}_1 \subseteq \mathcal{D}^*$. This means that when D^+ is completely symmetric, minimising $\text{tr}(D^+)$ over $\mathcal{D}^*$ is equivalent to minimising $\text{tr}(D^+)$ over $\mathcal{D}_1$. Hence d^* is universally optimal over $\mathcal{D}_1$.

2.5.6 Efficiency bounds

For competing designs the Φ_p-value can be compared to a lower bound, denoted by Φ_p^*-value. For a given $\text{tr}(D)$, a simple lower bound for the Φ_p-value is Φ_p^*-value $= (t-1)/\{\text{tr}(D)\}$. This bound is attained if D is completely symmetric. A global bound is obtained if the maximum of $\text{tr}(D)$ over $\mathcal{D}$ is used, or an upper bound for it.

A comparison of the Φ_p-value with a lower bound gives the

$$\Phi_p\text{-efficiency} = \frac{\left(\Phi_p^* - \text{value}\right)}{\left(\Phi_p - \text{value}\right)}.$$

If the lower bound is attainable, that is, if a design with Φ_p-value $= \Phi_p^*$-value exists, then clearly the design is Φ_p-optimal, and near-optimal designs will then have Φ_p-efficiency near to 1. However, if the Φ_p-optimal design has Φ_p-value considerably greater than the Φ_p^*-value (i.e. if the Φ_p^*-value is not a tight lower bound), the Φ_p-efficiency of the Φ_p-optimal and near-optimal designs will be much less than 1.

2.6 Simplification of the *C*-matrix

In this section a simplification to the *C*-matrix, (2.8), is given when model (2.1) with $Z = I_b \otimes B$ and $V = I_b \otimes \Lambda$ (see section 2.3) is assumed.

By using the properties of Kronecker products given in Appendix A1.3, the inverse of V is

$$V^{-1} = I_b \otimes \Lambda^{-1} \quad \text{(by (A1.11))}. \tag{2.24}$$

Then

$$(Z'V^{-1}Z)^+ = \{(I_b \otimes B')(I_b \otimes \Lambda^{-1})(I_b \otimes B)\}^+ \quad \text{(by (A1.10))}$$

$$= (I_b \otimes B'\Lambda^{-1}B)^+ \quad \text{(by (A1.12))}$$

$$= I_b \otimes (B'\Lambda^{-1}B)^+ \quad \text{(by (A1.11))}. \tag{2.25}$$

Substituting the expressions for V^{-1} and $(Z'V^{-1}Z)^+$ from (2.24) and (2.25), respectively, into the expression for Q_{ZV} in (2.10) gives

$$Q_{ZV} = (I_b \otimes \Lambda^{-1}) - (I_b \otimes \Lambda^{-1})(I_b \otimes B)\{I_b \otimes (B'\Lambda^{-1}B)^+\}(I_b \otimes B')(I_b \otimes \Lambda^{-1})$$

$$= (I_b \otimes \Lambda^{-1}) - I_b \otimes \Lambda^{-1}B(B'\Lambda^{-1}B)^+ B'\Lambda^{-1} \quad \text{(by (A1.12))}$$

$$= I_b \otimes \Omega^* \quad \text{(by (A1.13))},$$

where under gls

$$\Omega^* = \Lambda^{-1} - \Lambda^{-1}B(B'\Lambda^{-1}B)^+ B'\Lambda^{-1} = Q_{B,\Lambda}.$$

Under ols,

$$\Omega^* = I_k - B(B'B)^+ B' = Q_{B,J}.$$

Therefore, the expression for the C-matrix in (2.8) simplifies to

$$C = X'(I_b \otimes \Omega^*)X$$

for both ols and gls. Note that $Q_{B,\Lambda} = (Q_{B,J}\Lambda Q_{B,J})^+$.

A further simplification follows by taking $X' = (X_1', X_2', ..., X_b')$ where X_i is the $k \times t$ treatment design matrix for block i. This gives

$$C = \sum_{i=1}^{b} X_i' \Omega^* X_i, \tag{2.26}$$

and

$$\begin{aligned}
\mathrm{var}(\underline{q}) &= X'(I_b \otimes \Omega^*)(I_b \otimes \Lambda)(I_b \otimes \Omega^*)X\sigma^2 \\
&= X'(I_b \otimes \Omega^*\Lambda\Omega^*)X\sigma^2 \\
&= \sum_{i=1}^{b} X_i' \Omega^*\Lambda\Omega^* X_i\sigma^2.
\end{aligned} \tag{2.27}$$

2.7 The form of $X_i'WX_i$

Assuming that $Z = I_b \otimes B$ and $V = I_b \otimes \Lambda$, let W represent Ω^* under gls, and under ols, W can be replaced by either Ω^* or $\Omega^*\Lambda\Omega^*$. Let $(W)_{i,j} = w_{i,j}$. The rows and columns of W sum to zero, and the diagonal elements of W are positive. It is shown here that given $V = I_b \otimes \Lambda$, the elements of $X_i'WX_i$ can be written down easily.

Let $\Theta_{i,v}^{(1)}$ be the set of plots containing treatment v in block i, and if treatment v occurs more than once in block i, let $\Theta_{i,v}^{(2)}$ be the set of pairs of plots (l_1, l_2) that contain treatment v, such that $l_1 < l_2$. Also let $\Theta_{i,v_1,v_2}^{(3)}$ be the set of pairs

of plots (l_1, l_2) containing distinct treatments v_1 and v_2 in block i, such that $l_1 < l_2$. Then the vth diagonal element of $X_i'WX_i$ is

$$\left(X_i'WX_i\right)_{v,v} = \sum_{\Theta_{i,v}^{(1)}} w_{l,l} + 2\sum_{\Theta_{i,v}^{(2)}} w_{l_1,l_2} , \qquad (2.28)$$

and for $v_1 \ne v_2$, the $(v_1, v_2)^{\text{th}}$ element of $X_i'WX_i$ is

$$\left(X_i'WX_i\right)_{v_1,v_2} = \sum_{\Theta_{i,v_1,v_2}^{(3)}} w_{l_1,l_2} . \qquad (2.29)$$

It follows from (2.28) that

$$\operatorname{tr}(X_i'WX_i) = \operatorname{tr}(W) + 2\sum_{v=1}^{t}\sum_{\Theta_{i,v}^{(2)}} w_{l_1,l_2} , \qquad (2.30)$$

where $\sum_{\Theta_{i,v}^{(2)}} w_{l_1,l_2}$ is the sum of the off-diagonal elements of W corresponding to the pairs of plots in block i that contain treatment v. If block i is binary, $\Theta_{i,v}^{(2)} = \{\}$ for all v, so

$$\operatorname{tr}(X_i'WX_i) = \operatorname{tr}(W). \qquad (2.31)$$

As an example, consider a design with $p_1 = 2$, $p_2 = 3$ and $t = 5$. If the ith block is

2	3	2
1	5	3

,

then the elements of $\Theta_{i,v}^{(1)}$ and $\Theta_{i,v}^{(2)}$, for $v = 1, 2, ..., 5$ are

$\Theta_{i,1}^{(1)} = \{4\}$, $\Theta_{i,2}^{(1)} = \{1,3\}$, $\Theta_{i,3}^{(1)} = \{2,6\}$, $\Theta_{i,4}^{(1)} = \{\}$, $\Theta_{i,5}^{(1)} = \{5\}$, so

$\Theta_{i,1}^{(2)} = \Theta_{i,4}^{(2)} = \Theta_{i,5}^{(2)} = \{\}$, $\Theta_{i,2}^{(2)} = \{(1,3)\}$ and $\Theta_{i,3}^{(2)} = \{(2,6)\}$

and the elements of $\Theta_{i,v_1,v_2}^{(3)}$ are

$\Theta_{i,1,2}^{(3)} = \{(1,4),(3,4)\}$, $\Theta_{i,1,3}^{(3)} = \{(2,4),(4,6)\}$, $\Theta_{i,1,4}^{(3)} = \{\}$, $\Theta_{i,1,5}^{(3)} = \{(4,5)\}$,

$\Theta_{i,2,3}^{(3)} = \{(1,2),(1,6),(2,3),(3,6)\}$, $\Theta_{i,2,4}^{(3)} = \{\}$, $\Theta_{i,2,5}^{(3)} = \{(1,5),(3,5)\}$, $\Theta_{i,3,4}^{(3)} = \{\}$,

$\Theta_{i,3,5}^{(3)} = \{(2,5),(5,6)\}$, $\Theta_{i,4,5}^{(3)} = \{\}$.

Hence,

$$X_i'WX_i = \begin{pmatrix} w_{4,4} & \left(w_{1,4}+w_{3,4}\right) & \left(w_{2,4}+w_{4,6}\right) & 0 & w_{4,5} \\ \left(w_{1,4}+w_{3,4}\right) & \begin{pmatrix} w_{1,1}+w_{3,3} \\ +2w_{1,3} \end{pmatrix} & \begin{pmatrix} w_{1,2}+w_{1,6} \\ +w_{2,3}+w_{3,6} \end{pmatrix} & 0 & \left(w_{1,5}+w_{3,5}\right) \\ \left(w_{2,4}+w_{4,6}\right) & \begin{pmatrix} w_{1,2}+w_{1,6} \\ +w_{2,3}+w_{3,6} \end{pmatrix} & \begin{pmatrix} w_{2,2}+w_{6,6} \\ +2w_{2,6} \end{pmatrix} & 0 & \left(w_{2,5}+w_{5,6}\right) \\ 0 & 0 & 0 & 0 & 0 \\ w_{4,5} & \left(w_{1,5}+w_{3,5}\right) & \left(w_{2,5}+w_{5,6}\right) & 0 & w_{5,5} \end{pmatrix}$$

and

$$\mathrm{tr}(X_i'WX_i) = \mathrm{tr}(W) + 2(w_{1,3}+w_{2,6}).$$

3 Finding optimal and efficient designs

Under spatial dependence it is often difficult to obtain efficient or optimal designs. Martin (1996) lists several methods to find efficient designs under dependence:

i. *designs that are intuitively appealing can be constructed and their efficiency evaluated;*

ii. *designs can be sought for which the C-matrix is (close to being) completely symmetric, and their efficiency evaluated;*

iii. *optimality will usually depend on the model that is assumed for the dependence, and which estimator is used;*

iv. *optimality may depend not just on the model assumed, but on actual parameter values of Λ;*

v. *the structure of $\Omega^*\Lambda\Omega^*$ of (2.27) for ols estimation or Ω^* of (2.26) for gls estimation can be used to suggest what features lead to efficiency;*

vi. *if there are few competing designs, a complete enumeration and evaluation may be possible;*

vii. *well-structured searches, or other algorithmic methods, can be used.*

It can be seen that several of these techniques are used in the design problems considered in subsequent chapters. Some of these are discussed in more detail in this chapter.

3.1 Intuitively appealing designs

Designs which have a simple structure or form may be considered. For example, when the number of treatments is small, all $t!/(t-k)!$ arrangements of k of the t treatments may be used as the blocks of a design, with each arrangement allocated to the ordered plots 1 to k. As an illustration, for blocks of size 1×3 with $t=3$, the design with $b=3!=6$ is

$$\boxed{1\,2\,3}\,,\boxed{1\,3\,2}\,,\boxed{2\,1\,3}\,,\boxed{2\,3\,1}\,,\boxed{3\,1\,2}\,,\boxed{3\,2\,1}\,. \quad \text{D3.1}$$

3.1.1 Neighbour balance

More generally, designs which have some sort of *neighbour balance* may be
constructed. In the simplest sense, this means that the number of times
treatments are next to other treatments is the same. D3.1 clearly has
neighbour balance since each treatment occurs next to every other treatment
the same number of times. Exact neighbour balance is only possible for
particular combinations of t, b, p_1, p_2, and approximately balanced designs
may be used instead. Martin (1996) describes several types of neighbour
balance, some of which are summarised in sections 3.1.1.1 to 3.1.1.4.

3.1.1.1 Directional or non-directional neighbour balance

If the direction of the neighbours is important, say when left to right differs
from right to left and/or top to bottom differs from bottom to top, then
directional balance is needed. Note that D3.1 has directional balance since
each ordered pair of treatments occurs twice; for example, treatment 1 has
treatment 2 as a neighbour on the left twice and also on the right twice. Non-
directional neighbour balance is adequate when the direction is not important,
for example, when left to right is equivalent to right to left. As an example,
take the first three blocks of D3.1 to give the design:

$$\boxed{1}\boxed{2}\boxed{3}\ ,\ \boxed{1}\boxed{3}\boxed{2}\ ,\ \boxed{2}\boxed{1}\boxed{3}\ , \qquad\qquad \text{D3.2}$$

which has non-directional neighbour balance. Clearly a design with
directional neighbour balance also has non-directional neighbour balance.

3.1.1.2 Distinct pairs only or like pairs included

As well as considering balance with respect to distinct pairs of treatments, as
in D3.1 and D3.2, like pairs of treatments may also be included, with perhaps
each pair occurring equally often as the unlike pairs. Note that like treatments
which are neighbours are often called *self-adjacencies*.

3.1.1.3   Circular blocks

A one-dimensional block may be assumed to form an *annulus*, so that the last plot joins the first plot. For example, if the block

| 1 | 2 | 3 |

was a circular block then treatments 1 and 3 would be neighbours. If the blocks of D3.1 are circular then it is still neighbour balanced, with each ordered pair of treatments occurring 3 times as neighbours.

Recall from section 2.3.3.3 that the edges of a two-dimensional block may be joined to form a cylinder or a torus.

3.1.1.4   Higher level neighbours

As well as adjacent or first neighbours, higher level neighbours can also be considered. Plots are lag g_1 and lag g_2 neighbours, if they are g_1 plots apart in the horizontal direction and g_2 plots apart in the vertical direction, respectively. Assume that lag (g_1, g_2) is equivalent to lag $(-g_1, -g_2)$. As an illustration consider Figure 3.1, which shows the lag (g_1, g_2) neighbours of the plot marked X for a block of size 5×5. The adjacent neighbours have $(g_1, g_2) = (1, 0)$ or $(0, 1)$ and the diagonal neighbours have $(g_1, g_2) = (1, 1)$ or $(1, -1)$.

Figure 3.1
Lag (g_1, g_2) neighbours of the plot marked X for a block of size 5×5.

(2, 2)	(1, 2)	(0, 2)	(1,-2)	(2,-2)
(2, 1)	(1, 1)	(0, 1)	(1,-1)	(2,-1)
(2, 0)	(1, 0)	X	(1, 0)	(2, 0)
(2,-1)	(1,-1)	(0, 1)	(1, 1)	(2, 1)
(2,-2)	(1,-2)	(0, 2)	(1, 2)	(2, 2)

3.1.2 Positional balance

In addition to neighbour balance, designs with positional balance can also be considered. Positional balance means that each treatment occurs equally often in each plot position of a block. For example, D3.1 has both neighbour and positional balance since each treatment occurs in each plot position twice. However, D3.2 has neighbour balance but does not have positional balance, since, for example, treatment 1 occurs in plot 1 twice and in plot 2 once.

3.1.3 Semi-balanced arrays

Semi-balanced arrays (SBAs) of strength 2 were introduced by Rao (1961), where they were called orthogonal arrays of type II of strength 2. In this thesis they shall be called semi-balanced arrays, henceforth. A SBA of length k on t symbols is defined as a $k \times b$ array of t symbols, where, in every set of two rows the b columns contain each of the $\frac{1}{2}t(t-1)$ combinations of unordered pairs of symbols an equal number of times, c. That is, $b = \frac{1}{2}ct(t-1)$ for an integer c. For $k > 2$, if t is even then c must be even. Rao (1961) gives the minimum value of c, for a given t, as 1 ($b = \frac{1}{2}t(t-1)$) for t odd, and 2 ($b = t(t-1)$) for t even, and shows that a SBA can be constructed with the minimum value of c when a field with t elements, GF(t), exists. Constructions of SBAs have been given by Rao (1961) and Mukhopadhyay (1972). Figure 3.2 gives SBAs with the minimum value of c for $t = 3, 4$ and 5.

Figure 3.2
SBAs with the minimum value of c for a) $t = 3$,   b) $t = 4$,   c) $t = 5$.

1	2	3
2	3	1
3	1	2

$(c = 1)$

a)

1	1	1	2	2	2	3	3	3	4	4	4
2	3	4	1	3	4	1	2	4	1	2	3
3	4	2	4	1	3	2	4	1	3	1	2
4	2	3	3	4	1	4	1	2	2	3	1

$(c = 2)$

b)

1	1	2	2	3	3	4	4	5	5
2	4	3	5	1	4	2	5	1	3
3	2	4	3	4	5	5	1	2	1
4	5	5	1	2	1	3	2	3	4
5	3	1	4	5	2	1	3	4	2

$(c = 1)$

c)
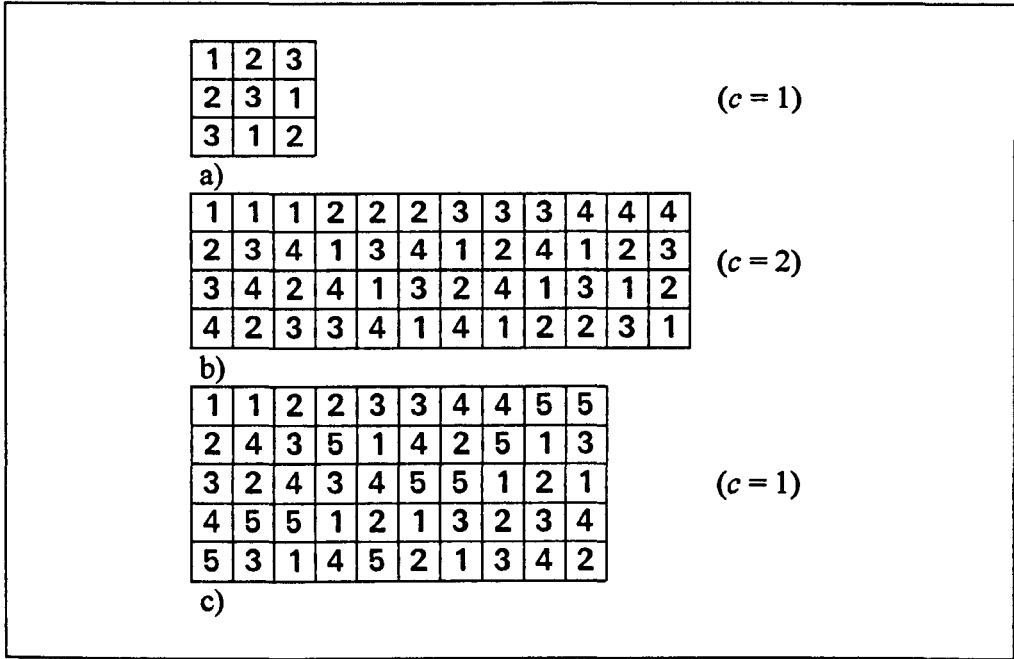
The columns of a SBA can be used to construct the blocks of a design which has neighbour balance at each level. For $k > 2$, the neighbour balance implies positional balance. For example, for blocks of size 1×3 with $t = 3$, the SBA in Figure 3.2a gives the design:

1	2	3

,

2	3	1

,

3	1	2

 .   D3.3

Also, note that the first 4 rows of the SBA in Figure 3.2c gives the design D2.1 in chapter 2, which has blocks of size 2×2 with $t = 5$. Designs constructed from SBAs in this way for $k > 2$ (i.e. when there is both neighbour and positional balance), have a completely symmetric C-matrix when $\Omega^{\bullet}$ is symmetric (Martin & Eccleston, 1991, also see section 5.2.4). Under ols, var $(\hat{\tau})$ is completely symmetric for a SBA when $\Omega^{\bullet} \Lambda \Omega^{\bullet}$ is symmetric (Martin & Eccleston, 1991).

For a one-dimensional array of plots, the SBA construction is also used in Jacroux *et al.* (1997) and Majumdar & Martin (2000) to find optimal designs under a polynomial trend and uncorrelated errors.

Many of the results on optimal designs considered in subsequent chapters assume that the designs are constructed from SBAs.

3.2 *C*-matrix close to complete symmetry

Some optimal designs, such as those constructed using SBAs, have a large number of blocks, which may be greater than resources allow for some situations. In this case, designs with a fewer number of blocks may be used, which may not have C and var $(\hat{\tau})$ completely symmetric. However, designs constructed so that C is close to complete symmetry may be possible, and if tr(C) is sufficiently large, such designs are likely to be very efficient.

3.3 Algorithmic methods

Given b, k and t there are a finite number of ways of allocating treatments to plots, and so it is theoretically possible to examine all competing designs and to choose the best design; this is *complete enumeration*. Unfortunately, as illustrated in the example below, for any non-trivial problem there are often too many designs for this approach to be feasible. Therefore, it is of interest to try to develop algorithms that are more *effective* than complete enumeration. Edmonds (1965) defined the concept of effectiveness in the following way:

> *An algorithm is considered to be effective if it can guarantee to solve any instance of the problem for which it was designed by performing a number of elementary computational steps and the number can be expressed as a polynomial function of the size of the problem.*

A problem is deemed to be NP (non-deterministic polynomial) if no effective algorithms are known for the problem. If an effective algorithm does not exist

- then, if the problem is small enough complete enumeration may be feasible;
- there may be algorithms which give optimal solutions for most cases in a reasonable time;
- *heuristic* procedures could be used; that is, procedures which do not guarantee to produce an optimal solution for every instance of the problem.

As an illustration of complete enumeration, assume that $t = k$ and only complete block designs are of interest. Also assume that the direction of the ordering of the plots is not relevant, so that, for example, the blocks

$\boxed{1\ 2\ 3}$ and $\boxed{3\ 2\ 1}$

are equivalent. Without loss of generality, it can be assumed that one of the b blocks has the same arrangement of treatments over all competing designs. For all other blocks, there are $\frac{1}{2}(k!)$ different permutations of treatments within a block. This means that an upper bound on the number of different designs is $\left\{\frac{1}{2}(k!)\right\}^{b-1}$. However, this does not take account of designs that are equivalent under block interchanges. For example, when $k = b = 3$, the design D3.3 is equivalent to the design

$\boxed{1\ 2\ 3}, \boxed{3\ 1\ 2}, \boxed{2\ 3\ 1}$,   D3.4

since blocks 2 and 3 are interchanged.

A tighter upper bound on the number of different designs, that takes block interchanges into account, is

$$\binom{\frac{1}{2}(k!)+b-2}{b-1}.$$

This is illustrated in Appendix A2.1 for $k = 3$ and $b = 3, 4, 5$.

As b and/or k increase this upper bound increases substantially. This is illustrated in Table 3.1, which gives the upper bound on the number of different designs in a complete enumeration, for $b = 3, 4, 5$ and $k = 3, 4, \ldots, 10$.

If it is assumed, perhaps unrealistically, that 1 million designs can be considered in 1 second, then for $b = 5$ and $k = 6$, the time taken will be about 12 minutes. For $b = 5$ and $k = 10$, the time taken will be over 14,000 million years! This example shows that a small problem could be feasibly solved by complete enumeration, but for larger problems, the time taken would clearly be prohibitive.

Table 3.1
Upper bound on the number of different designs in a complete enumeration for a complete block design with b blocks of size k.

k	$b = 3$	$b = 4$	$b = 5$
3	6	10	15
4	78	364	1,365
5	1,830	37,820	595,665
6	64,980	7,840,920	711,563,490
7	3,176,460	$\approx 2.67 \times 10^9$	$\approx 1.68 \times 10^{12}$
8	203,222,880	$\approx 1.37 \times 10^{12}$	$\approx 6.88 \times 10^{15}$
9	$\approx 1.65 \times 10^{10}$	$\approx 9.96 \times 10^{14}$	$\approx 4.52 \times 10^{19}$
10	$\approx 1.65 \times 10^{12}$	$\approx 9.96 \times 10^{17}$	$\approx 4.52 \times 10^{23}$

For design problems, heuristic techniques often involve defining *neighbours* of a feasible design. For example, the neighbourhood may consist of all designs which can be obtained by swapping treatments in or out of the current design.

Local optimisation is a method, where after selecting a starting design, a suitable neighbour, which gives an improvement, becomes the current design. This process is repeated until no neighbours of the current design yield an improvement. There are many ways of selecting a suitable neighbour. The neighbourhood may be sampled at random or in a fixed order and the first improvement selected or the whole neighbourhood may be scanned and the best improvement selected. Such searching techniques may yield locally optimal designs rather than the globally optimal design.

Simulated annealing (see Dowsland, 1995) attempts to overcome this problem by allowing some worse designs to be accepted as the current solution according to a probability function. This probability is determined by a parameter known as temperature, which usually decreases as the algorithm progresses. The lower the temperature the lower the probability of accepting a worse design. The temperature is reduced according to a cooling schedule, until some stopping criterion is satisfied.

Two other methods applicable to optimisation problems are tabu search and genetic algorithms. For the tabu search method (see Glover & Laguna, 1995) a fixed proportion of the neighbourhood is sampled at each iteration and the best design of those sampled is selected. The search is often controlled by 3 memory functions. Short term memory is managed in the form of a tabu list in which certain moves are not allowed in order to avoid returning to designs which have been considered recently. Medium term memory attempts to guide the search towards good designs by identifying common features of the best designs encountered so far, which can be difficult to do. Long term memory tries to spread the search over the set of feasible designs, either by identifying features which have occurred frequently to date and outlawing them or identifying features which have not appeared so far and forcing them

in to the design. Tabu status may be overridden if the optimality function for the tabu move is better than the best design found so far. Designing a tabu search algorithm to include all 3 features is a task that is very specific to the problem.

Genetic algorithms (see Reeves, 1995) work on populations, rather than on a sequential stream of designs. A method for producing an offspring design from two parents is defined and better designs are allowed to *breed* with higher probability than poorer ones. A new population is produced by a combination of exact copies, cross-over of 2 parents and mutation. The idea is that a survival of the fittest approach will eventually lead to a population of highly efficient designs.

4 Background material for NRC designs

In this chapter, additional background material, to that given in chapter 2, is provided for nested row-column (NRC) designs.

4.1 NRC design model

For a NRC design the plots are arranged in b blocks of size $p_1 \times p_2$, where p_1, $p_2 > 1$, and the plots are ordered lexicographically. For the NRC designs considered in this thesis, it is assumed, unless otherwise stated, that treatments are equally replicated.

Let the postulated model be

$$\underline{y} = X\underline{\tau} + Z_1\underline{\beta} + Z_2\underline{\gamma} + Z_3\underline{\delta} + \underline{\varepsilon} \tag{4.1}$$

where

$\underline{y}$, $\underline{\tau}$, X and $\underline{\varepsilon}$ are as defined for model (2.1);

$\underline{\beta}$ is a b-vector of fixed block effects;

$Z_1 = I_b \otimes 1_k$ is the $m \times b$ block design matrix. The $(l, i)^{\text{th}}$ element of Z_1 is equal to 1 when plot l is in block i, for $l = 1, \ldots, m$ and $i = 1, \ldots, b$, and 0 otherwise;

$\underline{\gamma}$ and $\underline{\delta}$ are bp_1- and bp_2- vectors of fixed row within-block effects and fixed column within-block effects, respectively;

$Z_2 = I_b \otimes I_{p_1} \otimes 1_{p_2}$ and $Z_3 = I_b \otimes 1_{p_1} \otimes I_{p_2}$ are the $m \times bp_1$ and $m \times bp_2$ row and column design matrices, respectively;

Model (4.1) can be re-parameterised as the model (2.1):

$$\underline{y} = X\underline{\tau} + Z\underline{\alpha} + \underline{\varepsilon},$$

by taking

$$\underline{\alpha}' = (\underline{\alpha}_1', \underline{\alpha}_2', \ldots, \underline{\alpha}_b'),$$

where

$$\underline{\alpha}_i' = (\beta_i, \gamma_{(i-1)p_1+1}, \gamma_{(i-1)p_1+2}, \ldots, \gamma_{ip_1}, \delta_{(i-1)p_2+1}, \delta_{(i-1)p_2+2}, \ldots, \delta_{ip_2})$$

is a $(1 + p_1 + p_2)$-vector of block, row and column effects for block i.

The matrix $Z = I_b \otimes B$, where

$$B = [\underline{1}_k \ (I_{p_1} \otimes \underline{1}_{p_2}) \ (\underline{1}_{p_1} \otimes I_{p_2})]$$

is the within-block design matrix.

For example, for a design with blocks of size 2×2, such as Example 2.1,

$$B = \begin{pmatrix} 1 & 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 0 & 1 \\ 1 & 0 & 1 & 1 & 0 \\ 1 & 0 & 1 & 0 & 1 \end{pmatrix}.$$

Recall that Z was also assumed to be of the form $Z = I_b \otimes B$ in sections 2.6 and 2.7, hence the results in these two sections are also valid here.

Model (4.1) can also be written as

$$y_{i,j_1,j_2} = \tau_{T(i,j_1,j_2)} + \beta_i + \gamma_{(i-1)p_1+j_1} + \delta_{(i-1)p_2+j_2} + \varepsilon_{i,j_1,j_2}, \tag{4.2}$$

where

$T(i, j_1, j_2)$ is the treatment applied to the plot in the j_1^{th} row and j_2^{th} column of block i, β_i is the ith block effect, $\gamma_{(i-1)p_1+j_1}$ is the j_1^{th} row effect for block i, $\delta_{(i-1)p_2+j_2}$ is the j_2^{th} column effect for block i.

4.2 Simplifications to B

Consider the case where row and/or column effects are not included, that is when the row and/or the column effect vectors in model (4.1) are zero vectors. This gives the four models in Table 4.1, which are labelled as models I, II, III and IV, as in Uddin & Morgan (1997a). Model I includes both row and column effects, and models II and III include only row and column effects, respectively. Model IV includes only block effects.

Table 4.1
Models I to IV

Model	Row effect	Column effect	Within-block design matrix, B	Rank(B)	Ω^* under ols
I	$\underline{\gamma} \neq \underline{0}_{bp_1}$	$\underline{\delta} \neq \underline{0}_{bp_2}$	$[(I_{p_1} \otimes \underline{1}_{p_2})(\underline{1}_{p_1} \otimes I_{p_2})]$	$p_1 + p_2 - 1$	$E_{p_1} \otimes E_{p_2}$
II	$\underline{\gamma} \neq \underline{0}_{bp_1}$	$\underline{\delta} = \underline{0}_{bp_2}$	$I_{p_1} \otimes \underline{1}_{p_2}$	p_1	$I_{p_1} \otimes E_{p_2}$
III	$\underline{\gamma} = \underline{0}_{bp_1}$	$\underline{\delta} \neq \underline{0}_{bp_2}$	$\underline{1}_{p_1} \otimes I_{p_2}$	p_2	$E_{p_1} \otimes I_{p_2}$
IV	$\underline{\gamma} = \underline{0}_{bp_1}$	$\underline{\delta} = \underline{0}_{bp_2}$	$\underline{1}_k$	1	E_k

If row and/or column effects are included in model (4.1) (models I, II and III) then $\underline{\beta} = \underline{0}_b$ can be assumed without affecting the estimated treatment contrasts since the rank of B is the same whether B includes the column vector $\underline{1}_k$ or not. In terms of model (4.2) this means that the block effect β_i is incorporated into the row and/or column effects; that is, model (4.2) may be re-written as

$$y_{i,j_1,j_2} = \tau_{T(i,j_1,j_2)} + \gamma^*_{(i-1)p_1+j_1} + \delta_{(i-1)p_2+j_2} + \varepsilon_{i,j_1,j_2},$$

say, where

$$\gamma^*_{(i-1)p_1+j_1} = \beta_i + \gamma_{(i-1)p_1+j_1}.$$

Therefore, in terms of model (2.1), the simplified within-block design matrices, given in Table 4.1 can be used for the four models, I to IV.

4.3 Ω^* for models I to IV

Under ols, simple forms for $\Omega^* = I_k - B(B'B)^+ B'$ (see section 2.6) can be derived using the simplified B matrices given in Table 4.1. For model I,

$$B'B = \begin{pmatrix} p_2 I_{p_1} & 1_{p_1} \otimes 1_{p_2}' \\ 1_{p_1}' \otimes 1_{p_2} & p_1 I_{p_2} \end{pmatrix}$$

and a generalised inverse of $B'B$ is

$$(B'B)^- = \begin{pmatrix} p_2^{-1} E_{p_1} & 0 \\ 0 & p_1^{-1} I_{p_2} \end{pmatrix}.$$

Then

$$B(B'B)^- B' = \left(\frac{1}{p_1} J_{p_1} \otimes I_{p_2} \right) + \left(I_{p_1} \otimes \frac{1}{p_2} J_{p_2} \right) - \left(\frac{1}{p_1} J_{p_1} \otimes \frac{1}{p_2} J_{p_2} \right).$$

Since $B(B'B)^+ B' = B(B'B)^- B'$, it follows that

$$\Omega^* = E_{p_1} \otimes E_{p_2}.$$

For model II,

$$B(B'B)^+ B' = B(B'B)^{-1} B' = I_{p_1} \otimes p_2^{-1} J_{p_2},$$

so $\Omega^* = I_{p_1} \otimes E_{p_2}$. Similarly for model III, $\Omega^* = E_{p_1} \otimes I_{p_2}$, and $\Omega^* = E_k$ for model IV. Therefore, under ols, for all four models I to IV, Ω^* is centro-symmetric (by (A1.21) and (A1.16) in Appendix A1.4).

Now consider gls for Λ centro-symmetric. For models I to IV, if Λ is centro-symmetric then $\Omega^* = \Lambda^{-1} - \Lambda^{-1} B(B'\Lambda^{-1}B)^+ B'\Lambda^{-1}$ (see section 2.6) is also centro-symmetric. This is now shown for model I.

It is first shown that

$$BH^{\bullet}_{p_1+p_2} = H_k B,$$

where H_n is a matrix with ones on the NE-SW diagonal and zeros elsewhere, as defined in Appendix A1.4 and $H^{\bullet}_{p_1+p_2} = \begin{pmatrix} H_{p_1} & 0 \\ 0 & H_{p_2} \end{pmatrix}$. First consider

$$BH^{\bullet}_{p_1+p_2} = [(I_{p_1} \otimes \underline{1}_{p_2})\ (\underline{1}_{p_1} \otimes I_{p_2})]\begin{pmatrix} H_{p_1} & 0 \\ 0 & H_{p_2} \end{pmatrix}$$

$$= [(H_{p_1} \otimes \underline{1}_{p_2})\ (\underline{1}_{p_1} \otimes H_{p_2})],$$

and since $H_{p_1 p_2} = H_{p_1} \otimes H_{p_2}$,

$$H_k B = \left(H_{p_1} \otimes H_{p_2}\right)[(I_{p_1} \otimes \underline{1}_{p_2})\ (\underline{1}_{p_1} \otimes I_{p_2})]$$

$$= [(H_{p_1} \otimes H_{p_2}\underline{1}_{p_2})\ (H_{p_1}\underline{1}_{p_1} \otimes H_{p_2})]$$

$$= BH^{\bullet}_{p_1+p_2},$$

since $H_n \underline{1}_n = \underline{1}_n$. ∎

Since Λ^{-1} is centro-symmetric (by (A1.18) in Appendix A1.4),

$$B'\Lambda^{-1}B = B'H_k\Lambda^{-1}H_k B$$

$$= H^{\bullet}_{p_1+p_2}B'\Lambda^{-1}BH^{\bullet}_{p_1+p_2}.$$

Since $H^{\bullet}_{p_1+p_2}H^{\bullet}_{p_1+p_2} = I_{p_1+p_2}$ it follows that

$$(B'\Lambda^{-1}B)^{+} = H^{\bullet}_{p_1+p_2}(B'\Lambda^{-1}B)^{+}H^{\bullet}_{p_1+p_2}.$$

Finally consider

$$B(B'\Lambda^{-1}B)^{+}B' = BH^{\bullet}_{p_1+p_2}(B'\Lambda^{-1}B)^{+}H^{\bullet}_{p_1+p_2}B'$$

$$= H_k B(B'\Lambda^{-1}B)^{+}B'H_k,$$

showing the centro-symmetry of $B(B'\Lambda^{-1}B)^{+}B'$. By (A1.19) and (A1.20) in Appendix A1.4, it follows that $\Omega^{\bullet}$ is centro-symmetric. Similarly $\Omega^{\bullet}$ can be shown to be centro-symmetric for models II to IV.

5   Some recent results on nested row-column designs

A review of some recent work on optimal and efficient NRC designs is given in this chapter. Section 5.1 provides a brief summary of results on NRC designs when errors are assumed to be uncorrelated. Correlated errors are assumed in sections 5.2 and 5.3, where a detailed review of results on one-dimensional block designs and NRC designs, respectively, are given.

Recall that the NRC design models I to IV were shown in chapter 4 to be equivalent to the block design model (2.1).

5.1   Nested row-column designs for uncorrelated errors

Section 5.1 considers some work on balanced, efficient and optimal NRC designs when errors are assumed to be uncorrelated. That is, for model (4.1):

$\underline{y} = X\underline{\tau} + Z_1\underline{\beta} + Z_2\underline{\gamma} + Z_3\underline{\delta} + \underline{\varepsilon}$, with $\text{var}(\underline{\varepsilon}) = I_m\sigma^2$. Note that a brief review

of NRC designs for uncorrelated observations is given in section 5.9 of John & Williams (1995), and a more detailed review is given in Morgan (1996). In the papers discussed in section 5.1, the block, row and column effects: $\underline{\beta}$, $\underline{\gamma}$ and $\underline{\delta}$, respectively, are either all fixed effects or all random effects. In section 5.1 the corresponding models will be referred to as *fixed* and *mixed effect models*, respectively. For the mixed effect model:

$$E(\underline{\beta}) = \underline{0}_b, \quad \text{var}(\underline{\beta}) = I_b\sigma_\beta^2;$$

$$E(\underline{\gamma}) = \underline{0}_{bp_1}, \quad \text{var}(\underline{\gamma}) = I_{bp_1}\sigma_\gamma^2;$$

$$E(\underline{\delta}) = \underline{0}_{bp_2}, \quad \text{var}(\underline{\delta}) = I_{bp_2}\sigma_\delta^2;$$

and $\underline{\varepsilon}$, $\underline{\beta}$, $\underline{\gamma}$ and $\underline{\delta}$ are mutually uncorrelated.

In what follows, the fixed effect model is assumed, unless otherwise stated.

5.1.1 Singh & Dey (1979)

Singh & Dey (1979) gave a procedure for the analysis of NRC designs. They defined a design with $k < t$ to be a *balanced incomplete block row-column* (BIBRC) design if

(i) every treatment occurs at most once in a block (i.e. blocks are binary), and

(ii) for any pair of distinct treatments (v_1, v_2),

$$(p_1 - 1)\omega_{r(v_1,v_2)} + (p_2 - 1)\omega_{c(v_1,v_2)} - \omega_{e(v_1,v_2)} = \omega,$$

where $\omega_{r(v_1,v_2)}$, $\omega_{c(v_1,v_2)}$ and $\omega_{e(v_1,v_2)}$ denote the number of blocks in which v_1 and v_2 occur together in the same row, column and elsewhere, respectively, and ω is an integer independent of the pair of treatments chosen.

This means that for a binary design, if each pair of treatments occur together equally often within rows, equally often within columns and equally often elsewhere within blocks, the design is a BIBRC design. In these designs every treatment occurs in exactly

$$r = \frac{\omega(t-1)}{(p_1 - 1)(p_2 - 1)}$$

blocks. Clearly $rt = bp_1 p_2$, therefore, for certain ω, these designs exist for

$$b = \frac{\omega\, t(t-1)}{p_1 p_2 (p_1 - 1)(p_2 - 1)}.$$

Let $\mathcal{D}^*$ be the set of binary designs in $\mathcal{D}$ (see Definition 2.2 in section 2.5.1). For designs in $\mathcal{D}^*$, by the equation in (2.31),

$$\mathrm{tr}(C) = b\,\mathrm{tr}(\Omega^*),$$

which is constant over designs in $\mathcal{D}^*$. Condition (ii) means that the C-matrix is completely symmetric. This gives the following theorem.

Theorem 5.1 (Singh & Dey, 1979)
For a fixed effect model with uncorrelated errors, BIBRC designs are universally optimal over all designs in $\mathcal{D}^*$.   ∎

Some methods of construction of BIBRC designs were given and several designs for blocks of size 2×2 were presented. These designs had $\omega = 1,2,3$ (i.e. $b = \frac{1}{4}t(t-1)$, $\frac{1}{2}t(t-1)$, $\frac{3}{4}t(t-1)$, respectively). An example of a cyclic BIBRC design with $t = 13$ and $2t = 26$ blocks of size 2×3 was also given.

5.1.2   Ipinyomi & John (1985)

Ipinyomi & John (1985) considered a class of NRC binary designs based on a cyclical method of construction. Unlike the designs in Singh & Dey (1979), these designs exist for many parameter combinations (t, b, p_1, p_2) and require a relatively small number of blocks. Let $\mathcal{D}^*$ be the set of cyclic NRC binary designs given by the development of a single initial block. The best designs in $\mathcal{D}^*$, with respect to the A-optimality criterion, were tabulated for $5 \leq t \leq 15$, $p_1 \leq 3$ and $p_2 \leq 7$. For blocks of size 2×2, cyclic designs with $b = t$ were presented, and for blocks of size 2×3, cyclic designs with t and $\frac{1}{2}t$ blocks were given.

5.1.3   Bagchi *et al.* (1990)

Bagchi *et al.* (1990) considered the optimality of NRC designs, and gave the following theorem.

Theorem 5.2   (Bagchi *et al.*, 1990)
For the fixed effect model when observations are uncorrelated, a design is universally optimal within the set of connected designs $\mathcal{D}$ if

i)   the number of times that treatment v appears in row j_1 of a block i is the same for each $j_1 = 1, \ldots, p_1$, and

ii)   the columns form a *balanced block design*.   ∎

A balanced block design is a binary equireplicate design with each pair of treatments occurring equally often in a block (see Appendix A1.7). Designs satisfying conditions (i) and (ii) are called balanced nested row-column (BNRC) designs. A BNRC design has, by condition (i), non-binary blocks.

An example for blocks of size 2×2 with $t = 4$ and $b = 6$ was given. The following two variance balanced designs with $b = \frac{1}{2}t(t-1)$ were considered.

$$
\begin{array}{|c|c|}\hline 1 & 2 \\ \hline 2 & 1 \\ \hline\end{array},\;
\begin{array}{|c|c|}\hline 1 & 3 \\ \hline 3 & 1 \\ \hline\end{array},\;
\begin{array}{|c|c|}\hline 1 & 4 \\ \hline 4 & 1 \\ \hline\end{array},\;
\begin{array}{|c|c|}\hline 2 & 3 \\ \hline 3 & 2 \\ \hline\end{array},\;
\begin{array}{|c|c|}\hline 2 & 4 \\ \hline 4 & 2 \\ \hline\end{array},\;
\begin{array}{|c|c|}\hline 3 & 4 \\ \hline 4 & 3 \\ \hline\end{array}
\qquad \text{D5.1}
$$

$$
\begin{array}{|c|c|}\hline 1 & 3 \\ \hline 4 & 2 \\ \hline\end{array},\;
\begin{array}{|c|c|}\hline 1 & 4 \\ \hline 2 & 3 \\ \hline\end{array},\;
\begin{array}{|c|c|}\hline 1 & 2 \\ \hline 3 & 4 \\ \hline\end{array},\;
\begin{array}{|c|c|}\hline 1 & 3 \\ \hline 4 & 2 \\ \hline\end{array},\;
\begin{array}{|c|c|}\hline 1 & 4 \\ \hline 2 & 3 \\ \hline\end{array},\;
\begin{array}{|c|c|}\hline 1 & 2 \\ \hline 3 & 4 \\ \hline\end{array}.
\qquad \text{D5.2}
$$

Since both these designs are variance balanced, the C-matrix is completely symmetric, that is $C = aE_4$. This means that the design with the larger a, is universally better (see section 2.5.4). The non-binary design D5.1 with $a = 4$, is universally better than the binary design D5.2 with $a = 2$. Design D5.1 is a BNRC design and is therefore universally optimal in the entire class of competing designs.

For the mixed effect model after recovering and combining information from the different strata, Theorem 5.3 below shows that optimality results are very sensitive to the relationship between the variance components, σ^2, σ_β^2, σ_γ^2 and σ_δ^2. Let

$$x_1 = (\sigma^2)^{-1}, \qquad\qquad x_2 = (\sigma^2 + p_2\sigma_\gamma^2)^{-1},$$

$$x_3 = (\sigma^2 + p_1\sigma_\delta^2)^{-1}, \quad x_4 = (\sigma^2 + p_2\sigma_\gamma^2 + p_1\sigma_\delta^2 + p_1 p_2\sigma_\beta^2)^{-1}$$

and $\quad x = x_1 - x_2 - x_3 + x_4.$

Theorem 5.3   (Bagchi *et al.*, 1990)

Under the mixed effect model when errors are uncorrelated, after recovering information from the different strata, if $x < 0$, then a BIBRC design, if it exists, is universally optimal within $\mathcal{D}$. If $x > 0$ then a BNRC design whose rows form a balanced block design is universally optimal within $\mathcal{D}$.   ∎

5.1.4   Leeming (1997)

Leeming (1997) considered blocks of size 2×2, where for each block there are two replications of a control treatment (labelled 0) which occur once per row and once per column, and the remaining plots are allocated the test treatments. Two designs were compared under the assumption that the test treatment versus control treatment comparisons are of interest. Design D5.3 has blocks of the form

$$\begin{array}{|c|c|} \hline a & 0 \\ \hline 0 & b \\ \hline \end{array} \,, \qquad\qquad\qquad\qquad \text{D5.3}$$

for each pair of distinct test treatments (a, b), repeated c times, where $c = 1$ for t odd and $c = 2$ for t even. Design D5.4 has blocks of the form

$$\begin{array}{|c|c|} \hline a & 0 \\ \hline 0 & a \\ \hline \end{array} \,, \qquad\qquad\qquad\qquad \text{D5.4}$$

for each test treatment a, repeated $\tfrac{1}{2}c(t-1)$ times. Hence, both designs have $b = \tfrac{1}{2}ct(t-1)$ blocks. For example, when $t = 4$, D5.3 has the blocks

$$\begin{array}{|c|c|} \hline 1 & 0 \\ \hline 0 & 2 \\ \hline \end{array} ,\; \begin{array}{|c|c|} \hline 1 & 0 \\ \hline 0 & 3 \\ \hline \end{array} ,\; \begin{array}{|c|c|} \hline 1 & 0 \\ \hline 0 & 4 \\ \hline \end{array} ,\; \begin{array}{|c|c|} \hline 2 & 0 \\ \hline 0 & 3 \\ \hline \end{array} ,\; \begin{array}{|c|c|} \hline 2 & 0 \\ \hline 0 & 4 \\ \hline \end{array} ,\; \begin{array}{|c|c|} \hline 3 & 0 \\ \hline 0 & 4 \\ \hline \end{array}$$

repeated twice, and D5.4 has the blocks

$$\begin{array}{|c|c|} \hline 1 & 0 \\ \hline 0 & 1 \\ \hline \end{array} ,\; \begin{array}{|c|c|} \hline 2 & 0 \\ \hline 0 & 2 \\ \hline \end{array} ,\; \begin{array}{|c|c|} \hline 3 & 0 \\ \hline 0 & 3 \\ \hline \end{array} ,\; \begin{array}{|c|c|} \hline 4 & 0 \\ \hline 0 & 4 \\ \hline \end{array}$$

repeated 3 times.

For the fixed effect analysis, it was shown that design D5.4, which has non-binary diagonals, is universally better than D5.3. When plot, row and column information are recovered and combined, the design which is universally better depends on the variance components.

As an example, Leeming (1997) considered a simplified version of a 2×2 NRC design from Kachlicka & Mejza (1995), which had 3 sub-plots for each whole plot. The design of Kachlicka & Mejza (1995) was for an experiment to observe potato crop yields under the influence of 3 levels of irrigation on the whole plots, and 3 levels of nitrogen on the sub-plots. The control treatment was the absence of irrigation. Leeming (1997) considered a similar experiment when potato yield was observed only under the influence of the 3 levels of irrigation.

5.2 One-dimensional designs for correlated errors

There has been much interest recently in the design of efficient experiments when plots are arranged in one-dimension under the assumption that errors are correlated. Discussed in section 5.2 are: Kiefer & Wynn (1981), Kunert (1987a), Cheng (1988), Martin & Eccleston (1991) and Martin (1998). These papers provide much of the foundation of the results on optimal NRC designs given in subsequent chapters of this thesis. Some others that have considered one-dimensional block designs under dependence are: Cheng (1983), Gill & Shukla (1985a), Kunert (1987b), Morgan & Chakravarti (1988) and Russell & Eccleston (1987a, 1987b).

Model IV is assumed throughout section 5.2. Kiefer & Wynn (1981) gave optimality conditions for the NN1 process under ols. For the AR(1) process under gls, optimality conditions were derived by Kunert (1987a). The optimality conditions from both Kiefer & Wynn (1981) and Kunert (1987a) are satisfied by SBAs. Cheng (1988) showed that SBAs are universally optimal over binary designs for any within-block covariance matrix Λ under gls, and also showed when non-binary designs are optimal for the NN1 process when $k = 3$ and 4. Martin & Eccleston (1991) gave a condition for the universal optimality of a SBA over all designs for any symmetric Λ, and also considered the optimality of non-binary blocks when $k = 3$ and 4. Martin

(1998) gave optimality results for $k = 3$ to 6, and also some results for general block sizes, over a range of dependence structures.

5.2.1 Kiefer & Wynn (1981)

Kiefer & Wynn (1981) considered optimal one-dimensional block designs for the NN1 process under ols. For blocks in which treatments v_1 and v_2 occur, let $n^*_{v_1,v_2}$ be the number of blocks in which v_1 and v_2 are lag 1 neighbours, and let $e^*_{v_1,v_2}$ be the number of blocks in which treatment v_1 occurs at an end plot plus the number of blocks in which treatment v_2 occurs at an end plot. Note that if both treatments occur at the end plots of a block, then the contribution of that block to $e^*_{v_1,v_2}$ is 2. Kiefer & Wynn (1981) gave the following theorem.

Theorem 5.4   (Kiefer & Wynn, 1981)
For the NN1 process, under ols, if a design

i)   is a balanced block design (see Appendix A1.7),   and

ii)   has $e^*_{v_1,v_2} + kn^*_{v_1,v_2}$ equal for all distinct pairs of treatments (v_1, v_2),

then the design is weakly universally optimal over all balanced block designs in $\mathcal{D}$. Note that such designs will only exist for certain b.   ■

For $t = 7$, $k = 4$ and $b = \frac{1}{2}t(t-1) = 14$, they gave an example of a weakly universally optimal design:

| 1 | 2 | 5 | 3 | , | 2 | 3 | 6 | 4 | , | 3 | 4 | 7 | 5 | , | 4 | 5 | 1 | 6 | ,

| 5 | 6 | 2 | 7 | , | 6 | 7 | 3 | 1 | , | 7 | 1 | 4 | 2 | ,

| 5 | 1 | 3 | 2 | , | 6 | 2 | 4 | 3 | , | 7 | 3 | 5 | 4 | , | 1 | 4 | 6 | 5 | ,

| 2 | 5 | 7 | 6 | , | 3 | 6 | 1 | 7 | , | 4 | 7 | 2 | 1 | ,   D5.5

which is a cyclic design developed from the initial blocks

| 1 | 2 | 5 | 3 | and | 5 | 1 | 3 | 2 | .

This design has $e^*_{v_1,v_2} = 8$ and $n^*_{v_1,v_2} = 2 \ \forall \ v_1 \neq v_2$. Note that designs D3.1 and D3.2 (in sections 3.1 and 3.1.1.1, respectively) are also weakly universally optimal with $e^*_{v_1,v_2} = 8$ and 4, and $n^*_{v_1,v_2} = 4$ and 2, respectively, $\forall \ v_1 \neq v_2$.

SBAs satisfy conditions (i) and (ii) of Theorem 5.4; in fact the properties of a SBA are more than what is needed. However, a design constructed from a SBA would have at least $b = \frac{1}{2}t(t-1)$.

5.2.2 Kunert (1987a)

Kunert (1987a) gave the following results for block designs under the AR(1) process and gls.

Lemma 5.5 (Kunert, 1987a)
For the AR(1) process under gls, $\text{tr}(C)$ is maximised for a binary design for all possible ρ_1 when $k = 3$, and for $\rho_1 \geq \rho^*_1(k)$ when $k \geq 4$, where

$$\rho^*_1(k) = \frac{\left\{k - 2 - \sqrt{(k^2 - 8)}\right\}}{(2k - 6)} < 0. \qquad \blacksquare$$

Note that $\rho_1 \geq \rho^*_1(k) \Leftrightarrow w_{1,2} < 0$, where $(\Omega^*)_{i,j} = w_{i,j}$.

Lemma 5.6 (Kunert, 1987a)
For the AR(1) process under gls, a binary design has a completely symmetric C-matrix if

i)   The design is a balanced block design,

ii) The design is lag 1 neighbour balanced,

and for all pairs of distinct treatments (v_1, v_2):

iii) $\sum_{i=1}^{b} \left(n_{v_1,i} e_{v_2,i} + n_{v_2,i} e_{v_1,i} \right)$ is constant, and

iv) $\sum_{i=1}^{b} e_{v_1,i} e_{v_2,i}$ is constant,

where $n_{v,i}$ is the number of times treatment v occurs in block i, and $e_{v,i}$ is the number of times treatment v occurs at an end plot in block i. ∎

This gives the following theorem.

Theorem 5.7   (Kunert, 1987a)
For the AR(1) process under gls, a design d^* satisfying (i) to (iv) of Lemma 5.6 is universally optimal over $\mathcal{D}$ for $\rho_1 \geq \rho_1^*(k)$. ∎

Note that d^* has $b = \frac{1}{2} ct(t-1)$ blocks for an integer c. As in Theorem 5.4 (Kiefer & Wynn, 1981), the properties of a SBA are more than what is needed for optimality.

5.2.3   Cheng (1988)

Cheng (1988) showed that, for any within-block covariance matrix Λ, the SBA gives a completely symmetric C-matrix. This is because for a SBA every pair of distinct treatments (v_1, v_2) occurs in every pair of distinct plots (l_1, l_2) an equal number of times, x_1, say. Hence, by the equation in (2.29),

$$\{X'(I_b \otimes W)X\}_{v_1,v_2} = x_1 \sum_{l_1 < l_2}\sum w_{l_1 l_2}$$

$$= \frac{x_1}{2}\{1_k' W 1_k - \text{tr}(W)\} \quad \forall \ v_1 \neq v_2.$$

Also, since for a SBA with $k > 2$, each treatment v occurs in each plot, x_2 times, say, by the equation in (2.28),

$$\{X'(I_b \otimes W)X\}_{v,v} = x_2 \sum_{l=1}^{k} w_{l,l}$$

$$= x_2 \text{tr}(W) \quad \forall \ v.$$

Therefore $C = X'(I_b \otimes \Omega^*)X$ is completely symmetric.

As in section 5.1.1, by the equation in (2.31), it clear that for a binary design,

$$\text{tr}\{X'(I_b \otimes W)X\} = b\,\text{tr}(W),$$

which is constant for all binary designs. This gives the following theorem.

Theorem 5.8   (Cheng, 1988)
A SBA is universally optimal over all binary designs in $\mathcal{D}$ for any within block covariance matrix Λ.   ∎

The NN1 process was considered in some detail for $k = 3$ and 4. Assuming that each block is of the same *type*, that is each block has the same structure of treatments on the ordered plots 1 to k, Cheng (1988) lists the different types of blocks, each contributing a different possible value to $\text{tr}\{X'(I_b \otimes W)X\}$. Four types are listed for $k = 3$:

$$[\text{aaa}], [\text{aab}], [\text{aba}] \text{ and } [\text{abc}], \tag{5.1}$$

where a, b and c are distinct labels. Note that reversing the order of the labels gives an equivalent type in terms of its contribution to $\text{tr}\{X'(I_b \otimes W)X\}$ since for the NN1 process, W is centro-symmetric (see Appendix A1.4). Hence the type [aab] is equivalent to the type [baa].

Consider a design with all its blocks of the same type. Then for any pair of blocks (i_1, i_2)

$$X_{i_1} = X_{i_2} P_{i_1 i_2}, \tag{5.2}$$

where, $P_{i_1 i_2} = P_{i_2 i_1}$ is a symmetric permutation matrix such that $P_{i_1 i_2} P_{i_1 i_2} = I_t$.

For example, consider the following non-binary unequally replicated design with $k = 3$, $b = 2$, $t = 5$ and blocks of type [aba]:

| 1 | 2 | 1 | , | 3 | 5 | 3 | .   D5.6

For this design,

$$X_1 = X_2 P_{1,2} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \end{pmatrix}, \quad X_2 = X_1 P_{1,2} = \begin{pmatrix} 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 \end{pmatrix},$$

where

$$P_{1,2} = \begin{pmatrix} 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 \end{pmatrix}.$$

Hence, by the equation in (5.2)

$$
\begin{aligned}
\mathrm{tr}(X_{i_1}'WX_{i_1}) &= \mathrm{tr}(P_{i_1,i_2} X_{i_2}'WX_{i_2} P_{i_1,i_2}) \\
&= \mathrm{tr}(X_{i_2}'WX_{i_2} P_{i_1,i_2} P_{i_1,i_2}) \\
&= \mathrm{tr}(X_{i_2}'WX_{i_2}) \\
&= c_W \quad \forall\ (i_1, i_2).
\end{aligned}
$$

That is, $\mathrm{tr}(X_i'WX_i)$ is the same for all the blocks. Therefore,

$$\mathrm{tr}\{X'(I_b \otimes W)X\} = bc_W. \tag{5.3}$$

Under gls, c_{Ω^*} was calculated for each of the 4 types, and so the type with maximum c_{Ω^*} gives the design with maximum $\mathrm{tr}(C)$. In this way, it was shown that for the NN1 process, the binary type [abc] has maximum c_{Ω^*} when $\rho_1 \leq \tfrac{1}{2}$, and the non-binary type [aba] has maximum c_{Ω^*} when $\rho_1 \geq \tfrac{1}{2}$. For a SBA, blocks are binary, so the SBA is universally optimal over all designs in $\mathcal{D}$ when $\rho_1 \leq \tfrac{1}{2}$. When $\rho_1 \geq \tfrac{1}{2}$, a design with blocks of type [aba] has completely symmetric C-matrix when the design is lag 1 neighbour balanced, so then the design is universally optimal over designs in $\mathcal{D}$. Lag 1 neighbour balance for a design with blocks of type [aba] means that a design with b equal to the number of pairs of distinct treatments, $\tfrac{1}{2}t(t-1)$,

is possible (including when t is even). Note that the design does not need to be equi-replicated.

Under ols, not all neighbour balanced designs have var($\hat{\underline{\tau}}$) = $D^+\sigma^2$
completely symmetric, so Cheng (1988) compared SBAs to designs with

> blocks of type [aba] such that treatments appear equally often
> at end plots,   D5.7

since these designs have D^+ completely symmetric. By considering tr$\{D^+\}$
for these two variance balanced designs. It was shown that the SBA is
universally better than D5.7 when $\rho_1 \leq \frac{1}{3}$, and D5.7 is universally better than
the SBA when $\rho_1 \geq \frac{1}{3}$.

For $k = 4$, 10 different types were listed by Cheng (1988):

> [aaaa], [aaab], [aaba], [aabb], [abab],
> [abba], [aabc], [abac], [abca], [abcd].   (5.4)

However, for a centro-symmetric W, there is an extra type which has been
noted by the author: [baac] (see the Acknowledgements in Martin, 1998).
Under gls for the NN1 process, there are 3 different types of universally
optimal design depending on the value of ρ_1, with the SBA being optimal
when $-\frac{1}{2} \leq \rho_1 \leq \frac{1}{4}$. Under ols, the SBA is the best of these three designs when
$-2/5 \leq \rho_1 \leq 2/7$. Note that for all the designs considered in Cheng (1988),
when $|\rho_1|$ is not too large, the SBA is universally optimal under gls, and is the
universally better design in comparisons between designs in $\mathcal{D}_1$ (see section
2.5.4) under ols.

5.2.4   Martin & Eccleston (1991)

Assuming that $b = \frac{1}{2}ct(t\text{-}1)$, for an integer c, Martin & Eccleston (1991) define
a binary block design to be <u>S</u>trongly <u>D</u>irectionally <u>E</u>qui<u>N</u>eighboured (SDEN)
if $X'(I_b \otimes W)X$ is completely symmetric for all symmetric W. For $k > 2$, a

SDEN design is a SBA (see section 3.1.3). When $k = 2$, Ω^* is a scalar multiple of E_2, so that $X'(I_b \otimes \Omega^*)X$ is completely symmetric when each treatment pair forms blocks. Also for $k = 2$, gls and ols are equivalent. Recall from section 3.1.3 that for a SBA with $k > 2$, if t is even then c must be even.

A binary block design is defined to be Strongly EquiNeighboured (SEN) if $X'(I_b \otimes W)X$ is completely symmetric for all symmetric and centro-symmetric W. Centro-symmetry essentially means that

(i) plots l and $k + 1 - l$ are equivalent, and

(ii) the pairs of plots (l_1, l_2) and $(k + 1 - l_1, k + 1 - l_2)$ are equivalent.

A SEN design

(i') has positional balance under (i), and

(ii') each unordered pair of distinct treatments occur equally often within the same block in each unordered pair of distinct plot positions, under (ii).

Clearly a SDEN design is a SEN design. However, for a SEN design if t is even and k is even then c can be odd. For example, when $t = k = 4$ a SEN design with $b = \frac{1}{2}t(t-1) = 6$ is given in Figure 5.1. This consists of half of the columns of the SBA in Figure3.2b.

Figure 5.1
A SEN design for $t = k = 4$ (columns are blocks) with the minimum value of c.

1	1	1	2	3	4
2	3	4	1	1	1
3	4	2	4	2	3
4	2	3	3	4	2

$(c = 1)$

Only those b for which SDENs or SENs exist are considered. If all blocks are of the same type (see section 5.2.3) then the equation in (5.3) is true, and c_W is given by the equation in (2.30). Also, if $X'(I_b \otimes W)X$ is completely

symmetric then $X'(I_b \otimes W)X = aE_t$, and so $\mathrm{tr}\{X'(I_b \otimes W)X\} = a(t-1)$. This gives $a = bc_W/(t-1)$, hence

$$X'(I_b \otimes W)X = \frac{bc_W}{(t-1)}E_t.$$

Recall that W can be replaced by Ω^* or $\Omega^*\Lambda\Omega^*$. (see section 2.7). Therefore $X'(I_b \otimes W)X$ completely symmetric means that C and $\mathrm{var}(\underline{q})$ are completely symmetric. Also, recall from section 2.5.4 that C and $\mathrm{var}(\underline{q})$ were taken as a_1E_t and $a_2E_t\sigma^2$, respectively.

Here,

$$a_1 = bc_{\Omega^*}/(t-1) \tag{5.5}$$

and,

$$a_2 = bc_{\Omega^*\Lambda\Omega^*}/(t-1), \tag{5.6}$$

which means that by the equation in (2.22)

$$D^+ = \frac{(t-1)c_{\Omega^*\Lambda\Omega^*}}{bc_{\Omega^*}^2}E_t. \tag{5.7}$$

Recall from section 5.2.3 that, for a binary design, c_W simplifies to $\mathrm{tr}(W)$, which is constant for all binary designs.

5.2.4.1   *Ordinary least squares results*

Under ols, $\Omega^* = E_k$ is centro-symmetric (see Table 4.1, model IV), and if Λ is centro-symmetric, so then is $\Omega^*\Lambda\Omega^* = E_k\Lambda E_k$. Therefore, for a SEN design

$$\mathrm{tr}\{D^+\} = \frac{(t-1)^2}{b(k-1)^2}\mathrm{tr}(E_k\Lambda E_k),$$

which is constant over all balanced block designs. This gives the following theorem.

Theorem 5.9 (Martin & Eccleston, 1991)
An SDEN/SEN design is weakly universally optimal under ols among all balanced block designs in $\mathcal{D}$ for all Λ/all centro-symmetric Λ. ∎

Note that for a stationary process, Kunert (1987b) showed that the SBA is a weakly universally optimal balanced block design under ols. However, Λ in Theorem 5.9 also includes non-stationary processes.

As in Cheng (1988), it is possible to construct balanced non-binary designs which can be more efficient than a binary design. Blocks of size $k = 3$ and 4 were considered for a centro-symmetric Λ, which includes the NN1 process considered by Cheng (1988). For $k = 3$, the variance balanced design D5.7 with blocks of type [aba] is compared to a SEN design with an equal number of blocks. It is shown that the SEN design is universally better than D5.7 if

$$4w_{1,1} \leq 7w_{2,2},$$

where $W = E_3 \Lambda E_3$. In terms of the elements of Λ this inequality is

$$u_{1,1} + 8u_{1,2} \leq 5u_{1,3} + 4u_{2,2}, \tag{5.8}$$

where

$$\Lambda = \begin{pmatrix} u_{1,1} & u_{1,2} & u_{1,3} \\ u_{1,2} & u_{2,2} & u_{1,2} \\ u_{1,3} & u_{1,2} & u_{1,1} \end{pmatrix}.$$

(cf. the result of Cheng, 1988).

For $k = 4$, Martin & Eccleston (1991) show when variance balanced block designs of types [aabb] and [abab] are universally better than the SEN design.

For the NN1 process with k even, conditions for when variance balanced designs with blocks of type [aabbcc...] and [abab...ab] are universally better than the SEN design, are also derived in Martin & Eccleston (1991).

5.2.4.2   Generalised least squares results

For any symmetric Ω^*, a binary design has

$$\text{tr}(C) = b\,\text{tr}(\Omega^*),$$

and by the equation in (2.30), for a non-binary design, $c_{\Omega^*} < \text{tr}(\Omega^*)$ if

$$\sum_{v=1}^{t} \sum_{\Theta_{i,v}^{(2)}} w_{l_1 l_2} < 0,$$

i.e. when

$$(\Omega^*)_{l_1 l_2} \leq 0 \quad \forall \quad l_1 \neq l_2. \tag{5.9}$$

That is, if the off-diagonal elements of Ω^* are non-positive. Therefore $\text{tr}(C)$ is maximal for a SEN design if any only if the condition in (5.9) is true. This gives the following theorem.

Theorem 5.10   (Martin & Eccleston, 1991)
An SDEN/SEN design is universally optimal under gls for all Ω^* /all centro-symmetric Ω^*
a) among all binary designs in $\mathcal{D}$
b) among all designs in $\mathcal{D}$ if the condition in (5.9) is true.   ∎

Theorem 5.10 is also valid when the data need to be differenced, as for the CG(d) model (see section 2.3.2.4). Recall that part a) of Theorem 5.10 was given by Cheng (1988), although he did not consider differenced data.

Martin & Eccleston (1991) note that many dependence structures have some positive off-diagonal elements in Ω^*. Two exceptions are the LV model and the AR(1) process with $\rho_1 \geq \rho_1^*(k)$, where $\rho_1^*(k)$ is given in Lemma 5.5.

Blocks of size $k = 3$ and 4 were considered by Martin & Eccleston (1991) for centro-symmetric Λ. When $k = 3$, only designs with blocks of two of the four

types listed in (5.1) (in section 5.2.3) can be universally optimal. If

$$2u_{1,2} \le u_{1,3} + u_{2,2} \qquad\qquad (5.10)$$

then the SEN design is universally optimal over $\mathcal{D}$, otherwise the design D5.7 is universally optimal (cf. the result of Cheng, 1988).

For $k = 4$, the 10 types listed in (5.4) were reduced to the 5 types

[aabb], [abab], [abba], [abca] and [abcd].

For each of these types, conditions in terms of the elements of Ω^* were given for which designs with C completely symmetric are universally optimal over $\mathcal{D}$. However, since the extra type [baac] was not considered here, these conditions are incorrect, but were corrected in Martin (1998).

5.2.5   Martin (1998)

Martin (1998) extends the results of Martin & Eccleston (1991), considering blocks of size 3 to 6 in detail, and also giving some results for general block sizes, over a range of dependence structures. Only $k \le t$ is discussed here, although Martin (1998) also considered the extended block case of $k > t$.

Most of the assumptions in Martin (1998) are as in Martin & Eccleston (1991). However, it is assumed throughout Martin (1998) that W is centro-symmetric as well as symmetric, and therefore a reference to w_{i_1, i_2} implies also the elements w_{i_2, i_1}, $w_{k+1-i_2, k+1-i_1}$ and $w_{k+1-i_1, k+1-i_2}$. Recall, from section 2.7, that the rows and columns of W sum to zero and the diagonal elements of W are positive.

Although some results for general dependence structures are given by Martin (1998), the main dependence structures considered are the NN1, HCS, AR(1), two special cases of the AR(2), the LV and the CG(2) models. The two special cases of the AR(2) (defined in section 2.3.2.2) are called the AR(2a) and the AR(2b). The AR(2a) has $\eta_1 = 2\eta$ and $\eta_2 = -\eta^2$ for $|\eta| < 1$, and the

AR(2b) has $\eta_1 = \eta$ and $\eta_2 = 2\eta^2$ for $|\eta| < \frac{1}{2}$. These 7 processes are all one-parameter processes. Martin (1998) defines *positive dependence* to mean any process formed by differencing (e.g. LV and CG(2)), and any correlation structure with $\rho_1 > 0$. *Negative dependence* means any correlation structure with $\rho_1 < 0$.

The designs considered here
 (i)   have $b = \frac{1}{2}ct(t\text{-}1)$ for an integer c,
 (ii) are equireplicated,
 (iii) have each block of the same type (see section 5.2.3), and
 (iv) have $X'(I_b \otimes W)X$ completely symmetric.

The complete symmetry of $X'(I_b \otimes W)X$ is achieved by using the columns of a SBA of length k on t symbols, as described in section 3.1.3. Let the number of different symbols in a type be $s \leq k$. The design is constructed from s rows of the SBA, with the columns forming the blocks. If a type has $s < k$ different symbols, the s rows are used in the appropriate plot positions, and the remaining $k - s$ plot positions are filled with the within-block replicates according to the type. For example, when $t = 5$, using the SBA given in Figure 3.2c, a binary design with blocks of type [abcd] formed from the columns of the first $s = 4$ rows of this SBA is the SDEN design with $b = 10$:

| 1 | 2 | 3 | 4 | , | 1 | 4 | 2 | 5 | , | 2 | 3 | 4 | 5 | , | 2 | 5 | 3 | 1 | ,

| 3 | 1 | 4 | 2 | , | 3 | 4 | 5 | 1 | , | 4 | 2 | 5 | 3 | , | 4 | 5 | 1 | 2 | ,

| 5 | 1 | 2 | 3 | , | 5 | 3 | 1 | 4 | .   D5.8

A non-binary design of type [aabb] has $s = 2$, and so the first two rows of the SBA can be used to construct the design:

| 1 | 1 | 2 | 2 | , | 1 | 1 | 4 | 4 | , | 2 | 2 | 3 | 3 | , | 2 | 2 | 5 | 5 | ,

| 3 | 3 | 1 | 1 | , | 3 | 3 | 4 | 4 | , | 4 | 4 | 2 | 2 | , | 4 | 4 | 5 | 5 | ,

| 5 | 5 | 1 | 1 | , | 5 | 5 | 3 | 3 | .   D5.9

It has been shown in section 5.2.3 that for a SDEN design, $X'(I_b \otimes W)X$ is completely symmetric. It is now shown that $X'(I_b \otimes W)X$ is also completely symmetric for non-binary designs constructed as described above.

Let $\Theta^{(4)}_{v_1,v_2} = \bigcup_{i=1}^{b} \Theta^{(3)}_{i,v_1,v_2}$ be the set of pairs of plots that contain the distinct treatments v_1 and v_2, and let $\Theta_v = \bigcup_{i=1}^{b} \Theta^{(2)}_{i,v}$ be the set of pairs of distinct plots containing treatment v. Then for any design, from the equation in (2.29),

$$\{X'(I_b \otimes W)X\}_{v_1,v_2} = x_1 \sum_{i=1}^{b} \sum_{\Theta^{(3)}_{i,v_1,v_2}} w_{j_1 j_2}$$

$$= x_1 \sum_{\Theta^{(4)}_{v_1,v_2}} w_{j_1 j_2},$$

and from the equation in (2.28),

$$\{X'(I_b \otimes W)X\}_{v,v} = x_2 \left\{ \sum_{l=1}^{k} w_{l,l} + 2 \sum_{i=1}^{b} \sum_{\Theta^{(2)}_{i,v}} w_{j_1 j_2} \right\}$$

$$= x_2 \left\{ \mathrm{tr}(W) + 2 \sum_{\Theta_v} w_{j_1 j_2} \right\},$$

where x_1 is the number of times each pair of distinct treatments occur in each pair of distinct plot positions, and x_2 is the number of times each treatment occurs in each plot position (as defined in section 5.2.3). For a design constructed from a SBA in the way described above, $\Theta^{(4)}_{v_1,v_2}$ is the same for all $v_1 \neq v_2$, and so the off-diagonal elements of $X'(I_b \otimes W)X$ are equal. Also, Θ_v is the same for all v, and so the diagonal elements of $X'(I_b \otimes W)X$ are equal.

It follows that

$$\text{tr}\{X'(I_b \otimes W)X\} = tx_2\left\{\text{tr}(W) + 2\sum_{\Theta_v} w_{l_1 l_2}\right\}$$

$$= b\,c_W \quad \text{(by the equation in (5.3))},$$

since

$$tx_2 = b \quad \text{and} \quad \text{tr}(W) + 2\sum_{\Theta_v} w_{l_1 l_2} = \text{tr}(X_i'WX_i) = c_W,$$

where $\sum_{\Theta_v} w_{l_1 l_2}$ is the sum of the $w_{l_1 l_2}$ for those plots $l_1 < l_2$ with the same

symbol in the type.

As an example consider designs D5.8 and D5.9. For both designs, $x_2 = 2$.

For the SDEN design D5.8, $\Theta_{v_1,v_2}^{(4)} = \{(1,2), (1,3), (1,4), (2,3), (2,4), (3,4)\}$ $\forall$

$v_1 \neq v_2$, and $\Theta_v = \{\}$ $\forall$ v, so $c_W = \text{tr}(W)$. For D5.9, $\Theta_{v_1,v_2}^{(4)} = \{(1,3), (1,4),$

$(2,3), (2,4)\}$ $\forall$ $v_1 \neq v_2$, and $\Theta_v = \{(1,2), (3,4)\}$ $\forall$ v, so $c_W = \text{tr}(W) +$

$2(w_{1,2} + w_{3,4})$. Clearly $\Theta_{v_1,v_2}^{(4)} \bigcup \Theta_v = \Theta_{v_1,v_2}^{(4)} \bigcap \Theta_v$ is the set of all pairs of

distinct plots.

Since $X'(I_b \otimes W)X$ is completely symmetric, C and $\text{var}(\underline{q})$ are completely

symmetric, as shown in section 5.2.4. Therefore D^+ is also completely

symmetric. Under gls, maximising c_{Ω^*} gives the universally optimal design

(by the equation in (5.5)). Under ols, $\Omega^* = E_k$ so minimising $c_{E_k \wedge E_k}/c_{E_k}^2$

gives the universally optimal design among designs for which C and $\text{var}(q)$ are

completely symmetric and the weakly universally optimal design over designs

with C completely symmetric (by the equation in (5.7)). Note that

$$c_{E_k} = k - k^{-1}\underline{r}'\underline{r},$$

where $\underline{r} = X_i'\underline{1}_k$ is the vector of within-block replicate numbers for any

block i.

For $k = 3, 4, 5, 6$, Martin (1998) gives a list of types corresponding to the different c_W possible for W centro-symmetric. Expressions for c_W are given for $k = 3, 4, 5$. There are 4, 11, 32 and 117 types for $k = 3, 4, 5$ and 6, respectively. The types and expressions for c_W are repeated here in Table 5.1 and Table 5.2 for $k = 3$ and 4, respectively.

Table 5.3 gives the list of types for $k = 6$. For a given k, types are numbered 1,2, ... When comparing two types e_1 and e_2, e_1 is defined to be *better* than e_2 if $c_{\Omega^* \wedge \Omega^*} / c_{\Omega^*}^2$ for e_1 is less or equal to $c_{\Omega^* \wedge \Omega^*} / c_{\Omega^*}^2$ for e_2. A design with blocks of type e is called a type e design. In comparing designs of different types it is assumed that c, and hence b are equal. A type is called optimal if the design of that type is optimal.

Table 5.1
List of types and expressions for c_W for $k = 3$.

type no.	type	c_W
1	[aaa]	0
2	[aab]	$2w_{1,1}$
3	[aba]	$2w_{2,2}$
4	[abc]	$2w_{1,1} + w_{2,2}$

Table 5.2
List of types and expressions for c_W for $k = 4$.

type no.	type	c_W
1	[aaaa]	0
2	[aaab]	$2w_{1,1}$
3	[aaba]	$2w_{2,2}$
4	[aabb]	$2w_{1,1} + 2w_{2,2} + 4w_{1,2}$
5	[abab]	$2w_{1,1} + 2w_{2,2} + 4w_{1,3}$
6	[abba]	$2w_{1,1} + 2w_{2,2} + 2w_{1,4} + 2w_{2,3}$
7	[aabc]	$2w_{1,1} + 2w_{2,2} + 2w_{1,2}$
8	[abac]	$2w_{1,1} + 2w_{2,2} + 2w_{1,3}$
9	[abca]	$2w_{1,1} + 2w_{2,2} + 2w_{1,4}$
10	[baac]	$2w_{1,1} + 2w_{2,2} + 2w_{2,3}$
11	[abcd]	$2w_{1,1} + 2w_{2,2}$

Table 5.3
List of types for $k = 6$.

type no.	type	type no.	type	type no.	type	type no.	type
1	[aaaaaa]	31	[aababc]	61	[aabcbc]	91	[acabdb]
2	[aaaaab]	32	[abaabc]	62	[aabccb]	92	[abbacd]
3	[aaaaba]	33	[baaabc]	63	[abacbc]	93	[abcabd]
4	[aaabaa]	34	[aabbac]	64	[abaccb]	94	[abcadb]
5	[aaaabb]	35	[ababac]	65	[abcabc]	95	[acbabd]
6	[aaabab]	36	[baabac]	66	[abcacb]	96	[acbadb]
7	[aabaab]	37	[abbaac]	67	[abccab]	97	[abbcad]
8	[abaaab]	38	[babaac]	68	[abbcca]	98	[abcbad]
9	[baaaab]	39	[bbaaac]	69	[abcbca]	99	[abcdab]
10	[aaabba]	40	[aaabcb]	70	[abccba]	100	[acbbad]
11	[aababa]	41	[aabacb]	71	[aaabcd]	101	[abbcda]
12	[abaaba]	42	[abaacb]	72	[aabacd]	102	[abcbda]
13	[aabbaa]	43	[baaacb]	73	[aabcad]	103	[abcdba]
14	[aaabbb]	44	[aabbca]	74	[aabcda]	104	[acbbda]
15	[aababb]	45	[ababca]	75	[abaacd]	105	[caabbd]
16	[abaabb]	46	[baabca]	76	[abacad]	106	[cababd]
17	[aabbba]	47	[abbaca]	77	[abacda]	107	[cabbad]
18	[ababab]	48	[babaca]	78	[abcaad]	108	[aabcde]
19	[ababba]	49	[bbaaca]	79	[baaacd]	109	[abacde]
20	[abbaab]	50	[aaacbb]	80	[baacad]	110	[abcade]
21	[aaaabc]	51	[aabcab]	81	[aabbcd]	111	[abcdae]
22	[aaabac]	52	[abacab]	82	[aabcbd]	112	[abcdea]
23	[aabaac]	53	[baacab]	83	[aabcdb]	113	[baacde]
24	[abaaac]	54	[aabcba]	84	[aacbbd]	114	[bacade]
25	[baaaac]	55	[abacba]	85	[aacbdb]	115	[bacdae]
26	[aaabca]	56	[baacba]	86	[aacdbb]	116	[bcaade]
27	[aabaca]	57	[abbcaa]	87	[ababcd]	117	[abcdef]
28	[abaaca]	58	[babcaa]	88	[abacbd]		
29	[aabcaa]	59	[bbacaa]	89	[abacdb]		
30	[aaabbc]	60	[aabbcc]	90	[acabbd]		

5.2.5.1 *Generalised least squares results for general k*

Now consider gls. As seen in Martin & Eccleston (1991) for $k = 3$ and 4,
when Λ is the within-block correlation matrix for a stationary process, $\{w_{l_1 l_2}\}$
can easily be written down in terms of $\{\rho_g\}$. Recall from Theorem 5.10 that
a SEN design is universally optimal among all designs when the condition in
(5.9) is true. This occurs for all the seven processes considered in Martin

(1998) in a parameter region around zero, but not for the CG(2). For the LV model it is true for all ψ, and for the AR(p) when all $\eta_i \geq 0$. Martin (1998) points out that for the AR(p), optimality of the SEN design can extend slightly outside the region $\{\eta_i \geq 0 \ \forall \ i\}$ (cf. the result for the AR(1) process in Theorem 5.7). He also gives a condition, in terms of η, when the SEN design is optimal for the AR(2b). It is noted further that for the AR(2a) and NN1, the range of the parameter in which the SEN design is optimal tends to zero as k increases.

Clearly if the condition in (5.9) is not true, then a non-binary type is optimal. If $w_{l_1,l_2} > 0$, then a type with the same symbol on plots l_1 and l_2, and different symbols on all the other plots, will have a larger c_W than for a binary design. Under the centro-symmetry of Ω^*, if $l_1 + l_2 \neq k + 1$, a different repeated symbol can be used on plots $k + 1 - l_1$ and $k + 1 - l_2$. Hence this design will be universally better than the SEN design, and is optimal if w_{l_1,l_2} is the only positive off-diagonal element.

Martin (1998) notes that as ρ_1 becomes more negative (i.e. increasing negative dependence), $w_{1,2}$ often becomes positive first, in which case a type with the same symbols on plots 1 and 2 (and a different repeated symbol on plots $k - 1$ and k, for $k > 3$), is likely to be optimal. For example, for $k = 3, 4, 5$ and 6, the resulting types are [aab], [aabb], [aacbb] and [aacdbb]. For general k, conditions for when $w_{1,2}$ becomes positive are given in Martin (1998) for the seven processes being considered.

For increasing positive dependence, $w_{2,4}$ often becomes positive first. The optimal type has the same symbol on plots 2 and 4 (and a different repeated symbol on plots $k - 3$ and $k - 1$, for $k = 6$ and $k > 7$). For example, the resulting types for $k = 5, 6, 7$ and 8, are [bacad], [cababd], [bacadef]

and [cadabebf]. For general k, conditions for when $w_{2,4}$ becomes positive are given in Martin (1998) for the seven processes being considered. As the positive or negative dependence increases, further w_{i_1,i_2} may become positive, and therefore optimal types are more difficult to deduce.

5.2.5.2 *Ordinary least squares results for general k*

Under ols, Martin (1998) points out that in general it is more difficult to see which types are optimal since optimality depends on $c_{E_k \wedge E_k} / c_{E_k}^2$, and it is difficult to see which off-diagonal elements of $E_k \wedge E_k$ are large and negative. However, some general results are given despite these difficulties, including some simple comparisons between binary and non-binary types.

5.2.5.3 *Optimal types for small k*

For $k = 3, 4, 5, 6$, optimal types and change points are given in Martin (1998) for $t \geq 2$ under both ols and gls for each of the processes under consideration.

Definition 5.1
A type is deemed to be *inadmissible* if, in the situation considered, there is another type which is always better. ∎

Type 1 is inadmissible for $k = 3, 4, 5, 6$. When $k = 3$, the 4 types listed by Cheng (1988) ((5.1) in section 5.2.3) are given in Table 5.1. Now consider gls. First assume $t \geq 3$. Since $w_{2,2} > 0$, type 4 is always better than type 2, so type 2 is inadmissible. Therefore type 4 is optimal if it is better than type 3, which is the case when $2w_{1,1} > w_{2,2}$. This is equivalent to $w_{1,3} < 0$ since the row/column sums of W are zero. Otherwise type 3 is optimal (cf. the result of Martin & Eccleston (1991), given as the inequality in (5.10)). When $t = 2$, type 3 is optimal if $w_{1,1} < w_{2,2}$, otherwise type 2 is optimal.

Under ols, c_{E_3} is $\frac{4}{3}$, $\frac{4}{3}$ and 2 for types 2, 3 and 4, respectively. Hence

$c_{E_3 \wedge E_3} / c_{E_3}^2$ is $\frac{9}{8} w_{1,1}$, $\frac{9}{8} w_{2,2}$ and $\frac{1}{4}(2w_{1,1} + w_{2,2})$ for types 2, 3 and 4, respectively.

First assume $t \geq 3$. Recall that Martin & Eccleston (1991) gave the condition for when type 4 is better than type 3 (the inequality in (5.8)). For a stationary process, the inequality in (5.8) is equivalent to

$$3 - 8\rho_1 + 5\rho_2 > 0.$$

Type 4 is better than type 2 if $5w_{1,1} > 2w_{2,2}$. For a stationary process this is equivalent to

$$3 + \rho_1 - 4\rho_2 > 0.$$

For $t = 2$ under stationarity, type 3 is optimal if $\rho_1 > \rho_2$, otherwise type 2 is optimal.

For $k = 4$, the complete list of 11 types is given in Table 5.2. Now consider gls for $t \geq 4$. Types 2 and 3 are inadmissible since type 11 is better. For type 7, c_W lies between c_W for types 4 and 11, and c_W for type 8 lies between c_W for types 5 and 11. Hence types 7 and 8 are also inadmissible. Therefore the optimal type depends on the maximum of $2w_{1,2}$, $2w_{1,3}$, $w_{1,4} + w_{2,3}$, $w_{1,4}$, $w_{2,3}$ and 0, for types 4, 5, 6, 9, 10 and 11, respectively. This corrects the result in Martin & Eccleston (1991), which omitted the optimality of type 10 for Λ centro-symmetric. For a stationary process, $w_{2,3} > 0$ requires $w_{1,4} > 0$. This means that type 6 is better than type 10. If $w_{2,3} < 0$ then type 11 is better than type 10. Hence, type 10 is inadmissible under stationarity.

Under ols for $t \geq 4$, type 10 is inadmissible for a stationary process since $c_{E_4 \wedge E_4} / c_{E_4}^2$ for type 10 lies between $c_{E_4 \wedge E_4} / c_{E_4}^2$ for types 7 and 9. Conditions are given in Martin (1998) for when types 4, 5 (Martin & Eccleston, 1991) and 9 are better than type 11 under stationarity.

For $k = 5$ under gls for $t \geq 5$, optimality conditions in terms of $\{\rho_i\}$ are complicated in general. Under ols for $t \geq 5$, it is simple to compare one type with another type for a stationary process, but the number of possible comparisons is very large.

For $k = 6$ under gls for $t \geq 6$, types 2, 3, 4, 30, 31, 35, 37, 40, 41, 48, 50, 52, 56, 59, 71, 72, 76, 78, 108, 109, 110, 111, 113 and 114 are inadmissible. This reduces the number of types from 117 to 93.

5.2.5.4 Discussion

In the Discussion section of Martin (1998), it is noted that

- general results on optimality are difficult to obtain even for small-sized blocks;
- it is difficult to give all the types for higher k;
- the parameter range in which the binary type is optimal can be very small, and can tend to zero as k increases;
- in practice, optimality is not important as long as an efficient design is used;
- designs robust to changes in the parameter values and the dependence structure are needed. Therefore a design that is optimal for only a small region for one particular process should not usually be used.

5.3 Two-dimensional designs for correlated errors

Section 5.3 considers some recent work on efficient two-dimensional NRC designs for correlated errors. Martin & Eccleston (1993) extended the ideas of Martin & Eccleston (1991) to designs with blocks having plots arranged in two dimensions, mainly considering model IV. Uddin & Morgan (1997a) found optimal NRC designs for blocks of size $p_1 \times 2$ under the AR(1)*AR(1) process for models I to IV. Uddin & Morgan (1997b) considered NRC

designs under model IV for blocks of size $p_1 \times 2$ under the AR(1)*AR(1) and 3-parameter CAR(2) processes. They derived conditions for the universal optimality of binary designs, and gave reasonably efficient cyclic designs which have a smaller number of blocks than the optimal designs when $t > 3$.

Morgan & Uddin (1991) and Uddin (2000) constructed optimal torus and cylindrical designs, and showed that (planar) NRC designs obtained from them have very good efficiency.

5.3.1 Martin & Eccleston (1993)

The results of Martin & Eccleston (1991) are generalised to a two-dimensional array of plots in Martin & Eccleston (1993). As well as centro-symmetry, reflection, axial and complete symmetry (see section 2.3.1) are also considered, and the corresponding designs that have $X'(I_b \otimes W)X$ completely symmetric are defined.

A binary <u>S</u>patial block design is <u>S</u>trongly <u>D</u>irectionally <u>E</u>qui<u>N</u>eighboured (SSDEN) if $X'(I_b \otimes W)X$ is completely symmetric for all symmetric W. Clearly a SSDEN design is a SDEN design (see section 5.2.4) in which the plots are spatially arranged. Consider the following example.

Example 5.1
This example consists of blocks of size 2×2 with $t = 4$ treatments. ∎

The columns of the SBA in Figure 3.2b give the following SSDEN design with $b = 12$ for Example 5.1.

$$\begin{array}{|c|c|}\hline 1 & 2 \\\hline 3 & 4 \\\hline\end{array}, \begin{array}{|c|c|}\hline 1 & 3 \\\hline 4 & 2 \\\hline\end{array}, \begin{array}{|c|c|}\hline 1 & 4 \\\hline 2 & 3 \\\hline\end{array}, \begin{array}{|c|c|}\hline 2 & 1 \\\hline 4 & 3 \\\hline\end{array}, \begin{array}{|c|c|}\hline 3 & 1 \\\hline 2 & 4 \\\hline\end{array}, \begin{array}{|c|c|}\hline 4 & 1 \\\hline 3 & 2 \\\hline\end{array},$$

$$\begin{array}{|c|c|}\hline 2 & 3 \\\hline 1 & 4 \\\hline\end{array}, \begin{array}{|c|c|}\hline 3 & 2 \\\hline 4 & 1 \\\hline\end{array}, \begin{array}{|c|c|}\hline 3 & 4 \\\hline 1 & 2 \\\hline\end{array}, \begin{array}{|c|c|}\hline 2 & 4 \\\hline 3 & 1 \\\hline\end{array}, \begin{array}{|c|c|}\hline 4 & 2 \\\hline 1 & 3 \\\hline\end{array}, \begin{array}{|c|c|}\hline 4 & 3 \\\hline 2 & 1 \\\hline\end{array}. \qquad\text{D5.10}$$

Design D2.1 for Example 2.1 ($t = 5$) is also a SSDEN design.

A binary $\underline{S}$patial block design is $\underline{S}$trongly $\underline{E}$qui$\underline{N}$eighboured (SSEN) if $X'(I_b \otimes W)X$ is completely symmetric for all symmetric and centro-symmetric W. A SSEN design is a SEN design (see section 5.2.4) in which the plots are spatially arranged. For Example 5.1, the SEN in Figure 5.1 gives the SSEN design with $b = 6$ (the first 6 blocks of design D5.10) :

$$\begin{array}{|c|c|}\hline 1 & 2 \\\hline 3 & 4 \\\hline\end{array} \,,\, \begin{array}{|c|c|}\hline 1 & 3 \\\hline 4 & 2 \\\hline\end{array} \,,\, \begin{array}{|c|c|}\hline 1 & 4 \\\hline 2 & 3 \\\hline\end{array} \,,\, \begin{array}{|c|c|}\hline 2 & 1 \\\hline 4 & 3 \\\hline\end{array} \,,\, \begin{array}{|c|c|}\hline 3 & 1 \\\hline 2 & 4 \\\hline\end{array} \,,\, \begin{array}{|c|c|}\hline 4 & 1 \\\hline 3 & 2 \\\hline\end{array} . \qquad \text{D5.11}$$

A binary $\underline{S}$patial block design is $\underline{S}$trongly $\underline{E}$qui$\underline{N}$eighboured under $\underline{R}$eflection symmetry (SSENR) if $X'(I_b \otimes W)X$ is completely symmetric for all symmetric, centro-symmetric and reflection symmetric W. On the given plot arrangement a SSDEN or SSEN design is a SSENR design. If p_1 and p_2 are both even, and $t = 4c'$ or $t = 4c'+1$ for an integer c', then a SSENR design with $b = \frac{1}{4}ct(t-1)$ may be possible. For Example 5.1, Martin & Eccleston (1993) give the following SSENR design with $b = 3$ ($c = c' = 1$):

$$\begin{array}{|c|c|}\hline 1 & 2 \\\hline 3 & 4 \\\hline\end{array} \,,\, \begin{array}{|c|c|}\hline 1 & 3 \\\hline 4 & 2 \\\hline\end{array} \,,\, \begin{array}{|c|c|}\hline 1 & 4 \\\hline 2 & 3 \\\hline\end{array} \,, \qquad \text{D5.12}$$

Here the blocks are the first 3 blocks of design D5.10.

A binary $\underline{S}$patial block design is $\underline{S}$trongly $\underline{E}$qui$\underline{N}$eighboured under $\underline{C}$omplete symmetry (SSENC) if $X'(I_b \otimes W)X$ is completely symmetric for all symmetric, centro-symmetric and completely symmetric W. Any SSDEN, SSEN or SSENR design with $p_1 = p_2$, on the given plot arrangement, is a SSENC design. However, a SSENC design with a smaller number of blocks may be possible. If p_1 is odd and $t = 4c'+1$ for an integer c', then a necessary condition for a SSENC design is that $b = \frac{1}{4}ct(t-1)$. SSENC designs with $b = \frac{1}{4}ct(t-1)$ may also be possible for p_1 even. For example, Martin & Eccleston (1993) give the following SSENC design with 5 blocks ($c = 1$) of size 2×2 with $t = 5$ treatments.

$$\begin{array}{|c|c|}\hline 1 & 5 \\\hline 4 & 3 \\\hline\end{array} \,,\, \begin{array}{|c|c|}\hline 2 & 1 \\\hline 5 & 4 \\\hline\end{array} \,,\, \begin{array}{|c|c|}\hline 3 & 2 \\\hline 1 & 5 \\\hline\end{array} \,,\, \begin{array}{|c|c|}\hline 4 & 3 \\\hline 2 & 1 \\\hline\end{array} \,,\, \begin{array}{|c|c|}\hline 5 & 4 \\\hline 3 & 2 \\\hline\end{array} . \qquad \text{D5.13}$$

Optimal NRC designs with blocks of size 2×2 are considered under both ols and gls, and it is shown that non-binary designs can be universally better than binary designs. Under centro-symmetry,

$$\Lambda = \begin{pmatrix} u_{1,1} & u_{1,2} & u_{1,3} & u_{1,4} \\ u_{1,2} & u_{2,2} & u_{2,3} & u_{1,3} \\ u_{1,3} & u_{2,3} & u_{2,2} & u_{1,2} \\ u_{1,4} & u_{1,3} & u_{1,2} & u_{1,1} \end{pmatrix}. \tag{5.11}$$

The completely symmetric structure has

$$u_{1,1} = u_{2,2}, \quad u_{1,2} = u_{1,3} \quad \text{and} \quad u_{1,4} = u_{2,3}.$$

This corrects a small slip in Martin & Eccleston (1993) which omitted the equality $u_{1,2} = u_{1,3}$. For a stationary process,

$$u_{1,1} = u_{2,2} = 1, \quad u_{1,2} = \rho_{1,0}, \quad u_{1,3} = \rho_{0,1},$$

$$u_{1,4} = \rho_{1,1} \quad \text{and} \quad u_{2,3} = \rho_{-1,1}. \tag{5.12}$$

Therefore under stationarity, the completely symmetric process has $\rho_{1,0} = \rho_{0,1}$ and $\rho_{1,1} = \rho_{-1,1}$. A special case of this is the completely symmetric separable process, which has

$$\Lambda = \begin{pmatrix} 1 & \rho_{1,0} \\ \rho_{1,0} & 1 \end{pmatrix} \otimes \begin{pmatrix} 1 & \rho_{1,0} \\ \rho_{1,0} & 1 \end{pmatrix},$$

(i.e. $\rho_{1,0} = \rho_{0,1}$ and $\rho_{1,1} = \rho_{-1,1} = \rho_{1,0}^2$).

When the plots are numbered, 1 to k, by rows from the top-left, the types and c_W values listed in Table 5.2 are valid here. Hence the type $[abcd]$ in Table 5.2 is given here as $\begin{bmatrix} ab \\ cd \end{bmatrix}$. As in Martin (1998), a type is called optimal if the variance balanced design of that type is optimal.

The results in Martin & Eccleston (1993) assume model IV. They note that results for models including row and/or column effects (models I, II and III) can be obtained in a similar way as those for model IV. They give their opinion that

> *fixed row and column effects are usually not necessary when a*
> *reasonable dependence structure is postulated*

but they add that

> *there are some who feel that both should be included in the model.*
> *Further research on optimal designs for this situation would then be of*
> *interest.*

5.3.1.1 *Ordinary least squares results*

In this section (5.3.1.1) ols is assumed. The following theorem is obtained by
the same reasoning as Martin & Eccleston (1991) used to obtain Theorem 5.9.

Theorem 5.11   (Martin & Eccleston, 1993)
A SSDEN/SSEN/SSENR/SSENC design is weakly universally optimal under
ols among all balanced block designs in $\mathcal{D}$ for all Λ/all centro-symmetric
Λ/all reflection symmetric Λ/all completely symmetric Λ.   ∎

Under a completely symmetric dependence structure, for blocks of size 2×2,

$$w_{1,1} = w_{2,2}, \quad w_{1,2} = w_{1,3} \quad \text{and} \quad w_{1,4} = w_{2,3}. \tag{5.13}$$

The equality $w_{1,2} = w_{1,3}$ was omitted in Martin & Eccleston (1993). Therefore

types 4 and 5 ($\begin{bmatrix} a\,a \\ b\,b \end{bmatrix}$ and $\begin{bmatrix} a\,b \\ a\,b \end{bmatrix}$, respectively) are equivalent, since they have

the same $c_W = 4w_{1,1} + 4w_{1,2}$. Henceforth, only the type with the lowest type

number will be given for equivalent types.

For a completely symmetric dependence structure under stationarity, by

comparing $c_W / c_{E_4}^2$ where $W = E_4 \Lambda E_4$, type 4 is shown to be better than the

binary type (type 11) if

$$(5/9)w_{1,1} + w_{1,2} \leq 0,$$

i.e. if

$$3 + 4\rho_{1,0} - 7\rho_{1,1} \leq 0. \tag{5.14}$$

Under a completely symmetric separable process, the inequality in (5.14) becomes

$$\rho_{1,0} \leq -3/7$$

Type 6 ($\begin{bmatrix} a & b \\ b & a \end{bmatrix}$) is also compared to type 11. For Λ centro-symmetric, type 6 is better than type 11 if

$$5(w_{1,1} + w_{2,2}) + 9(w_{1,4} + w_{2,3}) \leq 0,$$

i.e. if

$$3(u_{1,1} + u_{2,2}) - 14(u_{1,2} + u_{1,3}) + 11(u_{1,4} + u_{2,3}) \leq 0. \tag{5.15}$$

Under a completely symmetric stationary dependence structure, the inequality in (5.15) becomes

$$3 - 14\rho_{1,0} + 11\rho_{1,1} \leq 0, \tag{5.16}$$

and for a completely symmetric separable process, the inequality in (5.15) becomes

$$\rho_{1,0} \geq 3/11. \tag{5.17}$$

5.3.1.2   Generalised least squares results

Theorem 5.12, below, follows from Theorem 5.10 (Martin & Eccleston, 1991).

Theorem 5.12   (Martin & Eccleston, 1993)

A SSDEN/SSEN/SSENR/SSENC design is universally optimal under gls, using a known Ω^* for all Ω^*/all centro-symmetric Ω^*/all reflection symmetric Ω^*/all completely symmetric Ω^*

a) among all binary designs in $\mathcal{D}$

b) among all designs in $\mathcal{D}$ if $\left(\Omega^*\right)_{l_1,l_2} \leq 0 \quad \forall \quad l_1 \neq l_2$, the condition in (5.9), is

   true.   ∎

For blocks of size 2×2, under the completely symmetric structure, the equations in (5.13) means that types 2 and 3 from Table 5.2 are equivalent; as are types 4 and 5; 7 and 8; and types 9 and 10. As in section 5.2.5.3, types 1, 2 and 7 are inadmissible. Type 9 is also inadmissible since c_W lies between the c_W for types 6 and 11. Hence types 4, 6 and 11 can be optimal, depending on the maximum of $w_{1,2}$, $w_{1,4}$ and 0, respectively. When type 11 is optimal a SSENC design is universally optimal. When types 4 and 6 are optimal, the optimal design is a design for which C is completely symmetric. This corrects a small mistake in Martin & Eccleston (1993) which omitted the word 'completely'.

For a completely symmetric stationary process, the design with blocks of type 6 is universally optimal if

$$1 - 4\rho_{1,0} + 3\rho_{1,1} \leq 0,$$
(5.18)

Otherwise the SSENC is optimal. Under the completely symmetric separable process, the inequality in (5.18) simplifies to

$$\rho_{1,0} \geq \tfrac{1}{3}.$$
(5.19)

5.3.2   Uddin & Morgan (1997a)

Assuming that within-block observations are correlated, universally optimal NRC designs with blocks of size $p_1 \times 2$ have been obtained under gls for models I to IV and the AR(1)*AR(1) process by Uddin & Morgan (1997a). Results for blocks of size 2×2 under a general dependence structure for model I are given here in section 5.3.2.1. Optimality results are given in section 5.3.2.2. Some corrections are also given in section 5.3.2.3.

The plots in positions $(1,1)$, $(1,2)$, $(p_1, 1)$ and $(p_1, 2)$ will be referred to as *end plots*, and the other plots as *interior plots*.

5.3.2.1   Blocks of size 2×2 under model I

Assume that the within-block dependence structure is not necessarily the same for each block. Let Λ_i be the within-block dependence matrix for block i, and let $\underline{l} = \frac{1}{2}(1, -1, -1, 1)'$. Then if $\vartheta = \underline{l}' \Lambda_i \underline{l}$ does not depend on i, the C-matrix under gls is equal to $1/\vartheta$ times the C-matrix under ols. Therefore a design is optimal under gls if and only if it is optimal under ols with $V = I_{4b}$.

As seen in section 5.1.3, under ols with $V = I_{4b}$, a BNRC design is universally optimal; that is a design with blocks of type $\begin{bmatrix} ab \\ ba \end{bmatrix}$ for each unordered pair of treatments. This leads to the following theorem.

Theorem 5.13   (Uddin & Morgan, 1997a)
If $\vartheta = \underline{l}' \Lambda_i \underline{l}$ does not depend on i, then a design with blocks of type $\begin{bmatrix} ab \\ ba \end{bmatrix}$ for each unordered pair of treatments is universally optimal over $\mathcal{D}$ under gls for model I.   ∎

5.3.2.2   Results for the AR(1)*AR(1) process

Rather than considering the elements of Ω^* as in Martin & Eccleston (1991, 1993) and Martin (1998), Uddin & Morgan (1997a) give the C-matrices under the four models in terms of the following matrices and vectors.

The neighbour count matrices are the $t \times t$ matrices, N^C, N^D, N_I^R and N^R, where

$(N^C)_{v_1, v_2}$ is the number of plots containing treatments v_1 and v_2 as lag (0, 1) neighbours (i.e. column neighbours) – see Figure 3.1;

$(N^D)_{v_1, v_2}$ is the number of plots containing treatments v_1 and v_2 as lag (1, 1) or lag(-1, 1) neighbours (i.e. diagonal neighbours);

$(N_I^R)_{v_1, v_2}$ is the number of interior plots containing treatments v_1 and v_2 as lag (1, 0) neighbours (i.e. row neighbours);

$\left(N^R\right)_{\nu_1,\nu_2}$ is the number of plots containing treatments ν_1 and ν_2 as lag $(1, 0)$ neighbours;

C_E^O is the C-matrix under ols for the design with $2b$ blocks of size 2, given by the end rows of the b blocks;

C_I^O is the C-matrix under ols for the design with $(p-2)b$ blocks of size 2, given by the interior rows of the b blocks;

$\underline{r}_{Eih}$ is the t-vector whose ν^{th} element is the replication of treatment ν in the two end plots of column h of the ith block;

$\underline{r}_{Iih}$ is the t-vector whose ν^{th} element is the replication of treatment ν in the $(p-2)$ interior plots of column h of the ith block;

R_E is the $t \times t$ diagonal matrix whose ν^{th} diagonal element is the replication total of treatment ν in the $4b$ end plots of the b blocks.

For example, consider the following design consisting of one block, with $t = 4$.

1	4
3	1
1	1
2	2
1	2

D5.14

Here

$$N^C = \begin{pmatrix} 2 & 3 & 2 & 1 \\ 3 & 2 & 0 & 0 \\ 2 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}, \quad N^D = \begin{pmatrix} 4 & 3 & 1 & 0 \\ 3 & 2 & 0 & 0 \\ 1 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix},$$

$$N_I^R = \begin{pmatrix} 2 & 0 & 1 & 0 \\ 0 & 2 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad N^R = \begin{pmatrix} 2 & 1 & 1 & 1 \\ 1 & 2 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix},$$

$$r_{E11} = \begin{pmatrix} 2 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad r_{E12} = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 1 \end{pmatrix}, \quad r_{I11} = \begin{pmatrix} 1 \\ 1 \\ 1 \\ 0 \end{pmatrix}, \quad r_{I12} = \begin{pmatrix} 2 \\ 1 \\ 0 \\ 0 \end{pmatrix}$$

and $\quad R_E = \begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$

For model IV, the C-matrix is

$$C = (1 + \rho_{0,1}^2)X'X - \rho_{0,1}^2 R_E + \rho_{0,1}\rho_{1,0}N^D - \rho_{0,1}N^C - \rho_{1,0}N^R - \rho_{0,1}^2\rho_{1,0}N_I^R$$

$$- \frac{(1 - \rho_{0,1})(1 - \rho_{1,0})}{2\nmid(\rho_{0,1}, p_1)}\sum_{i=1}^{b}V_iV_i', \tag{5.20}$$

where

$$\nmid(\rho_{0,1}, p_1) = 2\rho_{0,1} + p_1(1 - \rho_{0,1})$$

and

$$V_i = r_{Ei1} + r_{Ei2} + (1 - \rho_{0,1})(r_{Ii1} + r_{Ii2}).$$

It is shown that if a design is optimal under model II (IV) and satisfies

$$r_{Ii1} = r_{Ii2} \quad \text{and} \quad r_{Ei1} = r_{Ei2} \quad \text{for all } i \tag{5.21}$$

then the design is also optimal under model I (III). Condition (5.21) means that for any block the treatments in the end (interior) plots of the first column are a permutation of the treatments in the end (interior) plots of the second column of that block.

The rest of this section gives the optimality results from Uddin & Morgan (1997a). The proofs are omitted here. The design construction is as described in Martin (1998), where the blocks are of the same type. To give a completely symmetric C-matrix: for types with only 2 symbols, each unordered pair of treatments gives a block, and for types with more than 2 symbols the SBA construction method is used. This means that $b = \frac{1}{2}ct(t-1)$ for an integer c.

Definition 5.2
Designs D5.15 to D5.20, with blocks of the following type, are now defined.

D5.15	D5.16	D5.17 †	D5.18 ‡	D5.19 ‡	D5.20

$\begin{bmatrix} ab \\ ba \\ ab \\ ba \\ \vdots \end{bmatrix}$ $\begin{bmatrix} ab \\ ab \\ \vdots \\ ab \end{bmatrix}$

D5.17: $\left.\begin{matrix} ab \\ ba \\ \vdots \\ ab \end{matrix}\right\} n_1 \text{ rows}$ $\left.\begin{matrix} ca \\ ac \\ \vdots \\ ca \end{matrix}\right\} n_2 \text{ rows}$ $\left.\begin{matrix} bc \\ cb \\ \vdots \\ bc \end{matrix}\right\} n_3 \text{ rows}$

D5.18: $\left.\begin{matrix} ab \\ ab \\ \vdots \\ ab \end{matrix}\right\} \frac{1}{2}p_1 \text{ rows}$ $\left.\begin{matrix} ba \\ ba \\ \vdots \\ ba \end{matrix}\right\} \frac{1}{2}p_1 \text{ rows}$

D5.19: $\left.\begin{matrix} ab \\ ab \\ \vdots \\ ab \end{matrix}\right\} \frac{1}{2}p_1 \text{ rows}$ $\left.\begin{matrix} ac \\ bc \\ ba \\ \vdots a \end{matrix}\right\} \frac{1}{2}p_1 \text{ rows}$ $\left.\begin{matrix} b\colon \\ ba \end{matrix}\right\}$

D5.20: $\begin{bmatrix} ab \\ ba \\ cd \\ dc \\ \vdots \end{bmatrix}$

† n_1, n_2, n_3 are odd, such that $n_1 + n_2 + n_3 = p_1$.
‡ for p_1 even. ∎

5.3.2.2.1 Optimal designs under model II

Theorem 5.14   (Uddin & Morgan, 1997a)
Under model II for the AR(1)*AR(1) process, D5.15 is universally optimal over $\mathcal{D}$ when $\rho_{0,1} > 0$, otherwise D5.16 is universally optimal. ∎

5.3.2.2.2 Optimal designs under model I
When p_1 is even, the condition in (5.21) is satisfied for D5.15. This gives the following theorem.

Theorem 5.15   (Uddin & Morgan, 1997a)

Under model I for the AR(1)*AR(1) process, for even $p_1 \geq 4$, D5.15 is
universally optimal over $\mathcal{D}$ when $\rho_{0,1} > 0$.   ■

Theorem 5.16   (Uddin & Morgan, 1997a)

For model I under the AR(1)*AR(1) process, when $\rho_{0,1} > 0$ and p_1 is odd,
D5.15 is universally optimal over $\mathcal{D}$ if

$$p_1 \geq \frac{(1 - 2\rho_{0,1})(1 + 3\rho_{0,1})}{2\rho_{0,1}(1 - \rho_{0,1})},$$

otherwise D5.17 is universally optimal.   ■

Theorem 5.17   (Uddin & Morgan, 1997a)

For model I under the AR(1)*AR(1) process, when $\rho_{0,1} < 0$ and p_1 is even,
D5.18 is universally optimal over $\mathcal{D}$ if

$$p_1 \leq -\frac{\left\{ 2\rho_{0,1}^2 + 3(1 - \rho_{0,1})^3 \right\}}{\left\{ \rho_{0,1}(1 - \rho_{0,1}) \right\}},$$

otherwise D5.19 is universally optimal.   ■

For p_1 odd and $\rho_{0,1} < 0$ optimal types are not given, but it is noted that more
than two types can be optimal.

5.3.2.2.3 Optimal designs under model IV

For model IV, only $\rho_{0,1}, \rho_{1,0} > 0$ was considered. The following theorems were given.

Theorem 5.18 (Uddin & Morgan, 1997a)

For model IV under the AR(1)*AR(1) process, when $\rho_{0,1}, \rho_{1,0} > 0$ the binary block design (constructed using SBAs) is universally optimal over $\mathcal{D}$ if

$$\frac{(1-\rho_{0,1})(1-\rho_{1,0})}{4\rho_{0,1}\rho_{1,0}} \geq 1 \quad \text{for } p_1 = 2,$$

$$\frac{(1-\rho_{0,1})^2(1+\rho_{1,0})}{2(1+\rho_{0,1})\rho_{1,0}} \geq 1 \quad \text{for } p_1 = 3,$$

$$\frac{(1-\rho_{0,1})^3(1-\rho_{1,0}) - 4\rho_{0,1}^2\rho_{1,0}}{2\rho_{0,1}(1-\rho_{0,1})\rho_{1,0}} \geq p_1 \quad \text{for } p_1 \geq 4. \qquad \blacksquare$$

Theorem 5.19 (Uddin & Morgan, 1997a)

For model IV under the AR(1)*AR(1) process, when $\rho_{0,1}, \rho_{1,0} > 0$ the design D5.15 is universally optimal over $\mathcal{D}$ if

$$\frac{8\rho_{0,1}\rho_{1,0}}{(1-\rho_{0,1})(1-\rho_{1,0})} \geq f(\rho_{0,1}, p_1) \quad \text{for even } p_1, \qquad (5.22)$$

$$\frac{8\rho_{0,1}\rho_{1,0}}{(1-\rho_{0,1})(1-\rho_{1,0})} + \frac{(1-\rho_{0,1})^2}{f(\rho_{0,1}, p_1)} \geq f(\rho_{0,1}, p_1) \quad \text{for odd } p_1. \qquad \blacksquare$$

Theorem 5.18 and Theorem 5.19 cover small and large combinations of ($\rho_{0,1}$, $\rho_{1,0}$). For other values, an integer programming problem is given by Uddin & Morgan (1997a), which can be solved on a computer to give the optimal type given the values of $\rho_{0,1}$, $\rho_{1,0}$ and p_1. Uddin & Morgan (1997a, page 1201), solve this integer programming problem for $p_1 = 3, 4, \dots, 10, 15, 20$ and $\rho_{1,0} = \rho_{0,1} = 0.1, 0.2, \dots, 0.9$. For $\rho_{0,1} \geq 0.6$ design D5.15 is optimal.

5.3.2.2.4 Optimal designs under model III

As for model IV, only $\rho_{0,1}, \rho_{1,0} > 0$ were considered for model III. When p_1 is even, the condition in (5.21) is satisfied for D5.15. This gives Theorem 5.20.

Theorem 5.20 (Uddin & Morgan, 1997a)

Under model III for the AR(1)*AR(1) process, for even p_1, D5.15 is universally optimal over $\mathcal{D}$ if the condition in (5.22) is satisfied. ∎

Although the optimality of other types is not shown for model III, design D5.20, which is likely to be highly efficient, is considered for p_1 even.

Under the AR(1)*AR(1) process, when $\rho_{0,1}, \rho_{1,0} > 0$, design D5.20 is likely to be highly efficient for model III with even $p_1 \geq 4$ if

$$\frac{2(1-\rho_{0,1})^2(1-\rho_{1,0}) - 2\rho_{0,1}^2\rho_{1,0}}{\rho_{0,1}(1-\rho_{0,1})\rho_{1,0}} > p_1 \quad \text{for } p_1 = 4,$$

$$\frac{(1-\rho_{0,1})^2(1-\rho_{1,0})(2-\rho_{0,1}) - 2\rho_{0,1}^2\rho_{1,0}}{\rho_{0,1}(1-\rho_{0,1})\rho_{1,0}} > p_1 \quad \text{for } p_1 = 6,$$

$$\frac{2(1-\rho_{0,1})^3(1-\rho_{1,0}) - 2\rho_{0,1}^2\rho_{1,0}}{\rho_{0,1}(1-\rho_{0,1})\rho_{1,0}} > p_1 \quad \text{for } p_1 \geq 8.$$

An integer programming problem, which yields efficient designs, is given in Uddin & Morgan (1997a) for model III. The solutions to this are given for the same values of p_1, $\rho_{0,1}$ and $\rho_{1,0}$ as for model IV (see section 5.3.2.2.3). The corresponding efficiency lower bounds are also given, and are greater than or equal to 0.997 for the cases considered. For the range of the p_1 covered, D5.15 is optimal for $\rho_{0,1} \geq 0.6$.

5.3.2.3   *Some corrections*

Some corrections to Uddin & Morgan (1997a) are given in this section.

The values of $T_1'T_1$ in Uddin & Morgan (1997a, page 1197) are incorrect, although the results in the theorems are unaffected. The corrected values of $T_1'T_1$, in the notation of Uddin & Morgan (1997a), are given in Table 5.4. For a definition of T_1, and cases (i') and (i''), the reader is referred to Uddin & Morgan (1997a).

Table 5.4
$T_1'T_1$ for cases (i') and (i'').

n_1	n_2	n_3	$T_1'T_1$ for	
			case (i')	case (i'')
even	even	odd	$2(1+\alpha+\alpha^2)$	$2(1+\alpha)^2$
even	odd	even	$2(1+2\alpha^2)$	$2(1+3\alpha^2)$
odd	even	even	$2(1+\alpha+\alpha^2)$	$2(1+\alpha)^2$
odd	odd	odd	$2(2+\alpha^2)$	$2(3+\alpha^2)$

Also, Table 1 in Uddin & Morgan (1997a, page 1201) has two incorrect entries. In the notation of Uddin & Morgan (1997a), the entry for $p=9$ and $\alpha=0.2$ should be (5,2,1), and the entry for $p=20$ and $\alpha=0.4$ should be (3,7,6).

5.3.2.4 Discussion

In the 'Summary discussion' section of Uddin & Morgan (1997a) it is noted that

- D5.15, which is a BNRC design is optimal or efficient for at least some $(\rho_{0,1}, \rho_{1,0})$ for all four models;

- binary block designs are only optimal for model IV, and then only for small $(\rho_{0,1}, \rho_{1,0})$ and small p_1;

- under models I and II binary rows are required, and under model III, for small correlations, binary columns are needed;

- although the designs given here have a large number of blocks

    knowledge of maximal trace blocks will certainly be required at the logical next step: determination of optimal designs which, due to smaller numbers of blocks, cannot enjoy complete symmetry.

5.3.3 Uddin & Morgan (1997b)

Under model IV and gls, Uddin & Morgan (1997b) consider the AR(1)*AR(1) process and the 3-parameter CAR(2) process for blocks of size $p_1 \times 2$. For the AR(1)*AR(1) process, $\rho_{0,1}, \rho_{1,0} \geq 0$ is assumed, and for the 3-parameter CAR(2) process it is assumed that $\zeta_{0,1}, \zeta_{1,0}, \zeta_{1,1} \geq 0$.

The off-diagonal elements of Ω^* are given for the two processes. However, they are slightly incorrect. For the AR(1)*AR(1) process, the corrections are not given here specifically for blocks of size $p_1 \times 2$. However, for the general case where blocks are of size $p_1 \times p_2$ the elements of Ω^* are given in section 8.2.1. For the 3-parameter CAR(2) process, the off-diagonal elements for given $p_1 \geq 3$ and $p_1 = 2$ are actually for $p_1 \geq 4$ and $p_1 = 3$, respectively. Therefore conditions for when all the off-diagonal elements are non-positive (i.e. when the condition in (5.9) is true) are also incorrect. The corrected conditions are as follows.

For the AR(1)*AR(1) process,

$$\left(\Omega^*\right)_{l_1 l_2} \leq 0 \quad \forall \ l_1 \neq l_2 \quad \Leftrightarrow$$

$$\begin{cases} \rho_{0,1}\rho_{1,0} - \dfrac{(1-\rho_{1,0})(1-\rho_{0,1})^3}{2\phi(\rho_{0,1},p_1)} \leq 0 & \text{for } p_1 \geq 4, \\[3mm] \rho_{0,1}\rho_{1,0} - \dfrac{(1-\rho_{1,0})(1-\rho_{0,1})^{p_1-1}}{2\phi(\rho_{0,1},p_1)} \leq 0 & \text{otherwise,} \end{cases} \qquad (5.23)$$

where $\phi(\rho_{0,1},p_1)$ is as defined in section 5.3.2.2.

For the 3-parameter CAR(2) process,

$$\left(\Omega^*\right)_{l_1 l_2} \leq 0 \quad \forall \ l_1 \neq l_2 \quad \Leftrightarrow$$

$$\begin{cases} 1-\zeta_{1,0}-2\zeta_{0,1}-2\zeta_{1,1} > 0 & \text{for } p_1 \geq 4, \\[3mm] 1-\zeta_{1,0}-2\zeta_{0,1}-2\zeta_{1,1} > \dfrac{-\min(\zeta_{0,1},\zeta_{1,1})(6-6\zeta_{1,0}-8\zeta_{0,1}-8\zeta_{1,1})}{(1-\zeta_{1,0}-\zeta_{0,1}-\zeta_{1,1})} & \text{for } p_1 = 3, \\[3mm] \text{any } \zeta_{1,0}, \zeta_{0,1}, \zeta_{1,1} & \text{for } p_1 = 2. \end{cases} \qquad (5.24)$$

These corrections were pointed out by Dr. R. J. Martin and the author, and the conditions (5.23) and (5.24) appear in the corrections to Uddin & Morgan (1997b).

Optimality conditions for binary designs are given for the two processes. Let the *corner* and *interior* designs be the designs formed from the end and interior plots, respectively.

Theorem 5.21   (Uddin & Morgan, 1997b)

A binary design

i)   that is neighbour balanced (i.e. each distinct pair of treatments occur equally often as row, column and diagonal neighbours);

ii)   that is a balanced block design;

iii)   for which the interior design is a balanced block design when $p_1 \geq 3$;

iv)   for which the corner design is a balanced block design when $p_1 \geq 3$;

v)   for which the end rows give a balanced block design when $p_1 \geq 4$,

is universally optimal for model IV under the AR(1)*AR(1) process among all binary designs in $\mathcal{D}$, and among all designs in $\mathcal{D}$ if the condition in (5.23) is true. ∎

Theorem 5.22   (Uddin & Morgan, 1997b)
A binary design that satisfies (i) to (iv) of Theorem 5.21 is universally optimal for model IV under the 3-parameter CAR(2) process among all binary designs in $\mathcal{D}$, and among all designs in $\mathcal{D}$ if the condition in (5.24) is true. ∎

The two processes considered here are described by Uddin & Morgan (1997b) as 'distinctly different', however, as pointed out in the review of their paper by Martin (1999), both processes are second order reflection symmetric conditional autoregressions with non-negative row and column dependence parameters. Therefore they have very similar Λ^{-1} matrices and so it is not surprising that the optimality conditions are also similar.

SBAs satisfy both theorems, but designs that satisfy these theorems with a smaller number of blocks may exist. An example from Uddin & Morgan (1997b) for $t = 12$ and $p_1 = 3$ has $b = \frac{1}{2}t(t-1) = 66$ blocks. Labelling the treatments 0, 1, ... , 10, ∞, this design is constructed by cyclically developing 6 initial blocks by adding 1 modulo 11 to each treatment label, except for the treatment label ∞, which is invariant. The 6 initial blocks are:

0	5		0	9		0	3		∞	1		∞	1		1	9
9	10	,	3	7	,	1	6	,	4	2	,	8	5	,	∞	5
4	3		5	1		9	4		3	5		4	0		3	4

D5.21

As an illustration of the cyclical development, the following 11 blocks are cyclically developed from the 4th initial block.

∞	1		∞	2		∞	3		∞	4		∞	5		∞	6
4	2	,	5	3	,	6	4	,	7	5	,	8	6	,	9	7
3	5		4	6		5	7		6	8		7	9		8	10

∞	7		∞	8		∞	9		∞	10		∞	0
10	8	,	0	9	,	1	10	,	2	0	,	3	1
9	0		10	1		0	2		1	3		2	4

Uddin & Morgan (1997b) also give another example for $t = 8$ and $p_1 = 4$ which has $b = \frac{1}{4}t(t-1) = 14$ blocks. Martin (1999) notes that this example is a SSENR design, and so is universally optimal over all binary designs in $\mathcal{D}$ for all reflection symmetric dependence structures. In fact, the design D5.21 is also a SSENR design.

In justifying their restriction to binary designs, Uddin and Morgan (1997b) comment that non-binary designs are unlikely to be used in practice when $k \leq t$. However, they also note that for the AR(1)*AR(1) process, considerable gains can be obtained by using a non-binary design, and that the parameter range for which the binary design is optimal is limited. For the 3-parameter CAR(2) process, it is noted that the parameter range for which the binary design is optimal is much larger, and there is little gain in using a non-binary design.

The designs satisfying Theorem 5.21 and Theorem 5.22 have a large number of blocks for t not small. However, the optimality conditions in these theorems have been used to suggest the structure of efficient designs with a smaller number of blocks. For blocks of size $\frac{1}{2}t \times 2$ and $\frac{1}{2}(t-1) \times 2$ for t even and odd, respectively, reasonably efficient cyclic binary designs with $t-1$ and t blocks, respectively, are given in Uddin & Morgan (1997b) for $t \leq 30$.

5.3.4   Morgan & Uddin (1991)

Morgan & Uddin (1991) construct optimal designs for correlated errors on b toruses of size $p_1 \times p_2$ under gls. The torus equivalent of model IV is assumed. The within-torus error process is the torus version of the CAR(2) process (see section 2.3.3.3).

A *planar version* of a torus design is obtained by cutting the torus between any two rows and any two columns. Clearly the planar version of a design on b toruses is a NRC design with b blocks. The planar versions of the optimal torus designs given by Morgan & Uddin (1991) are shown to have very good efficiency. The CAR(2) with $\zeta_{0,1} = \zeta_{1,0}$ and $\zeta_{1,1} = \zeta_{-1,1}$ is used for the efficiency calculations.

5.3.5   Uddin (2000)

Uddin (2000) finds optimal designs under gls for correlated errors on b cylinders each of size $p_1 \times p_2$. The cylinder equivalent of model IV is assumed. The dependence structure is the cylinder version of the CAR(2) with $\zeta_{1,1} = \zeta_{-1,1}$ (see section 2.3.3.3).

Assuming that the rows are circular, a planar version of a cylindrical design is obtained by cutting the cylinders between any two columns. As in Morgan & Uddin (1991), efficiency calculations for the planar versions of some of the optimal cylinder designs, using the CAR(2) process with $\zeta_{1,1} = \zeta_{-1,1}$, show that these planar designs are very efficient.

6 Optimal nested row-column designs for blocks of size 2×2 under dependence

In this chapter, NRC designs with blocks of size 2×2 are examined under models I to IV. The results in this chapter appear in Chauhan & Martin (1999) and Chauhan (1998). Section 6.1 provides an introduction and preliminary material. Optimality results under gls and ols are given in sections 6.2 and 6.3, respectively.

6.1 Introduction and preliminaries

6.1.1 Introduction

As seen in chapter 5, there has been considerable interest recently in optimal NRC designs under dependence. Martin & Eccleston (1993) gave some general results under model IV – given as Theorem 5.11 and Theorem 5.12 here. Specific results for blocks of size 2×2 were also obtained. Uddin & Morgan (1997a) gave optimality results for a very general dependence structure for blocks of size 2×2 under model I (see Theorem 5.13). For blocks of size $p_1 \times 2$, they considered the AR(1)*AR(1) process under models I to IV and gls. However, some of their results are for positive correlation values only.

As seen in section 5.1, 2×2 designs, under model I when errors are uncorrelated and all treatment comparisons are of equal interest, were considered by Singh & Dey (1979), Ipinyomi & John (1985) and Bagchi *et al.* (1990). Also, John & Williams (1995, section 5.9) give an example of a cyclic 2×2 design with $t = 7$. Kachlicka & Mejza (1995) and Leeming (1997) considered the 2×2 layout when control versus test treatment contrasts are of interest.

For blocking to be effective, blocks should consist of relatively homogeneous plots. Using blocks consisting of only two rows and two columns should produce good homogeneity. Although designs that are used, for example, in variety trials and plant breeding experiments usually have more than two rows and columns, the results given here may provide some insight into the structure of efficient designs for larger-sized blocks.

6.1.2   Dependence structure

Assume that blocks are of size 2×2. Let $(\Lambda)_{i,j} = u_{i,j}$. If Λ is assumed to be symmetric there are at most 10 distinct parameters in Λ. Under centro-symmetry, Λ is given as the expression in (5.11) in section 5.3.1, which has at most 6 distinct parameters. This simplifies to Λ having at most 4 and 3 distinct parameters under reflection symmetry and complete symmetry, respectively. Under stationarity, taking Λ to be a within-block correlation matrix, the diagonal elements of Λ are equal to 1. Here the most general form of Λ has Λ centro-symmetric with at most 4 distinct correlations (excluding $\rho_{0,0} = 1$), as given by the expression in (5.12). Under reflection symmetry, the 2 within-diagonal correlations $\rho_{1,1}$ and $\rho_{-1,1}$ are equal, so Λ has at most 3 distinct correlations (excluding $\rho_{0,0} = 1$), and is of the form

$$\Lambda = \begin{pmatrix} 1 & \rho_{1,0} & \rho_{0,1} & \rho_{1,1} \\ \rho_{1,0} & 1 & \rho_{1,1} & \rho_{0,1} \\ \rho_{0,1} & \rho_{1,1} & 1 & \rho_{1,0} \\ \rho_{1,1} & \rho_{0,1} & \rho_{1,0} & 1 \end{pmatrix}. \tag{6.1}$$

The following processes are special cases of the reflection symmetric process under stationarity.

(i)   completely symmetric process (i.e. $\rho_{1,0} = \rho_{0,1}$);

(ii)   separable process (i.e. $\rho_{1,1} = \rho_{1,0}\rho_{0,1}$). This is equivalent to the AR(1)*AR(1) and NN(1)*NN(1) processes when blocks are of size 2×2;

(iii) *nearest neighbour* process, which has $\rho_{1,1} = 0$;

(iv)   completely symmetric and separable process (i.e. $\rho_{1,0} = \rho_{0,1}$ and $\rho_{1,1} = \rho_{1,0}^2$).

In section 2.3, it is stated that the true dependence structure is not usually known exactly, and so simple structures are often considered. Also, the conclusion of Martin (1986) (see section 2.4) suggests that a reasonable approach is to specify the correlation by a small number of parameters. With this in mind, Λ is assumed to be reflection symmetric here. Reflection symmetry includes several interesting special cases, as seen above, and is a more general dependence structure than considered in Uddin & Morgan (1997a) and Martin & Eccleston (1993), excepting the result in Theorem 5.13 in section 5.3.2.1, and the result given as (5.15) in section 5.3.1.1. Recall that Theorem 5.13 gives the optimal design for the general case where the within-block dependence is not necessarily the same for each block, and the result (5.15) compares two types under ols when Λ is centro-symmetric.

Definition 6.1
The matrix W, which represents either Ω^{*} or $\Omega^{*}\Lambda\Omega^{*}$ has the following form

$$
\begin{pmatrix}
w_1 & w_2 & w_3 & w_4 \\
w_2 & w_1 & w_4 & w_3 \\
w_3 & w_4 & w_1 & w_2 \\
w_4 & w_3 & w_2 & w_1
\end{pmatrix},
$$

with $w_1 > 0$ and $\sum w_i = 0$. $\blacksquare$

Definition 6.2
The correlation parameters $\rho_{1,0}$, $\rho_{0,1}$ and $\rho_{1,1}$ are relabelled as ρ_2, ρ_3 and ρ_4, respectively. The subscripts have been chosen for consistency with the elements of W so that optimality results can be given succinctly. $\blacksquare$

Definition 6.3
The eigenvalues of Λ are

$$\lambda_1 = 1 + \rho_2 + \rho_3 + \rho_4, \qquad \lambda_2 = 1 + \rho_2 - \rho_3 - \rho_4,$$

$$\lambda_3 = 1 - \rho_2 + \rho_3 - \rho_4, \qquad \lambda_4 = 1 - \rho_2 - \rho_3 + \rho_4, \qquad \blacksquare$$

It is assumed that Λ is positive definite, so these eigenvalues are positive. Hence, the valid parameter space is the interior of a tetrahedron – see Figure 6.1. For the nearest neighbour and completely symmetric special cases, the valid parameter spaces, which are planar sections of this tetrahedron, are $|\rho_2| + |\rho_3| < 1$ and $2|\rho_2| < (1 + \rho_4) < 2$, respectively. For the separable structure, the constraints are $|\rho_2|, |\rho_3| < 1$, and for the completely symmetric separable process, the constraint is $|\rho_2| < 1$.

Figure 6.1
Valid parameter space of (ρ_2, ρ_3, ρ_4) for blocks of size 2×2 under a stationary reflection symmetric dependence structure.
$\lambda_1 = 0$, $\lambda_2 = 0$, $\lambda_3 = 0$ and $\lambda_4 = 0$ correspond to the planes which pass through the vertices (B, C, D), (A, B, D), (A, B, C) and (A, C, D), respectively.
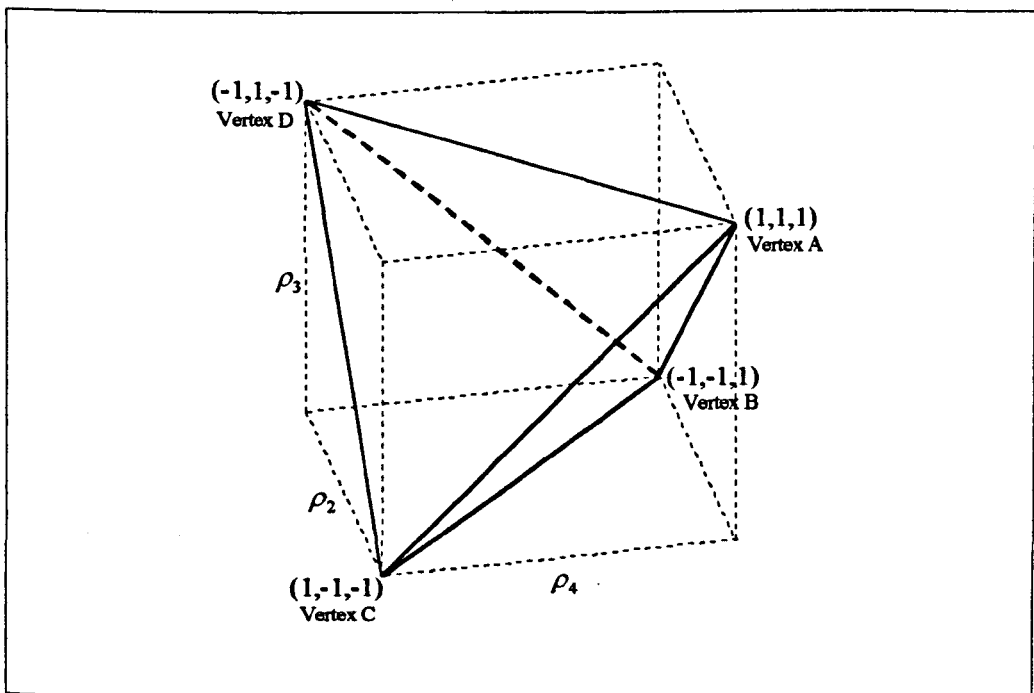
6.1.3 A mixed effects model with uncorrelated errors

Consider a mixed effects model with uncorrelated errors, random row and column effects, and fixed block and treatment effects (cf. the model of Leeming (1997), which has random row, column and block effects). It is now shown that for blocks of size 2×2, this mixed effects model is equivalent to

model IV under a special case of reflection symmetry. Using the same notation as for model (4.1), let the mixed effects model be

$$y = X\underline{\tau} + Z_1\underline{\beta} + Z_2\underline{\gamma} + Z_3\underline{\delta} + \underline{\varepsilon}, \tag{6.2}$$

with

$$E(\underline{\varepsilon}) = \underline{0}_m, \quad \text{var}(\underline{\varepsilon}) = I_m\sigma_1^2,$$

$$E(\underline{\gamma}) = E(\underline{\delta}) = \underline{0}_{2b}, \quad \text{var}(\underline{\gamma}) = I_{2b}\sigma_2^2, \quad \text{var}(\underline{\delta}) = I_{2b}\sigma_3^2$$

and $\underline{\varepsilon}$, $\underline{\gamma}$ and $\underline{\delta}$ are mutually uncorrelated.

Here

$$E(\underline{y}) = X\underline{\tau} + Z_1\underline{\beta}, \tag{6.3}$$

and

$$\begin{aligned}
\text{var}(\underline{y}) &= Z_2\,\text{var}(\underline{\gamma})Z_2' + Z_3\,\text{var}(\underline{\delta})Z_3' + \text{var}(\underline{\varepsilon}) \\
&= Z_2Z_2'\sigma_2^2 + Z_3Z_3'\sigma_3^2 + I_m\sigma_1^2 \\
&= (I_b \otimes I_2 \otimes J_2)\sigma_2^2 + (I_b \otimes J_2 \otimes I_2)\sigma_3^2 + (I_b \otimes I_2 \otimes I_2)\sigma_1^2 \\
&= I_b \otimes \Lambda_1,
\end{aligned}$$

where

$$\Lambda_1 = (I_2 \otimes J_2)\sigma_2^2 + (J_2 \otimes I_2)\sigma_3^2 + (I_2 \otimes I_2)\sigma_1^2$$

$$= \begin{pmatrix}
\sigma_1^2 + \sigma_2^2 + \sigma_3^2 & \sigma_2^2 & \sigma_3^2 & 0 \\
\sigma_2^2 & \sigma_1^2 + \sigma_2^2 + \sigma_3^2 & 0 & \sigma_3^2 \\
\sigma_3^2 & 0 & \sigma_1^2 + \sigma_2^2 + \sigma_3^2 & \sigma_2^2 \\
0 & \sigma_3^2 & \sigma_2^2 & \sigma_1^2 + \sigma_2^2 + \sigma_3^2
\end{pmatrix}.$$

Recall that for model IV under a stationary reflection symmetric process, $E(\underline{y})$ is the same as (6.3), and $\text{var}(\underline{y}) = \sigma^2(I_b \otimes \Lambda)$, where Λ is given as (6.1). It is clear that $\Lambda\sigma^2 = \Lambda_1$ when

$$\sigma^2\rho_i = \sigma_i^2 \quad \text{for } i = 2, 3;$$

$$\rho_4 = 0 \quad \text{and} \quad \sigma^2(1 - \rho_2 - \rho_3) = \sigma_1^2.$$

The variance components of the mixed effects model are positive and so $\rho_2, \rho_3 > 0$ is required. Note that $1 - \rho_2 - \rho_3 > 0$ since Λ is positive definite.

Therefore model IV under reflection symmetry with $\rho_4 = 0$ and $\rho_2, \rho_3 > 0$ is equivalent to this mixed effects model.

6.1.4 Design construction

Recall from Theorem 5.12 in section 5.3.1.2 (Martin & Eccleston, 1993) that for blocks consisting of $k \leq t$ plots under a reflection symmetric dependence structure, a binary design called a SSENR design is, under gls, universally optimal among all binary designs in $\mathcal{D}$, and is universally optimal among all designs in $\mathcal{D}$ if and only if all the off-diagonal elements of Ω^* are non-positive. Here, $\mathcal{D}$ is the set of all connected designs with t treatments and b blocks of size 2×2. Under ols, the SSENR design is weakly universally optimal among all balanced block designs in $\mathcal{D}$ (Theorem 5.11). A SSENR design with $b = \frac{1}{4}ct(t\text{-}1)$ exists for certain integers c, including $c = 1$ for certain t. SBAs are also SSENR designs, for which the minimum values of c which may be possible are 2 and 4 for t odd and t even, respectively. Sometimes a SSENR design can be constructed from a quarter of the columns of a SBA (see, for example, D5.12)

As in Martin (1998) assume that each block is of the same type with $s \leq k$ different symbols. For suitable b, designs are constructed using s rows of a SBA of length min(t, k) on t symbols. For example, when $t = 5$, the binary (SSDEN) design D2.1 (in section 2.2) is constructed from the first 4 rows of the SBA in Figure 3.2c; this is equivalent to the SDEN design D5.8 (in section 5.2.5) for one-dimensional blocks consisting of 4 plots. A non-binary design of type $\begin{bmatrix} a & a \\ b & b \end{bmatrix}$ can be constructed from the first 2 rows of this SBA to obtain the following design, which is equivalent to the one-dimensional design D5.9.

$$\begin{array}{|c|c|} \hline 1 & 1 \\ \hline 2 & 2 \\ \hline \end{array}, \begin{array}{|c|c|} \hline 1 & 1 \\ \hline 4 & 4 \\ \hline \end{array}, \begin{array}{|c|c|} \hline 2 & 2 \\ \hline 3 & 3 \\ \hline \end{array}, \begin{array}{|c|c|} \hline 2 & 2 \\ \hline 5 & 5 \\ \hline \end{array}, \begin{array}{|c|c|} \hline 3 & 3 \\ \hline 1 & 1 \\ \hline \end{array},$$

$$\begin{array}{|c|c|} \hline 3 & 3 \\ \hline 4 & 4 \\ \hline \end{array}, \begin{array}{|c|c|} \hline 4 & 4 \\ \hline 2 & 2 \\ \hline \end{array}, \begin{array}{|c|c|} \hline 4 & 4 \\ \hline 5 & 5 \\ \hline \end{array}, \begin{array}{|c|c|} \hline 5 & 5 \\ \hline 1 & 1 \\ \hline \end{array}, \begin{array}{|c|c|} \hline 5 & 5 \\ \hline 3 & 3 \\ \hline \end{array}. \qquad \text{D6.1}$$

For designs constructed in this way, C and var($\underline{q}$) are completely symmetric. Therefore, from the results in sections 2.5.4 and 5.2.4,

Φ_p-value $= a_2 / a_1^2$ for all $p \geq 0$,

where

$a_1 = bc_{\Omega^*} / (t-1)$ and $a_2 = bc_{\Omega^*\Lambda\Omega^*} / (t-1)$

In the rest of this chapter references to the Φ_p-value are for all $p \geq 0$. The Φ_p-value simplifies to

Φ_p-value $= c_{\Omega^*\Lambda\Omega^*} / c_{\Omega^*}^2$,

and under gls simplifies further to

Φ_p-value $= 1/c_{\Omega^*}$

since $\Omega^*\Lambda\Omega^* = \Omega^*$. Let the Φ_p-value of an optimal design be called the Φ_p^*-value. Then the Φ_p-efficiency of a design with Φ_p-value is

$$\Phi_p\text{-efficiency} = \frac{\left(\Phi_p^* \text{ - value}\right)}{\left(\Phi_p \text{ - value}\right)}$$

(see section 2.5.6).

As in section 2.5, let $\mathcal{D}_1$ be the set of designs in $\mathcal{D}$ for which C and var($\underline{q}$) are completely symmetric, and let $\mathcal{D}^*$ be the set of designs in $\mathcal{D}$ which have C-matrix completely symmetric under ols. Throughout this chapter, under gls, an optimal design will refer to a design that is universally optimal over $\mathcal{D}$. Under ols, an optimal design will mean a design that is universally optimal over $\mathcal{D}_1$ and weakly universally optimal over $\mathcal{D}^*$.

For $k = 4$ and $t \geq 4$, the list of 11 different types from Martin (1998) when Ω^* or $\Omega^*\Lambda\Omega^*$ are centro-symmetric, given as Table 5.2, is reduced to the 9 types in Table 6.1, since, in the notation of Table 5.2, $w_{1,1} = w_{2,2}$ and $w_{1,4} = w_{2,3}$ here. In Table 6.1 these 9 types are re-labelled as types 0 to 8. This re-labelling means that for types i and $i+3$ ($i = 2, 3, 4$) the off-diagonal element

of W in the expression for c_W is w_i, and so optimality results can be given succinctly. Clearly for $t = 3$ and $t = 2$, only types 0 to 7 and 0 to 4, respectively, are possible.

Table 6.1
List of types and expressions for c_W for blocks of size 2×2 under reflection symmetry.

Type no.	type	(n_2, n_3, n_4)	c_W
0	$\begin{bmatrix} aa \\ aa \end{bmatrix}$	$(0, 0, 0)$	0
1	$\begin{bmatrix} aa \\ ab \end{bmatrix}$	$(1, 1, 1)$	$2w_1$
2	$\begin{bmatrix} aa \\ bb \end{bmatrix}$	$(0, 2, 2)$	$4w_1 + 4w_2$
3	$\begin{bmatrix} ab \\ ab \end{bmatrix}$	$(2, 0, 2)$	$4w_1 + 4w_3$
4	$\begin{bmatrix} ab \\ ba \end{bmatrix}$	$(2, 2, 0)$	$4w_1 + 4w_4$
5	$\begin{bmatrix} aa \\ bc \end{bmatrix}$	$(1, 2, 2)$	$4w_1 + 2w_2$
6	$\begin{bmatrix} ab \\ ac \end{bmatrix}$	$(2, 1, 2)$	$4w_1 + 2w_3$
7	$\begin{bmatrix} ab \\ ca \end{bmatrix}$	$(2, 2, 1)$	$4w_1 + 2w_4$
8	$\begin{bmatrix} ab \\ cd \end{bmatrix}$	$(2, 2, 2)$	$4w_1$

Reflection symmetry is a special case of centro-symmetry, so for any type, reversing the symbols on the ordered plots 1 to 4 results in an equivalent type. Also, by the reflection symmetry, a vertical or horizontal reflection of the symbols gives equivalent types. For example, type 1,

$\begin{bmatrix} aa \\ ab \end{bmatrix}$,

is equivalent to types

$\begin{bmatrix} ba \\ aa \end{bmatrix}$, $\begin{bmatrix} aa \\ ba \end{bmatrix}$ and $\begin{bmatrix} ab \\ aa \end{bmatrix}$,

by reversal, vertical reflection and horizontal reflection, respectively. Also, for the special case of the completely symmetric dependence structure, $w_2 = w_3$, so a diagonal reflection of a type gives an equivalent type. For example, type $\begin{bmatrix} a\,a \\ b\,b \end{bmatrix}$ is equivalent to type $\begin{bmatrix} a\,b \\ a\,b \end{bmatrix}$ (see section 5.3.1.1).

For model I under gls, and under ols with uncorrelated errors, type 4 is optimal (Theorem 5.13 in section 5.3.2.1). Therefore only models II, III and IV are examined here. Note also that optimality results for model II are equivalent to model III results if ρ_2 and ρ_3 are interchanged, w_2 and w_3 are interchanged and the types reflected about a diagonal (that is, types 2 and 3 are interchanged and also types 5 and 6 are interchanged). Therefore, optimality results for model III immediately follow from the results for model II.

In sections 6.2 and 6.3, it is useful to see that there is a relationship between the within-row, within-column and within-diagonal correlation parameters (ρ_2, ρ_3, ρ_4) and the optimality regions of the types with binary rows, columns and diagonals, respectively. Let (n_2, n_3, n_4) describe a type with n_2 binary rows, n_3 binary columns, and n_4 binary diagonals. The values of (n_2, n_3, n_4) are given with the types listed in Table 6.1. If ρ_2 and ρ_3 are interchanged then types with (n_2, n_3, n_4) and (n_3, n_2, n_4) are interchanged. That is, the optimality regions for types 2 and 3 (and types 5 and 6) are symmetric about $\rho_2 = \rho_3$. Similarly, interchanging ρ_2 and ρ_4 means that types with (n_2, n_3, n_4) and (n_4, n_3, n_2) are interchanged, and so types 2 and 4, and types 5 and 7 are swapped; and interchanging ρ_3 and ρ_4 means that types with (n_2, n_3, n_4) and (n_2, n_4, n_3) are interchanged, so types 3 and 4, and types 6 and 7 are swapped.

6.2   Generalised least squares estimation

Under gls, for designs constructed using SBAs, a type with maximum c_{Ω^*} gives an optimal design. Table 6.1 gives $c_W = c_{\Omega^*}$ for the 9 types. Clearly type 0 is inadmissible.

Definition 6.4

Let $\theta = \{2, 3, 4\}$ and assume throughout sections 6.2 and 6.3 that $i \in \theta$, $j \in \theta \setminus \{i\}$ and $\{j_1, j_2\} = \theta \setminus \{i\}$.   ∎

6.2.1   Optimal designs for model IV under gls

For model IV, the elements of Ω^* are

$$w_1 = \tfrac{1}{4}\left(\lambda_2^{-1} + \lambda_3^{-1} + \lambda_4^{-1}\right), \quad w_i = \tfrac{1}{2}\lambda_i^{-1} - w_1.$$

When $t \geq 4$, type 1 is inadmissible since type 8 is better. Also type $i + 3$ is inadmissible since type i is better if $w_i \geq 0$, otherwise type 8 is better. Therefore the optimal design depends on the maximum of $\{w_i\}$ and 0. It is shown in Appendix A2.2 that w_i is maximal if $w_i \geq 0$, and so the design of type i is optimal if $w_i \geq 0$, otherwise the binary design (type 8) is optimal. This gives the following theorem.

Theorem 6.1
For blocks of size 2×2 with $t \geq 4$, under model IV, a stationary reflection symmetric dependence structure and gls, a design of type i is optimal if

$$(\rho_{j_1} - \rho_{j_2})^2 \leq (1 - \rho_i)(1 - \rho_i - 2\lambda_i)$$

and type 8 is optimal otherwise.   ∎

The regions in which designs of these types are optimal are shown in parts a), b) and c) of Figure 6.2 for $\rho_4 = -\frac{1}{2}$, 0 and $\frac{1}{2}$, respectively. For fixed ρ_4, the rectangular region enclosed by the lines $\lambda_1 = 0$, $\lambda_2 = 0$, $\lambda_3 = 0$ and $\lambda_4 = 0$ (see Figure 6.2) is the region in which Λ is positive definite. Rotating this region by a quarter turn and interchanging ρ_2 and ρ_3 gives the region in which Λ is positive definite for ρ_4 replaced by $-\rho_4$.

Figure 6.2
Optimality regions for blocks of size 2×2 under reflection symmetry, model IV and gls, for $t \geq 4$. Vertical axis: ρ_3, horizontal axis: ρ_2.
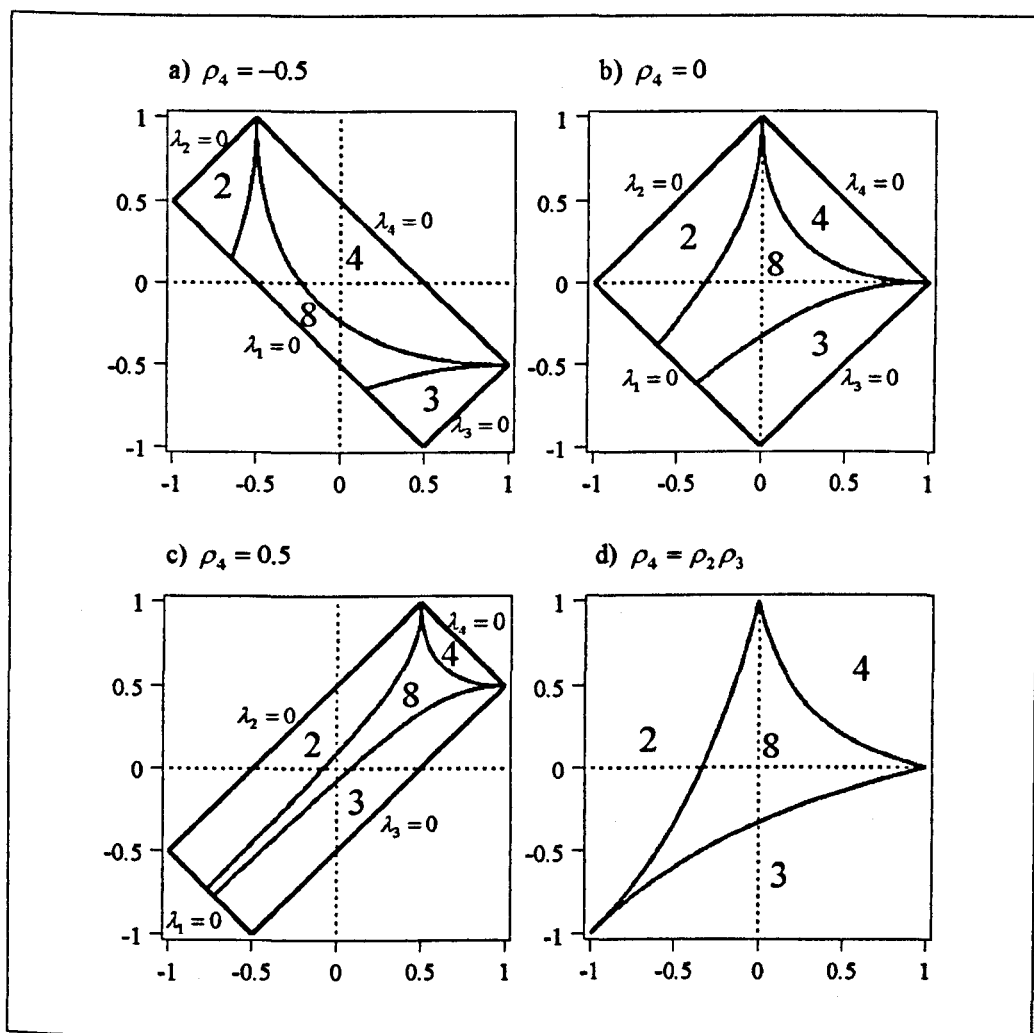
For ρ_4 near -1, type 4 is optimal for most of the region. When ρ_4 is near to 1, types 2 and 3 are optimal for most of the region where $\rho_3 > \rho_2$ and $\rho_3 < \rho_2$, respectively. As would be expected from the results in chapter 5, when the dependence is low, that is when ρ_2, ρ_3 and ρ_4 are near zero, the binary design is optimal. Note that on the boundaries between optimality regions more than one type is optimal.

Now consider the special cases given in section 6.1.2, when $t \geq 4$. The optimality regions for the nearest neighbour process are shown in Figure 6.2b. The completely symmetric process, for which optimality results were obtained by Martin & Eccleston (1993) (see section 5.3.1), corresponds to the diagonal $\rho_2 = \rho_3$ in Figure 6.2a to Figure 6.2c. Here type 4 is optimal if $4\rho_2 \geq (1 + 3\rho_4)$, otherwise type 8 is optimal (this is the optimality condition in (5.18)). For the separable process, type 2 is optimal if $(1 - \rho_2)(1 - \rho_3) \leq -4\rho_2$; type 3 is optimal if $(1 - \rho_2)(1 - \rho_3) \leq -4\rho_3$; type 4 is optimal if $(1 - \rho_2)(1 - \rho_3) \leq 4\rho_2\rho_3$; otherwise type 8 is optimal. This is illustrated in Figure 6.2d. The optimality conditions under separability for types 4 and 8 were given by Uddin & Morgan (1997a) for ρ_2, $\rho_3 > 0$ (Theorem 5.18 and Theorem 5.19 in section 5.3.2.2.3). The completely symmetric separable process corresponds to the diagonal $\rho_2 = \rho_3$ in Figure 6.2d. Here type 4 is optimal if $\rho_2 \geq \frac{1}{3}$ and type 8 is optimal otherwise (the optimality condition in (5.19)).

For some $\{\rho_i\}$ there can be a substantial loss in Φ_p-efficiency if the binary design is used when it is not optimal. When a design of type i is optimal,
$$\Phi_p^*\text{-value} = (4w_1 + 4w_i)^{-1}.$$
A design of type 8 has
$$\Phi_p\text{-value} = (4w_1)^{-1},$$

so the Φ_p-efficiency of the binary design when the non-binary design of type i is optimal is

$$\Phi_p\text{-efficiency} = \frac{w_1}{(w_1 + w_i)} = \tfrac{1}{2}\left\{1 + \lambda_i\left(\lambda_{j_1}^{-1} + \lambda_{j_2}^{-1}\right)\right\}.$$

Near the line $\lambda_i = 0$ in Figure 6.2a to Figure 6.2c, λ_i is close to zero and the Φ_p-efficiency is near to $\tfrac{1}{2}$.

Now consider the case when $t = 3$. The optimal design is one of types 1 to 7. As for $t \geq 4$, type i is optimal when $w_i \geq 0$. If $w_i \leq 0$ then type $i+3$ is better than type i. Type 1 cannot be optimal since the necessary condition for type 1 to be optimal: $w_1 + 2w_i \leq 0 \ \forall \ i$ (i.e. type 1 better than types 2, 3 and 4), is not possible for Λ positive definite. Type $i+3$ is better than types j and $j+3$ if $2w_j \leq w_i$ and $w_j \leq w_i$, respectively. However, if $w_j \leq w_i \leq 0$ then $2w_j \leq w_i$. Hence, type $i+3$ is optimal if $w_j \leq w_i \leq 0 \ \forall \ j$. The optimality conditions for types 2, 3 and 4 are as for $t \geq 4$, and types 5, 6 and 7 are optimal in the region where the binary type was optimal for $t \geq 4$ (see Figure 6.3). Theorem 6.2 gives the optimality conditions in terms of $\{\rho_i\}$.

Theorem 6.2
For blocks of size 2×2 with $t = 3$, under model IV, a stationary reflection symmetric dependence structure and gls, the optimality condition for a design of type i is as in Theorem 6.1. Type $i+3$ is optimal if

$$(\rho_{j_1} - \rho_{j_2})^2 \geq (1 - \rho_i)(1 - \rho_i - 2\lambda_i) \quad \text{and} \quad \rho_i = \min_{h \in \theta}(\rho_h). \qquad \blacksquare$$

For $t = 2$, type 1 cannot be optimal so optimality depends on the maximum of $\{w_i\}$. Hence, type i is optimal if $w_i \geq w_j \ \forall \ j$. This gives the following theorem.

Theorem 6.3

For blocks of size 2×2 with $t = 2$, under model IV, a stationary reflection symmetric dependence structure and gls, type i is optimal if

$$\rho_i = \min_{h \in \theta}(\rho_h). \qquad \blacksquare$$

This means that when $t = 2$, the type with both rows/columns/diagonals non-binary (type 2/3/4) is optimal if the within-row/column/diagonal correlation is lowest.

Figure 6.3

Optimality regions for blocks of size 2×2 under reflection symmetry, model IV and gls, for $t = 3$. Vertical axis: ρ_3, horizontal axis: ρ_2.
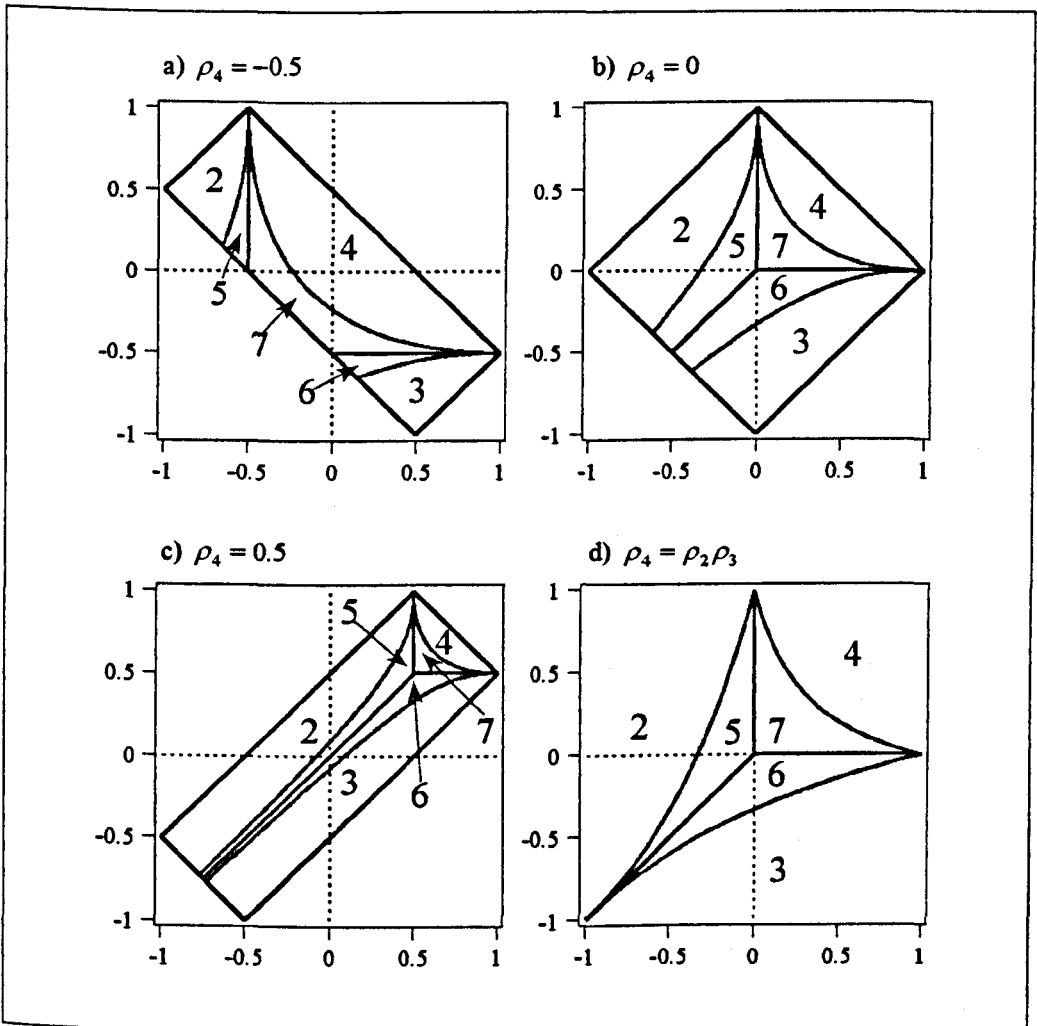
6.2.2   Optimal designs for model II under gls

Under model II the elements of Ω^* are:

$$w_1 = (1-\rho_2)/(2\lambda_3\lambda_4), \qquad w_2 = -w_1,$$

$$w_3 = (\rho_4 - \rho_3)/(2\lambda_3\lambda_4), \qquad w_4 = -w_3.$$

This means that types 0 and 2 are equivalent, as are types 1 and 5. For $t \geq 2$, it is clear that types 1, 6, 7 and 8 are inadmissible since either type 3 or 4 is better. Therefore type 3 is optimal if $w_3 \geq 0$, otherwise type 4 is optimal.

Note that both these types have binary rows. Theorem 6.4 gives this result in terms of $\{\rho_i\}$.

Theorem 6.4
For blocks of size 2×2 with $t \geq 2$, under model II, a stationary reflection symmetric dependence structure and gls, type 3 is optimal if

$$\rho_3 \leq \rho_4$$

and type 4 is optimal otherwise.   ∎

For the separable process, type 3 is optimal if $\rho_3 \leq 0$, otherwise type 4 is optimal (see Theorem 5.14 in section 5.3.2.2.1).

The Φ_p-efficiency of type 8 when type 3 is optimal is

$$\Phi_p\text{-efficiency} = \frac{(4w_1 + 4w_3)^{-1}}{(4w_1)^{-1}} = \frac{w_1}{w_1 + w_3} = \frac{1-\rho_2}{\lambda_4}.$$

This simplifies to $\frac{1}{2}(1 + \lambda_3/\lambda_4)$ since $2(1-\rho_2) = \lambda_3 + \lambda_4$. Similarly, the Φ_p-efficiency of type 8 when type 4 is optimal can be shown to be $\frac{1}{2}(1 + \lambda_4/\lambda_3)$. These Φ_p-efficiencies equal 1 when $\rho_3 = \rho_4$. If $\rho_3 \neq \rho_4$, the Φ_p-efficiency of type 8, given that type 3 is optimal, is near to $\frac{1}{2}$ when λ_3 is near zero and λ_4 is large. Similarly, assuming that $\rho_3 \neq \rho_4$ and type 4 is optimal, the Φ_p-efficiency of type 8 is near to $\frac{1}{2}$ when λ_4 is near zero and λ_3 is large.

6.2.3 Optimal designs for model III under gls

The relationship between model II and III, described in section 6.1.4, gives the following theorem.

Theorem 6.5
For blocks of size 2×2 with $t \geq 2$, under model III, a stationary reflection symmetric dependence structure and gls, type 2 is optimal if

$$\rho_2 \leq \rho_4$$

and type 4 is optimal otherwise.   ∎

6.3 Ordinary least squares estimation

Under ols estimation, Ω^* and $\Omega^* \Lambda \Omega^*$ have simple forms but finding the type with minimum $\mathrm{tr}\{D^+\}$ involves both c_{Ω^*} and $c_{\Omega^* \Lambda \Omega^*}$.

6.3.1 Optimal designs for model IV under ols

Under model IV, $\Omega^* = E_4$ and so $c_{\Omega^*} = 4 - \frac{1}{4}\underline{r}'\underline{r}$, where $\underline{r}$ is an s-vector of the number of times each label occurs in the type (as given in section 5.2.5). For the 9 types under consideration, $c_W = c_{\Omega^* \Lambda \Omega^*}$ is given in Table 6.1, and Table 6.2 gives c_{Ω^*} and $c_{\Omega^* \Lambda \Omega^*}/c_{\Omega^*}^2$. The elements of $\Omega^* \Lambda \Omega^*$ are

$$w_1 = \tfrac{1}{4}(4 - \lambda_1), \quad w_i = \tfrac{1}{4}(4\rho_i - \lambda_1) = \tfrac{1}{2}\lambda_i - w_1.$$

When $t \geq 4$, type 8 is better than type 1. Necessary conditions for type $i+3$ to be optimal are $w_i \geq -(9/17)w_1$ and $w_i \leq -(11/18)w_1$ (i.e. type $i+3$ better than types i and 8, respectively), which cannot be true. Therefore the optimal design depends on the minimum of $w_1 + w_i$ and $\frac{4}{3}w_1$. This gives Theorem 6.6.

Table 6.2

List of types, c_{Ω^*} and $c_{\Omega^*\wedge\Omega^*}/c_{\Omega^*}^2$ for blocks of size 2×2 under reflection symmetry, model IV and ols. $\dagger$ indicates that $c_{\Omega^*} = c_{\Omega^*\wedge\Omega^*} = 0$.

Type No.	Model IV	
	c_{Ω^*}	$c_{\Omega^*\wedge\Omega^*}/c_{\Omega^*}^2$
0	0	$\dagger$
1	3/2	$8w_1/9$
2		$w_1 + w_2$
3	2	$w_1 + w_3$
4		$w_1 + w_4$
5		$8(2w_1 + w_2)/25$
6	5/2	$8(2w_1 + w_3)/25$
7		$8(2w_1 + w_4)/25$
8	3	$4w_1/9$

Theorem 6.6

For blocks of size 2×2 with $t \geq 4$, under model IV, a stationary reflection symmetric dependence structure and ols, type i is optimal if

$$7\lambda_i \leq 4(1 - \rho_i) \quad \text{and} \quad \rho_i = \min_{h\in\theta}(\rho_h),$$

otherwise type 8 is optimal. ∎

The regions of optimality, illustrated in Figure 6.4, are similar to those for $t \geq 4$ under gls (Figure 6.2). However, the regions of optimality for types 4 and 8 are larger and smaller, respectively, than under gls. The Φ_p-efficiency of type 8 when type i is optimal is

$$\Phi_p\text{-efficiency} = \frac{(w_1 + w_i)}{(4/9)w_1} = \frac{9\lambda_i}{\{2(4 - \lambda_1)\}},$$

which is near to zero when λ_i is near zero. Note that the boundaries $\lambda_i = 0$ are as shown in Figure 6.2.

Recall that for model IV under ols when Λ is centro-symmetric, the condition for when type 4 is better than type 8 is given as the inequality in (5.15) in section 5.3.1.1. Under stationarity, the completely symmetric dependence structure corresponds to the diagonal $\rho_2 = \rho_3$ in Figure 6.4, and the inequality in (5.15) simplifies to $\rho_2 \geq (3 + 11\rho_4)/14$ (given as the condition in (5.16)). Also, type 2 is better than type 8 if $\rho_2 \leq -\frac{1}{4}(3 - 7\rho_4)$ (the condition in (5.14)).

Figure 6.4

Optimality regions for blocks of size 2×2 under reflection symmetry, model IV and ols for $t \geq 4$. Vertical axis: ρ_3, horizontal axis: ρ_2.
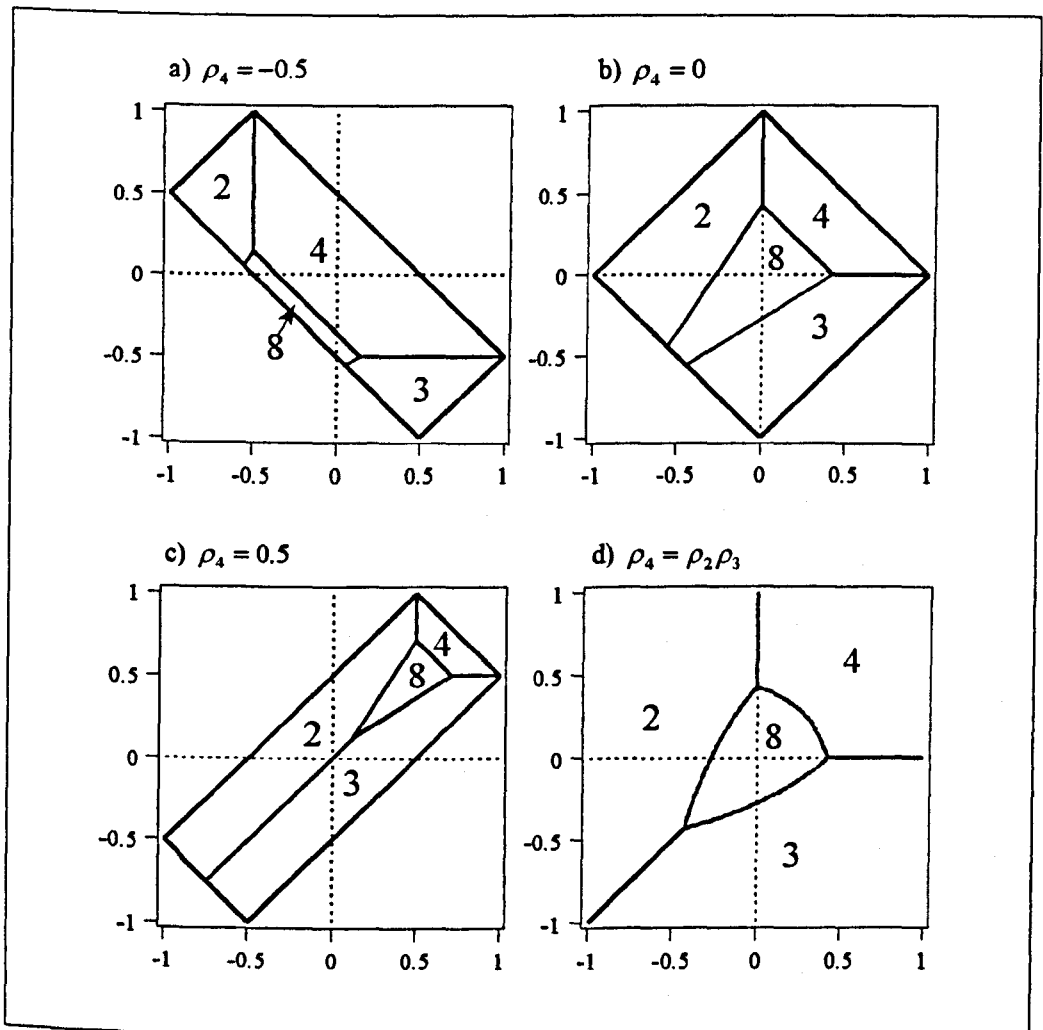
When $t = 3$, type 1 cannot be optimal since $w_i \geq -w_1/9 \; \forall \; i$ (i.e. type 1 better than types 2, 3 and 4) cannot be true. If $w_i \leq w_j \; \forall \; j$, then type i is better than type $j \; \forall \; j$, and type $i+3$ is better than type $j+3 \; \forall \; j$. Therefore for type i to be optimal, $w_i \leq w_j \; \forall \; j$, and $w_i \leq -9w_1/17$ (i.e. type i better than type $i+3$) are required. Type $i+3$ is optimal if $w_i \leq w_j \; \forall \; j$ and $w_i \geq -9w_1/17$.

Theorem 6.7
For blocks of size 2×2 with $t = 3$, under model IV, a stationary reflection symmetric dependence structure and ols, type i is optimal if

$$\rho_i = \min_{h \in \theta}(\rho_h) \quad \text{and} \quad 13\lambda_i \leq 8(1 - \rho_i),$$

and type $i+3$ is optimal if

$$\rho_i = \min_{h \in \theta}(\rho_h) \quad \text{and} \quad 13\lambda_i \geq 8(1 - \rho_i). \qquad\qquad \blacksquare$$

The optimality regions (see Figure 6.5) are similar to those obtained for $t = 3$ under gls (Figure 6.3). However, the regions of optimality for types 5, 6 and 7 are smaller than under gls, and much smaller for $\rho_4 < 0$. For example, in Figure 6.5a, the optimality region for types 5 and 6 are small triangles at either end of the optimality region for type 7. Also, unlike under gls, the optimality region for types 5, 6 and 7 together, is slightly smaller than the optimality region for type 8 when $t \geq 4$.

When $t = 2$, type 1 is inadmissible, and type i is optimal if $w_i \leq w_j \; \forall \; j$, which gives precisely the same optimality conditions as under gls.

Figure 6.5
Optimality regions for blocks of size 2×2 under reflection symmetry, model IV and ols for $t = 3$. Vertical axis: ρ_3, horizontal axis: ρ_2.

a) $\rho_4 = -0.5$

b) $\rho_4 = 0$

c) $\rho_4 = 0.5$

d) $\rho_4 = \rho_2 \rho_3$
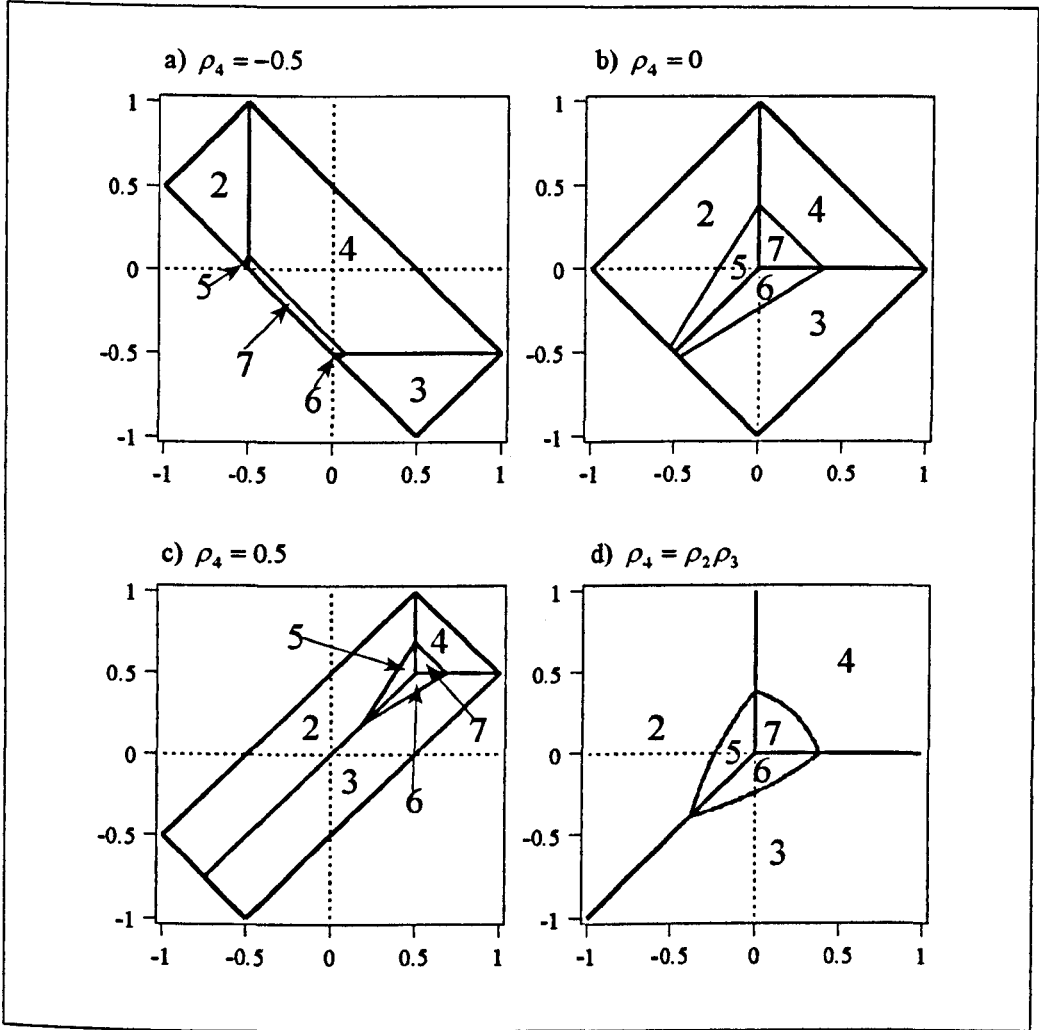
6.3.2   Optimal designs for model II under ols

Under model II, $\Omega^* = I_2 \otimes E_2$ and so $c_{\Omega^*} = n_2$, the number of binary rows in the type (Table 6.3). The elements of $\Omega^* \Lambda \Omega^*$ are

$$w_1 = \tfrac{1}{2}(\lambda_3 + \lambda_4), \quad w_2 = -w_1, \quad w_3 = \tfrac{1}{2}(\lambda_3 - \lambda_4), \quad w_4 = -w_3.$$

Table 6.3
List of types, $c_{\varrho^\bullet}$ and $c_{\varrho^\bullet \wedge \varrho^\bullet}/c^2_{\varrho^\bullet}$ for blocks of size 2×2 under reflection symmetry, model II and ols. † indicates $c_{\varrho^\bullet} = c_{\varrho^\bullet \wedge \varrho^\bullet} = 0$.

Type	Model II	
No.	$c_{\varrho^\bullet}$	$c_{\varrho^\bullet \wedge \varrho^\bullet}/c^2_{\varrho^\bullet}$
0	0	†
1	1	$2w_1$
2	0	†
3	2	$w_1 + w_3$
4	2	$w_1 - w_3$
5	1	$2w_1$
6	2	$w_1 + \frac{1}{2}w_3$
7	2	$w_1 - \frac{1}{2}w_3$
8	2	w_1

As under gls, types 0 and 2 are equivalent, and also types 1 and 5. It follows that for $t \geq 2$, if $w_3 \leq 0$ type 3 is optimal, otherwise type 4 is optimal. This leads to exactly the same optimality conditions in $\{\rho_i\}$ as under gls (see section 6.2.2). However, the Φ_p-efficiencies of type 8 when types 3 and 4 are optimal are different:

$$\Phi_p\text{-efficiency} = \frac{w_1 + w_3}{w_1} = \frac{2}{(1 + \lambda_4/\lambda_3)}$$

and

$$\Phi_p\text{-efficiency} = \frac{w_1 - w_3}{w_1} = \frac{2}{(1 + \lambda_3/\lambda_4)},$$

respectively, which are the reciprocals of the Φ_p-efficiencies of type 8 when types 4 and 3, respectively, are optimal under gls. These Φ_p-efficiencies equal 1 when $\rho_3 = \rho_4$. If $\rho_3 \neq \rho_4$ and type 3 is optimal, the Φ_p-efficiency of type 8 is near to zero when λ_3 is near zero and λ_4 is large. Similarly, assuming that $\rho_3 \neq \rho_4$ and type 4 is optimal, the Φ_p-efficiency of type 8 is near to zero when λ_4 is near zero and λ_3 is large.

6.4 Discussion

As in sections 5.2 and 5.3, optimal designs are highly specific to the correlation parameters. The optimality results obtained here are similar under gls and ols for the model with block effects only (model IV). For models with row and/or column effects (models I, II and III), the optimality results under gls and ols are identical, and the optimal designs have blocks with two different treatments each replicated twice. Under the model with row/column effect only, if the within-column/row correlation is less than the within-diagonal correlation, the design with binary rows/columns is optimal (cf. the comment from Uddin & Morgan (1997a) given in section 5.3.2.4), otherwise the design with both binary rows and columns is optimal. Note that although the binary design might usually be preferred in practice, the Φ_p-efficiency of the binary design can be very low for some correlation values.

When t is not small the designs here have a large number of blocks, which may not be practically feasible. However, under gls, the results obtained here on the maximisation of c_{Ω^*} will provide a lower bound for the Φ_p-value for all $p \geq 0$ over all designs with t treatments and any number of blocks of size 2×2, including designs with a smaller number of blocks than required for a SBA. In general, for designs with t treatments and b blocks of size $p_1 \times p_2$, given that c_{Ω^*} is maximised, a lower bound for the Φ_p-value (for all $p \geq 0$) over all designs with t treatments and blocks of size $p_1 \times p_2$ is

$$\frac{1}{a_1} = \frac{(t-1)}{bc_{\Omega^*}}.$$

This lower bound can be used to provide an upper bound on the Φ_p-efficiency. When this lower bound is not attainable, it is the Φ_p-value of a hypothetical design that has b blocks with C-matrix completely symmetric and $\text{tr}(C)$ maximised.

Also, results on the minimisation of $c_{\Omega^*\Lambda\Omega^*}/c^2_{\Omega^*}$ (or equivalently the maximisation of c_{Ω^*} under gls) allow the Φ_p-efficiency of a binary design to be calculated. This means that an upper bound on the loss in Φ_p-efficiency of using a binary design when a non-binary design is optimal can be found.

As well as providing a lower bound for the Φ_p-value, the optimal designs obtained here may indicate the form of the optimal or near-optimal designs for a smaller number of blocks, as in Uddin & Morgan (1997b).

Unless block sizes are very small, optimality results can be difficult to obtain even when C and var(q) are completely symmetric. However, some results for NRC designs with blocks having more than 2 rows and/or columns are given in chapters 7 and 8.

7 Optimal nested row-column designs for blocks of size 3×2 under dependence

In this chapter, optimal NRC designs are obtained for blocks of size 3×2 and $t \geq 6$ treatments under model IV and gls, for a separable dependence structure. Preliminary material is given in sections 7.1 to 7.4, and optimality regions are specified in section 7.5.

7.1 Introduction

Finding optimal NRC designs is difficult for blocks of size 3×2 and hence only model IV under gls with $t \geq 6$ is considered here. The separable dependence structure is assumed, which has the AR(1)*AR(1) process as a special case. Design construction and the method of obtaining optimality conditions are as in chapter 6, and therefore are not repeated here.

Under a centro-symmetric Λ, Martin (1998) lists 11 types for blocks consisting of 4 plots. When $k = 6$, there are 117 types, which is over 10 times more types than for $k = 4$. Hence finding the type with maximum c_W is much more complicated for blocks of size 3×2 than for the 2×2 layout.

For uncorrelated errors under model I, examples of 2×3 NRC designs appear in several papers. The examples in Singh & Dey (1979) and Ipinyomi & John (1985) are cyclic designs (see sections 5.1.1 and 5.1.2). Also, Morgan (1996) has an example of a 2×3 BIBRC design with $t = 9$, $b = \frac{4}{3}t = 6$.

For correlated errors, the results of Uddin & Morgan (1997a, 1997b) for blocks of size $p_1 \times 2$ include the case where $p_1 = 3$. The AR(1)*AR(1) process is considered in these two papers. Recall that optimality results for the AR(1)*AR(1) process under model IV and gls (for positive correlation values)

are given here as Theorem 5.18 and Theorem 5.19 in section 5.3.2.2.3. For $p_1 = 3$, these theorems show when the binary and non-binary types

$$\begin{bmatrix} ab \\ cd \\ ef \end{bmatrix} \text{ and } \begin{bmatrix} ab \\ ba \\ ab \end{bmatrix},$$

respectively, are optimal. The optimality of other types (for positive correlation values) can be found by solving an integer programming problem. Also, Uddin & Morgan (1997b) give a cyclic SSENR design with blocks of size 3×2, which is given here as design D5.21 in section 5.3.3.

Recall from section 6.1 that small-sized blocks, such as the blocks of size 3×2 considered here, should produce good homogeneity.

7.2   Dependence structure

For blocks of size 3×2, Λ is a 6×6 matrix. If Λ is symmetric it consists of at most 21 distinct parameters. Under centro-symmetry this is reduced to at most 12 distinct parameters. For a stationary process, there are at most 7 distinct correlations (excluding $\rho_{0,0} = 1$), and

$$\Lambda = \begin{pmatrix} 1 & \rho_{1,0} & \rho_{0,1} & \rho_{1,1} & \rho_{0,2} & \rho_{1,2} \\ \rho_{1,0} & 1 & \rho_{-1,1} & \rho_{0,1} & \rho_{-1,2} & \rho_{0,2} \\ \rho_{0,1} & \rho_{-1,1} & 1 & \rho_{1,0} & \rho_{0,1} & \rho_{1,1} \\ \rho_{1,1} & \rho_{0,1} & \rho_{1,0} & 1 & \rho_{-1,1} & \rho_{0,1} \\ \rho_{0,2} & \rho_{-1,2} & \rho_{0,1} & \rho_{-1,1} & 1 & \rho_{1,0} \\ \rho_{1,2} & \rho_{0,2} & \rho_{1,1} & \rho_{0,1} & \rho_{1,0} & 1 \end{pmatrix}. \tag{7.1}$$

Given that a simple structure with a small number of parameters is usually desirable (see sections 2.3 and 2.4), the maximum number of distinct correlations (excluding $\rho_{0,0} = 1$) in (7.1) may still be considered to be large. Under stationarity and reflection symmetry, Λ consists of at most 5 distinct correlations (excluding $\rho_{0,0} = 1$) since $\rho_{1,1} = \rho_{-1,1}$ and $\rho_{1,2} = \rho_{-1,2}$. Although reflection symmetry was considered for blocks of size 2×2, here the 5

possible distinct correlations would mean that optimality results would be much more difficult to obtain. For this reason, and to have a simple Λ, optimality results are obtained for a separable process, which has at most 3 distinct correlations (excluding $\rho_{0,0} = 1$).

Definition 7.1
For the separable process, $\Lambda = \Lambda_2 \otimes \Lambda_1$, where

$$\Lambda_1 = \begin{pmatrix} 1 & \rho_{1,0} \\ \rho_{1,0} & 1 \end{pmatrix} \quad \text{and} \quad \Lambda_2 = \begin{pmatrix} 1 & \rho_{0,1} & \rho_{0,2} \\ \rho_{0,1} & 1 & \rho_{0,1} \\ \rho_{0,2} & \rho_{0,1} & 1 \end{pmatrix}.$$

$\blacksquare$

The separable process is a special case of reflection symmetry under stationarity with $\rho_{1,1} = \rho_{0,1}\rho_{1,0}$ and $\rho_{1,2} = \rho_{0,2}\rho_{1,0}$. Several interesting special cases are contained within the separable process. These are the:

i)   AR(1)*AR(1) process, where $\rho_{0,2} = \rho_{0,1}^2$;

ii) NN1*NN1 process, where $\rho_{0,2} = 0$;

iii) Completely symmetric and separable process, where $\rho_{0,1} = \rho_{1,0}$.

Definition 7.2
In order to simplify the notation a little, the correlation parameters $\rho_{0,1}$, $\rho_{0,2}$ and $\rho_{1,0}$ are re-labelled as ρ_1, ρ_2 and ρ_3, respectively. $\blacksquare$

7.3 Types

When Λ represents a stationary process, $W = \Omega^*$ is centro-symmetric, so the 117 types due to Martin (1998), listed in Table 5.3, need to be considered. Under reflection symmetry,

$$w_{1,1} = w_{2,2}, \quad w_{1,3} = w_{2,4}, \quad w_{1,4} = w_{2,3} \quad \text{and} \quad w_{1,6} = w_{2,5},$$

so giving the following definition.

Definition 7.3
Under reflection symmetry Ω^* has the following form:

$$\Omega^* = \begin{pmatrix} w_{1,1} & w_{1,2} & w_{1,3} & w_{1,4} & w_{1,5} & w_{1,6} \\ w_{1,2} & w_{1,1} & w_{1,4} & w_{1,3} & w_{1,6} & w_{1,5} \\ w_{1,3} & w_{1,4} & w_{3,3} & w_{3,4} & w_{1,3} & w_{1,4} \\ w_{1,4} & w_{1,3} & w_{3,4} & w_{3,3} & w_{1,4} & w_{1,3} \\ w_{1,5} & w_{1,6} & w_{1,3} & w_{1,4} & w_{1,1} & w_{1,2} \\ w_{1,6} & w_{1,5} & w_{1,4} & w_{1,3} & w_{1,2} & w_{1,1} \end{pmatrix}. \tag{7.2}$$

where

$$\sum_{i=1}^{6} w_{1,i} = 0 \tag{7.3}$$

and $2(w_{1,3} + w_{1,4}) + (w_{3,3} + w_{3,4}) = 0.$ (7.4)

■

It follows from the zero row/column sums of Ω^* in (7.2) that

$$w_{1,1} + w_{1,2} + w_{1,5} + w_{1,6} = w_{1,3} + w_{1,4} + w_{3,3} + w_{3,4}.$$

Note that the form of Ω^* for a separable process is also given by (7.2).

Under Λ reflection symmetric, as for the 2×2 layout considered in chapter 6, a reversal, vertical reflection or horizontal reflection of the symbols in any type will result in an equivalent type with respect to the value of c_W. When plots are numbered 1 to k, by rows from the top-left, the 117 types in Table 5.3

give the list of types for W centro-symmetric. For example, the type [abcdef] in Table 5.3 is represented here as the type

$$\begin{bmatrix} ab \\ cd \\ ef \end{bmatrix}.$$

The type numbers from Table 5.3 are used here.

Under reflection symmetry the number of different types is reduced from 117 to 74, due to vertical and horizontal reflections. Table 7.1 lists the types from Table 5.3 that are equivalent under reflection symmetry. For example, types 2 and 3,

$$\begin{bmatrix} aa \\ aa \\ ab \end{bmatrix} \text{ and } \begin{bmatrix} aa \\ aa \\ ba \end{bmatrix},$$

respectively, are equivalent due to a vertical reflection, and types 50 and 59,

$$\begin{bmatrix} aa \\ ac \\ bb \end{bmatrix} \text{ and } \begin{bmatrix} bb \\ ac \\ aa \end{bmatrix},$$

are equivalent due to a horizontal reflection.

For a given type, the expression for c_W is of the form

$$c_W = 4w_{1,1} + 2w_{3,3} + 2x_{3,4}w_{3,4} + 2\sum_{j=2}^{6} x_{1,j}w_{1,j}, \tag{7.5}$$

where $x_{i,j}$ is the coefficient of $2w_{i,j}$ ($i \neq j$) in c_W. This means that c_W can be specified by the 6-vector

$$(x_{1,2}, x_{1,3}, x_{1,4}, x_{1,5}, x_{1,6}, x_{3,4}).$$

For each of the types listed in Table 7.1, expressions for c_W are also given.

From the reduced set of 74 types, two pairs are equivalent since they have the same c_W values, although they are not horizontal or vertical reflections of each other. The pair of types 87 and 91,

$$\begin{bmatrix} ab \\ ab \\ cd \end{bmatrix} \text{ and } \begin{bmatrix} ac \\ ab \\ db \end{bmatrix},$$

respectively, are equivalent. Expressions for c_W for types 87 and 91 are

$$4w_{1,1} + 2w_{3,3} + 2(w_{1,3} + w_{2,4})$$

and $\quad 4w_{1,1} + 2w_{3,3} + 2(w_{1,3} + w_{4,6}),$

respectively. These two types are equivalent since $w_{2,4} = w_{4,6} (= w_{1,3})$ under reflection symmetry. Also, types 92 and 96,

$$\begin{bmatrix} ab \\ ba \\ cd \end{bmatrix} \text{ and } \begin{bmatrix} ac \\ ba \\ db \end{bmatrix},$$

respectively, are equivalent since the expressions for c_W,

$$4w_{1,1} + 2w_{3,3} + 2(w_{1,4} + w_{2,3})$$

and $\quad 4w_{1,1} + 2w_{3,3} + 2(w_{1,4} + w_{3,6}),$

respectively, are equivalent because $w_{2,3} = w_{3,6} (= w_{1,4})$.

Therefore, the list of types is reduced to 72 under reflection symmetry. This list is reduced further by eliminating inadmissible types, that is, types for which there are always better types. Fifty-four types, marked in Table 7.1 by round brackets, are shown to be inadmissible in Appendix A2.4). The inadmissibility of some of the types marked by round brackets in Table 7.1 follows from Lemma 7.1 (given below). Hence, the number of types that need to be considered under reflection symmetry is just 18.

Lemma 7.1

Under reflection symmetry (when Ω^* has the form given by (7.2)),

$$w_{3,3} + w_{3,4} \geq 0; \qquad w_{1,3} + w_{1,4} \leq 0; \qquad w_{1,1} + w_{1,2} \geq 0;$$

$$w_{1,1} + w_{1,5} \geq 0; \qquad w_{1,1} + w_{1,6} \geq 0.$$

<u>Proof</u>

Since Ω^* is a non-negative definite matrix, it follows from the result (A1.25) in Appendix A1.8, that the sub-matrix

$$\begin{pmatrix} w_{3,3} & w_{3,4} \\ w_{3,4} & w_{3,3} \end{pmatrix},$$

of Ω^*, given in (7.2), is also a non-negative definite matrix. It then follows that $w_{3,3} + w_{3,4} \geq 0$, and from equation (7.4), $w_{3,3} + w_{3,4} \geq 0$ implies $w_{1,3} + w_{1,4} \leq 0$. Similarly, it can be shown that $w_{1,1} + w_{1,j} \geq 0$ for $j = 2,5,6$.

■

Definition 7.4

For a reflection symmetric dependence structure, let Ξ be the set of admissible types. That is,

$$\Xi = \{13, 18, 20, 29, 60, 61, 62, 63, 65, 67, 70, 86, 87, 92, 99, 103, 116, 117\}.$$

■

Table 7.1

List of types and expressions for c_W, for blocks of size 3×2 under reflection symmetry.

The vector $(x_{1,2}, x_{1,3}, x_{1,4}, x_{1,5}, x_{1,6}, x_{3,4})$ (see equation (7.5)) is included when the elements of this vector are not immediately obvious from the expression given for c_W.

Note: type numbers in round brackets are inadmissible under reflection symmetry.

type no.	type	equivalent types	expression for c_W and $(x_{1,2}, x_{1,3}, x_{1,4}, x_{1,5}, x_{1,6}, x_{3,4})$
(1)	$\begin{bmatrix} aa \\ aa \\ aa \end{bmatrix}$		0 $(2, 4, 4, 2, 2, 1)$
(2)	$\begin{bmatrix} aa \\ aa \\ ab \end{bmatrix}$	3	$2w_{1,1}$ $(1, 3, 3, 1, 1, 1)$
(4)	$\begin{bmatrix} aa \\ ab \\ aa \end{bmatrix}$		$2w_{3,3}$ $(2, 2, 2, 2, 2, 0)$
(5)	$\begin{bmatrix} aa \\ aa \\ bb \end{bmatrix}$		$4w_{1,1} + 4w_{1,2}$ $(2, 2, 2, 0, 0, 1)$
(6)	$\begin{bmatrix} aa \\ ab \\ ab \end{bmatrix}$	11	$2w_{1,1} + 2w_{3,3} + 4w_{1,3}$ $(1, 3, 1, 1, 1, 0)$
(7)	$\begin{bmatrix} aa \\ ba \\ ab \end{bmatrix}$	10	$2w_{1,1} + 2w_{3,3} + 4w_{1,4}$ $(1, 1, 3, 1, 1, 0)$
(8)	$\begin{bmatrix} ab \\ aa \\ ab \end{bmatrix}$		$4w_{1,1} + 4w_{1,5}$ $(0, 2, 2, 2, 0, 1)$
(9)	$\begin{bmatrix} ba \\ aa \\ ab \end{bmatrix}$	12	$4w_{1,1} + 4w_{1,6}$ $(0, 2, 2, 0, 2, 1)$
13	$\begin{bmatrix} aa \\ bb \\ aa \end{bmatrix}$		$4w_{3,3} + 4w_{3,4}$ $(2, 0, 0, 2, 2, 1)$
(14)	$\begin{bmatrix} aa \\ ab \\ bb \end{bmatrix}$	15	$4w_{1,1} + 2w_{3,3} + 4w_{1,2} + 4w_{1,3} + 4w_{1,4}$ $(2, 2, 2, 0, 0, 0)$
(16)	$\begin{bmatrix} ab \\ aa \\ bb \end{bmatrix}$	17	$2w_{1,1} + 2w_{3,3} + 2w_{3,4}$ $(1, 1, 1, 1, 1, 1)$

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Table 7.1 continued.

type no.	type	equivalent types	c_W
18	$\begin{bmatrix} ab \\ ab \\ ab \end{bmatrix}$		$4w_{1,1} + 2w_{3,3} + 8w_{1,3} + 4w_{1,5}$
(19)	$\begin{bmatrix} ab \\ ab \\ ba \end{bmatrix}$		$4w_{1,1} + 2w_{3,3} + 4w_{1,3} + 4w_{1,4} + 4w_{1,6}$
20	$\begin{bmatrix} ab \\ ba \\ ab \end{bmatrix}$		$4w_{1,1} + 2w_{3,3} + 8w_{1,4} + 4w_{1,5}$
(21)	$\begin{bmatrix} aa \\ aa \\ bc \end{bmatrix}$		$4w_{1,1} + 2w_{1,2}$ $(1, 2, 2, 0, 0, 1)$
(22)	$\begin{bmatrix} aa \\ ab \\ ac \end{bmatrix}$	27	$2w_{1,1} + 2w_{3,3} + 2w_{1,3}$ $(1, 2, 1, 1, 1, 0)$
(23)	$\begin{bmatrix} aa \\ ba \\ ac \end{bmatrix}$	26	$2w_{1,1} + 2w_{3,3} + 2w_{1,4}$ $(1, 1, 2, 1, 1, 0)$
(24)	$\begin{bmatrix} ab \\ aa \\ ac \end{bmatrix}$		$4w_{1,1} + 2w_{1,5}$ $(0, 2, 2, 1, 0, 1)$
(25)	$\begin{bmatrix} ba \\ aa \\ ac \end{bmatrix}$	28	$4w_{1,1} + 2w_{1,6}$ $(0, 2, 2, 0, 1, 1)$
29	$\begin{bmatrix} aa \\ bc \\ aa \end{bmatrix}$		$4w_{3,3} + 2w_{3,4}$ $(2, 0, 0, 2, 2, 0)$
(30)	$\begin{bmatrix} aa \\ ab \\ bc \end{bmatrix}$	41	$4w_{1,1} + 2w_{3,3} + 2w_{1,2} + 2w_{1,3} + 4w_{1,4}$
(31)	$\begin{bmatrix} aa \\ ba \\ bc \end{bmatrix}$	40	$4w_{1,1} + 2w_{3,3} + 2w_{1,2} + 4w_{1,3} + 2w_{1,4}$
(32)	$\begin{bmatrix} ab \\ aa \\ bc \end{bmatrix}$	43	$4w_{1,1} + w_{3,3} + 2w_{1,6} + w_{3,4}$ $(0, 1, 1, 0, 1, 1)$
(33)	$\begin{bmatrix} ba \\ aa \\ bc \end{bmatrix}$	42	$4w_{1,1} + w_{3,3} + 2w_{1,5} + w_{3,4}$ $(0, 1, 1, 1, 0, 1)$
(34)	$\begin{bmatrix} aa \\ bb \\ ac \end{bmatrix}$	44	$2w_{1,1} + 3w_{3,3} + 3w_{3,4}$ $(1, 0, 0, 1, 1, 1)$

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Table 7.1 continued.

type no.	type	equivalent types	c_W
(35)	$\begin{bmatrix} ab \\ ab \\ ac \end{bmatrix}$	48	$4w_{1,1} + 2w_{3,3} + 6w_{1,3} + 2w_{1,5}$
(36)	$\begin{bmatrix} ba \\ ab \\ ac \end{bmatrix}$	47	$4w_{1,1} + 2w_{3,3} + 2w_{1,3} + 4w_{1,4} + 2w_{1,6}$
(37)	$\begin{bmatrix} ab \\ ba \\ ac \end{bmatrix}$	46	$4w_{1,1} + 2w_{3,3} + 6w_{1,4} + 2w_{1,5}$
(38)	$\begin{bmatrix} ba \\ ba \\ ac \end{bmatrix}$	45	$4w_{1,1} + 2w_{3,3} + 4w_{1,3} + 2w_{1,4} + 2w_{1,6}$
(39)	$\begin{bmatrix} bb \\ aa \\ ac \end{bmatrix}$	49	$4w_{1,1} + w_{3,3} + 2w_{1,2} + w_{3,4}$ $(1, 1, 1, 0, 0, 1)$
(50)	$\begin{bmatrix} aa \\ ac \\ bb \end{bmatrix}$	59	$4w_{1,1} + 2w_{3,3} + 4w_{1,2} + 2w_{1,3} + 2w_{1,4}$
(51)	$\begin{bmatrix} aa \\ bc \\ ab \end{bmatrix}$	57	$2w_{1,1} + 3w_{3,3} + 2w_{1,4} + w_{3,4}$ $(1, 0, 1, 1, 1, 0)$
(52)	$\begin{bmatrix} ab \\ ac \\ ab \end{bmatrix}$		$4w_{1,1} + 2w_{3,3} + 4w_{1,3} + 4w_{1,5}$
(53)	$\begin{bmatrix} ba \\ ac \\ ab \end{bmatrix}$	55	$4w_{1,1} + 2w_{3,3} + 2w_{1,3} + 2w_{1,4} + 4w_{1,6}$
(54)	$\begin{bmatrix} aa \\ bc \\ ba \end{bmatrix}$	58	$2w_{1,1} + 3w_{3,3} + 2w_{1,3} + w_{3,4}$ $(1, 1, 0, 1, 1, 0)$
(56)	$\begin{bmatrix} ba \\ ac \\ ba \end{bmatrix}$		$4w_{1,1} + 2w_{3,3} + 4w_{1,4} + 4w_{1,5}$
60	$\begin{bmatrix} aa \\ bb \\ cc \end{bmatrix}$		$4w_{1,1} + 2w_{3,3} + 4w_{1,2} + 2w_{3,4}$
61	$\begin{bmatrix} aa \\ bc \\ bc \end{bmatrix}$		$4w_{1,1} + 2w_{3,3} + 2w_{1,2} + 4w_{1,3}$
62	$\begin{bmatrix} aa \\ bc \\ cb \end{bmatrix}$		$4w_{1,1} + 2w_{3,3} + 2w_{1,2} + 4w_{1,4}$

Table 7.1 continued.

type no.	type	equivalent types	c_W
63	$\begin{bmatrix} ab \\ ac \\ bc \end{bmatrix}$	69	$4w_{1,1} + 2w_{3,3} + 4w_{1,3} + 2w_{1,6}$
(64)	$\begin{bmatrix} ab \\ ac \\ cb \end{bmatrix}$	66	$4w_{1,1} + 2w_{3,3} + 2w_{1,3} + 2w_{1,4} + 2w_{1,5}$
65	$\begin{bmatrix} ab \\ ca \\ bc \end{bmatrix}$	68	$4w_{1,1} + 2w_{3,3} + 4w_{1,4} + 2w_{1,6}$
67	$\begin{bmatrix} ab \\ cc \\ ab \end{bmatrix}$		$4w_{1,1} + 2w_{3,3} + 4w_{1,5} + 2w_{3,4}$
70	$\begin{bmatrix} ab \\ cc \\ ba \end{bmatrix}$		$4w_{1,1} + 2w_{3,3} + 4w_{1,6} + 2w_{3,4}$
(71)	$\begin{bmatrix} aa \\ ab \\ cd \end{bmatrix}$	72	$4w_{1,1} + 2w_{3,3} + 2w_{1,2} + 2w_{1,3} + 2w_{1,4}$
(73)	$\begin{bmatrix} aa \\ bc \\ ad \end{bmatrix}$	74	$2w_{1,1} + 3w_{3,3} + w_{3,4}$ $(1, 0, 0, 1, 1, 0)$
(75)	$\begin{bmatrix} ab \\ aa \\ cd \end{bmatrix}$	79	$4w_{1,1} + w_{3,3} + w_{3,4}$ $(0, 1, 1, 0, 0, 1)$
(76)	$\begin{bmatrix} ab \\ ac \\ ad \end{bmatrix}$		$4w_{1,1} + 2w_{3,3} + 4w_{1,3} + 2w_{1,5}$
(77)	$\begin{bmatrix} ab \\ ac \\ da \end{bmatrix}$	80	$4w_{1,1} + 2w_{3,3} + 2w_{1,3} + 2w_{1,4} + 2w_{1,6}$
(78)	$\begin{bmatrix} ab \\ ca \\ ad \end{bmatrix}$		$4w_{1,1} + 2w_{3,3} + 4w_{1,4} + 2w_{1,5}$
(81)	$\begin{bmatrix} aa \\ bb \\ cd \end{bmatrix}$		$4w_{1,1} + 2w_{3,3} + 2w_{1,2} + 2w_{3,4}$
(82)	$\begin{bmatrix} aa \\ bc \\ bd \end{bmatrix}$	85	$4w_{1,1} + 2w_{3,3} + 2w_{1,2} + 2w_{1,3}$
(83)	$\begin{bmatrix} aa \\ bc \\ db \end{bmatrix}$	84	$4w_{1,1} + 2w_{3,3} + 2w_{1,2} + 2w_{1,4}$

Table 7.1 continued.

type no.	type	equivalent types	c_W
86	$\begin{bmatrix} aa \\ cd \\ bb \end{bmatrix}$		$4w_{1,1} + 2w_{3,3} + 4w_{1,2}$
87	$\begin{bmatrix} ab \\ ab \\ cd \end{bmatrix}$		$4w_{1,1} + 2w_{3,3} + 4w_{1,3}$
(88)	$\begin{bmatrix} ab \\ ac \\ bd \end{bmatrix}$	102	$4w_{1,1} + 2w_{3,3} + 2w_{1,3} + 2w_{1,6}$
(89)	$\begin{bmatrix} ab \\ ac \\ db \end{bmatrix}$	98	$4w_{1,1} + 2w_{3,3} + 2w_{1,3} + 2w_{1,5}$
(90)	$\begin{bmatrix} ac \\ ab \\ bd \end{bmatrix}$	95	$4w_{1,1} + 2w_{3,3} + 2w_{1,3} + 2w_{1,4}$
91	$\begin{bmatrix} ac \\ ab \\ db \end{bmatrix}$	106	$4w_{1,1} + 2w_{3,3} + 4w_{1,3}$
92	$\begin{bmatrix} ab \\ ba \\ cd \end{bmatrix}$		$4w_{1,1} + 2w_{3,3} + 4w_{1,4}$
(93)	$\begin{bmatrix} ab \\ ca \\ bd \end{bmatrix}$	101	$4w_{1,1} + 2w_{3,3} + 2w_{1,4} + 2w_{1,6}$
(94)	$\begin{bmatrix} ab \\ ca \\ db \end{bmatrix}$	97	$4w_{1,1} + 2w_{3,3} + 2w_{1,4} + 2w_{1,5}$
96	$\begin{bmatrix} ac \\ ba \\ db \end{bmatrix}$	105	$4w_{1,1} + 2w_{3,3} + 4w_{1,4}$
99	$\begin{bmatrix} ab \\ cd \\ ab \end{bmatrix}$		$4w_{1,1} + 2w_{3,3} + 4w_{1,5}$
(100)	$\begin{bmatrix} ac \\ bb \\ ad \end{bmatrix}$		$4w_{1,1} + 2w_{3,3} + 2w_{1,5} + 2w_{3,4}$
103	$\begin{bmatrix} ab \\ cd \\ ba \end{bmatrix}$		$4w_{1,1} + 2w_{3,3} + 4w_{1,6}$
(104)	$\begin{bmatrix} ac \\ bb \\ da \end{bmatrix}$	107	$4w_{1,1} + 2w_{3,3} + 2w_{1,6} + 2w_{3,4}$

Table 7.1 continued.

type no.	type	equivalent types	c_W
(108)	$\begin{bmatrix} a\,a \\ b\,c \\ d\,e \end{bmatrix}$		$4w_{1,1} + 2w_{3,3} + 2w_{1,2}$
(109)	$\begin{bmatrix} a\,b \\ a\,c \\ d\,e \end{bmatrix}$	114	$4w_{1,1} + 2w_{3,3} + 2w_{1,3}$
(110)	$\begin{bmatrix} a\,b \\ c\,a \\ d\,e \end{bmatrix}$	113	$4w_{1,1} + 2w_{3,3} + 2w_{1,4}$
(111)	$\begin{bmatrix} a\,b \\ c\,d \\ a\,e \end{bmatrix}$		$4w_{1,1} + 2w_{3,3} + 2w_{1,5}$
(112)	$\begin{bmatrix} a\,b \\ c\,d \\ e\,a \end{bmatrix}$	115	$4w_{1,1} + 2w_{3,3} + 2w_{1,6}$
116	$\begin{bmatrix} b\,c \\ a\,a \\ d\,e \end{bmatrix}$		$4w_{1,1} + 2w_{3,3} + 2w_{3,4}$
117	$\begin{bmatrix} a\,b \\ c\,d \\ e\,f \end{bmatrix}$		$4w_{1,1} + 2w_{3,3}$

7.4 Elements of Ω^*

Definition 7.5
The eigenvalues of Λ_1 are

$$\lambda_{1,1} = 1 + \rho_3 \quad \text{and} \quad \lambda_{1,2} = 1 - \rho_3,$$

and the eigenvalues of Λ_2 are

$$\lambda_{2,1} = 1 - \rho_2,$$

$$\lambda_{2,2} = \tfrac{1}{2}\left(2 + \rho_2 + \sqrt{\rho_2^2 + 8\rho_1^2}\right)$$

and $\lambda_{2,3} = \tfrac{1}{2}\left(2 + \rho_2 - \sqrt{\rho_2^2 + 8\rho_1^2}\right).$ ∎

This means that the eigenvalues of Λ are $\lambda_{1,i}\lambda_{2,j}$ for $i = 1,2$ and $j = 1,2,3$. For Λ to be positive definite $\lambda_{1,i}\lambda_{2,j} > 0$ is necessary for all i,j. Since $|\rho_1|, |\rho_2|, |\rho_3| < 1$, $\lambda_{1,1}$, $\lambda_{1,2}$, $\lambda_{2,1}$ and $\lambda_{2,2}$ are positive. Therefore for Λ to be positive definite $\lambda_{2,3} > 0$ is required. The condition $\lambda_{2,3} > 0$ is equivalent to $\vartheta_1 > 0$, where ϑ_1 is given in the following definition.

Definition 7.6
Let

$$\vartheta_1 = \lambda_{2,2}\lambda_{2,3} = 1 + \rho_2 - 2\rho_1^2, \qquad \vartheta_2 = 3 - 4\rho_1 + \rho_2,$$

$$\vartheta_3 = 1 - 2\rho_1 + \rho_2, \qquad\qquad \vartheta_4 = 1 - \rho_1,$$

$$\vartheta_5 = 1 + \rho_1, \qquad\qquad \vartheta^* = 2\lambda_{1,1}\lambda_{1,2}\lambda_{2,1}\vartheta_1\vartheta_2 \qquad\blacksquare$$

Note that ϑ_i ($i = 1,2,4,5$) and ϑ^* are positive when Λ is positive definite, and ϑ_3 can be positive or negative.

Expressions for the elements of Ω^* for the separable process are derived in Appendix A2.3, and are listed in Definition 7.7, with common denominator ϑ^*.

Definition 7.7

The elements of Ω^* for a separable process are

$$w_{1,1} = \vartheta_4\left(2\vartheta_2\vartheta_5 - \lambda_{1,2}\lambda_{2,1}\vartheta_4\right)/\vartheta^*,$$

$$w_{1,2} = -\vartheta_4\left(2\rho_3\vartheta_2\vartheta_5 + \lambda_{1,2}\lambda_{2,1}\vartheta_4\right)/\vartheta^*,$$

$$w_{1,3} = -\lambda_{2,1}\left(2\rho_1\vartheta_2 + \lambda_{1,2}\vartheta_3\vartheta_4\right)/\vartheta^*,$$

$$w_{1,4} = \lambda_{2,1}\left(2\rho_1\rho_3\vartheta_2 - \lambda_{1,2}\vartheta_3\vartheta_4\right)/\vartheta^*,$$

$$w_{1,5} = -\left\{2(\rho_2 - \rho_1^2)\vartheta_2 + \lambda_{1,2}\lambda_{2,1}\vartheta_4^2\right\}/\vartheta^*,$$

$$w_{1,6} = \left\{2\rho_3(\rho_2 - \rho_1^2)\vartheta_2 - \lambda_{1,2}\lambda_{2,1}\vartheta_4^2\right\}/\vartheta^*,$$

$$w_{3,3} = \lambda_{2,1}\left(2\vartheta_2\vartheta_5 - \lambda_{1,2}\vartheta_3^2\right)/\vartheta^*,$$

$$w_{3,4} = -\lambda_{2,1}\left\{2\rho_3(1 + \rho_2)\vartheta_2 + \lambda_{1,2}\vartheta_3^2\right\}/\vartheta^*. \qquad \blacksquare$$

For ease of reference, the terms given in Definition 7.5 and Definition 7.6 are now given here again:

$$\lambda_{1,1} = 1 + \rho_3, \qquad \lambda_{1,2} = 1 - \rho_3, \qquad \lambda_{2,1} = 1 - \rho_2,$$

$$\lambda_{2,2} = \tfrac{1}{2}\left(2 + \rho_2 + \sqrt{\rho_2^2 + 8\rho_1^2}\right), \qquad \lambda_{2,3} = \tfrac{1}{2}\left(2 + \rho_2 - \sqrt{\rho_2^2 + 8\rho_1^2}\right),$$

$$\vartheta_1 = \lambda_{2,2}\lambda_{2,3} = 1 + \rho_2 - 2\rho_1^2, \qquad \vartheta_2 = 3 - 4\rho_1 + \rho_2,$$

$$\vartheta_3 = 1 - 2\rho_1 + \rho_2, \qquad \vartheta_4 = 1 - \rho_1,$$

$$\vartheta_5 = 1 + \rho_1, \qquad \vartheta^* = 2\lambda_{1,1}\lambda_{1,2}\lambda_{2,1}\vartheta_1\vartheta_2.$$

7.5 Optimal designs

Specifying the regions of optimality for non-binary types is cumbersome, and so exact optimality regions are derived only for the six types: 117, 13, 18, 20, 60 and 67, in sections 7.5.1 to 7.5.6, respectively. The five non-binary types, 13, 18, 20, 60 and 67, are considered here since they cover much of the region in which Λ is positive definite when ρ_2 is not too large. When ρ_2 is non-positive these types cover most of the positive definite region. The optimality

regions for these types, for fixed $\rho_2 = -0.9, -0.5, 0, 0.5, 0.9$, are illustrated in Figure 7.1 to Figure 7.5, respectively.

A grid search over the parameter spaces of ρ_1, ρ_2 and ρ_3 (i.e. finding the type with maximum c_W for each (ρ_1, ρ_2, ρ_3) setting in the grid) indicates when other types are optimal. However, it is possible that types for which the optimality region is very small, may have been missed in the grid search. This means that optimality regions, for those types for which exact optimality regions have not been derived, can be extrapolated from the grid search results by comparing the c_W values for neighbouring types. These optimality regions may not be exact and therefore are called *tentative* optimality regions. The grid search also provides a check that the exact optimality regions for the six types listed above are correct.

Recall that Λ is positive definite when $\vartheta_1 > 0$. This means that $|\rho_1| < \sqrt{\frac{1}{2}(1 + \rho_2)}$ is needed. The vertical lines, $\rho_1 = \pm\sqrt{\frac{1}{2}(1 + \rho_2)}$, in Figure 7.1 to Figure 7.5, and the horizontal lines, $\rho_3 = \pm 1$, give a rectangle, the interior of which is the positive definite region.

Figure 7.3 illustrates the optimality regions for the NN1*NN1 process. The completely symmetric and separable process corresponds to the diagonal $\rho_1 = \rho_3$ in Figure 7.1 to Figure 7.5. The optimality regions for the AR(1)*AR(1) process are shown in Figure 7.6 in section 7.5.8.

The key, given below, shows the optimal types for Figure 7.1 to Figure 7.5.

KEY:

13	18	20	60	61	63	65	67
$\begin{bmatrix} aa \\ bb \\ aa \end{bmatrix}$	$\begin{bmatrix} ab \\ ab \\ ab \end{bmatrix}$	$\begin{bmatrix} ab \\ ba \\ ab \end{bmatrix}$	$\begin{bmatrix} aa \\ bb \\ cc \end{bmatrix}$	$\begin{bmatrix} aa \\ bc \\ bc \end{bmatrix}$	$\begin{bmatrix} ab \\ ac \\ bc \end{bmatrix}$	$\begin{bmatrix} ab \\ ca \\ bc \end{bmatrix}$	$\begin{bmatrix} ab \\ cc \\ ab \end{bmatrix}$

86	87	92	99	103	116	117
$\begin{bmatrix} aa \\ cd \\ bb \end{bmatrix}$	$\begin{bmatrix} ab \\ ab \\ cd \end{bmatrix}$	$\begin{bmatrix} ab \\ ba \\ cd \end{bmatrix}$	$\begin{bmatrix} ab \\ cd \\ ab \end{bmatrix}$	$\begin{bmatrix} ab \\ cd \\ ba \end{bmatrix}$	$\begin{bmatrix} bc \\ aa \\ de \end{bmatrix}$	$\begin{bmatrix} ab \\ cd \\ ef \end{bmatrix}$

Figure 7.1
Optimality regions for blocks of size 3×2 under a separable dependence structure, model IV and gls, for $\rho_2 = -0.9$.
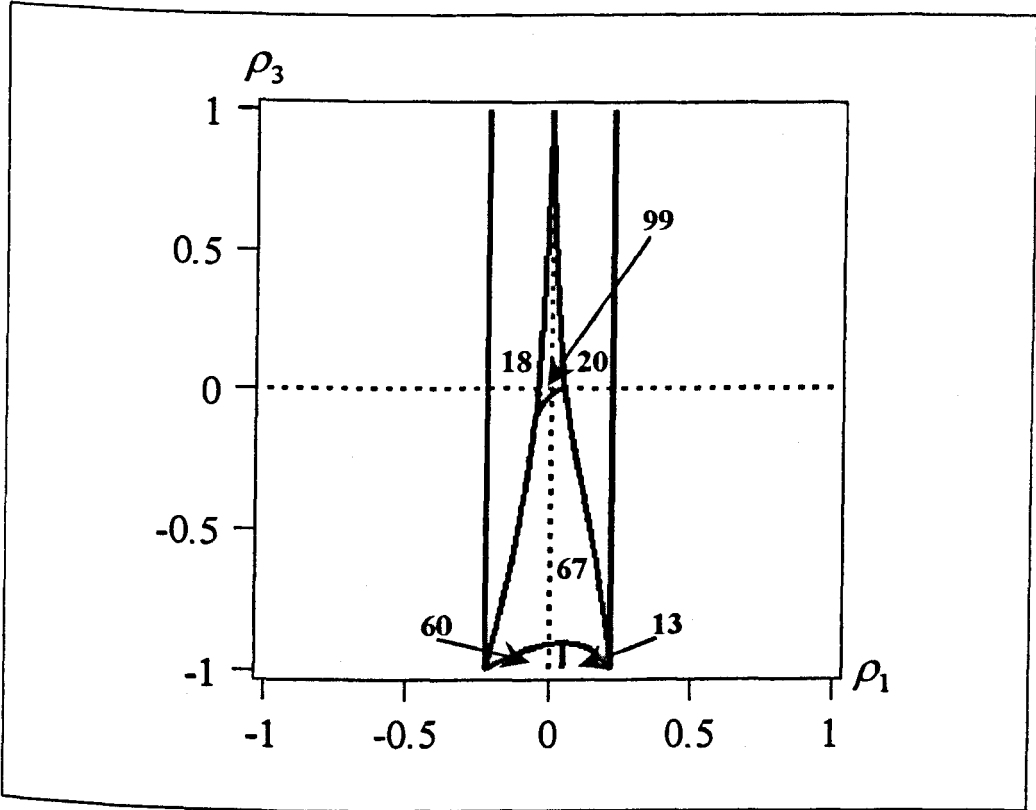
Figure 7.2   Optimality regions for $\rho_2 = -0.5$.
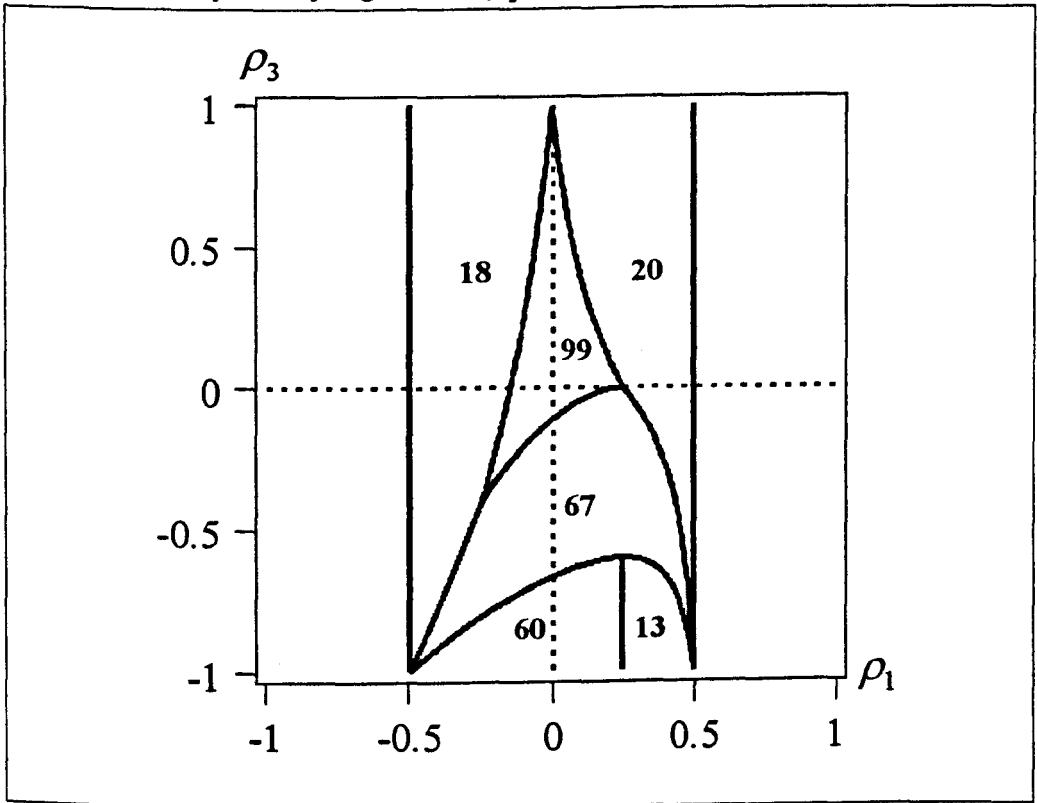
Figure 7.3   Optimality regions for $\rho_2 = 0$.
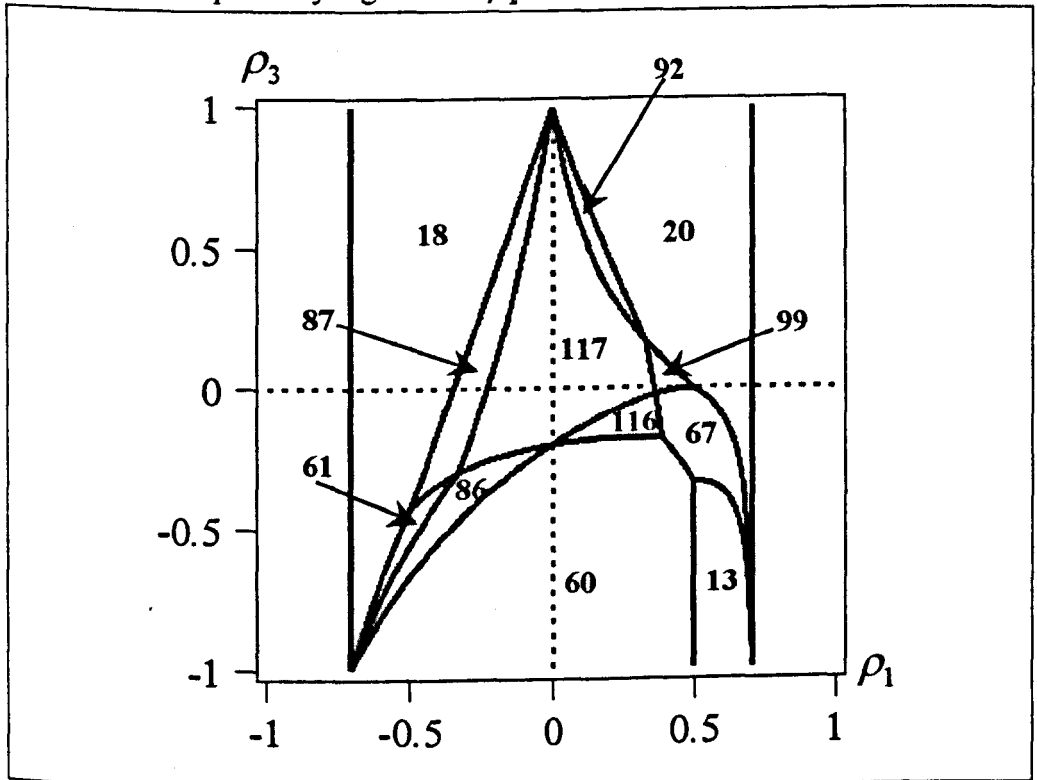
Figure 7.4 Optimality regions for $\rho_2 = 0.5$.
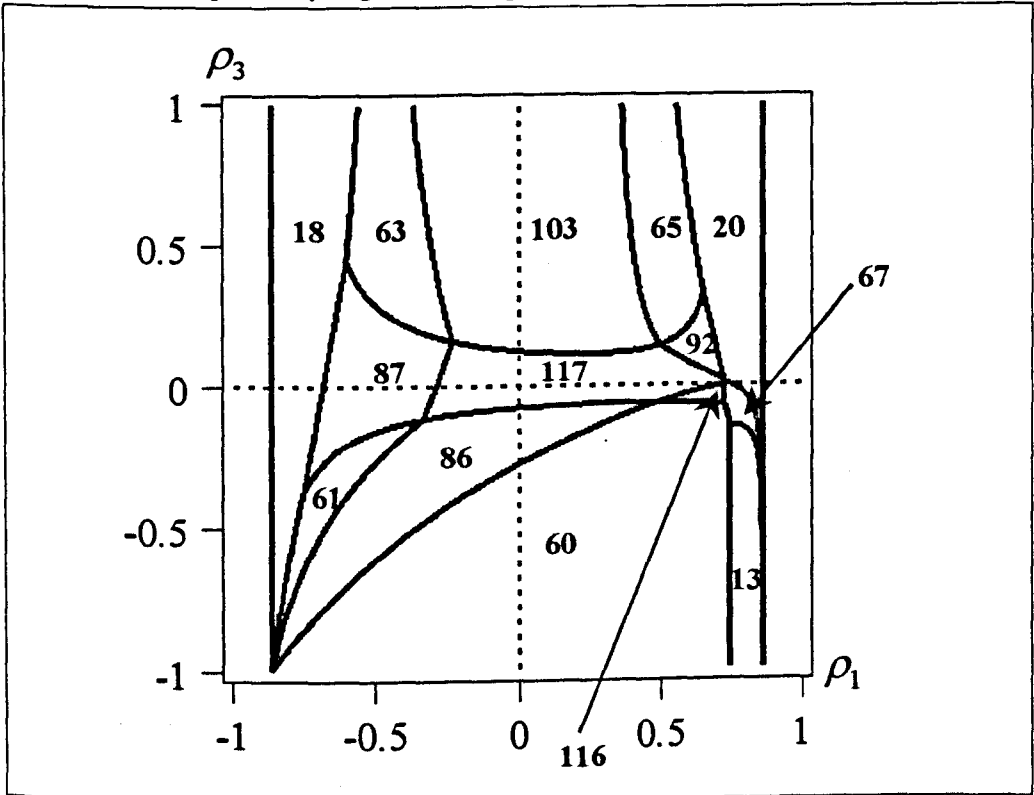
Figure 7.5 Optimality regions for $\rho_2 = 0.9$.
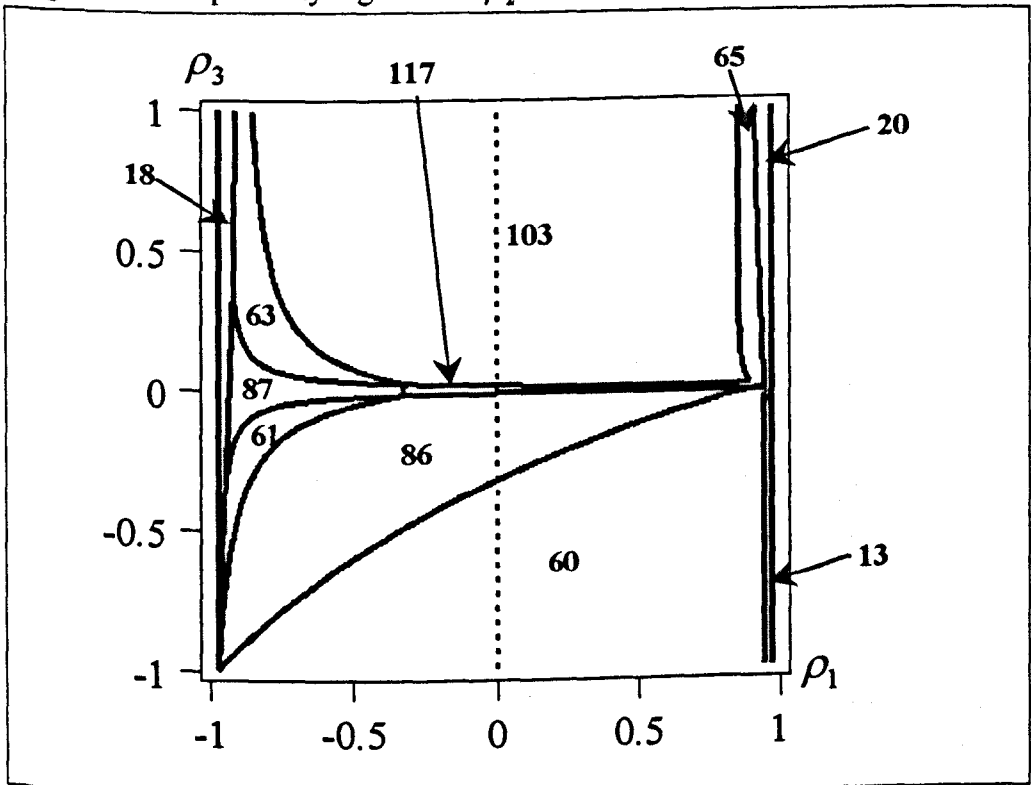
7.5.1   Optimality of type 117

In this section, the optimality region for the binary type (117) is specified. From Theorem 5.10 (in section 5.2.4.2), all the off-diagonal elements of Ω^* need to be non-positive for type 117 to be optimal over all $\mathcal{D}$. Here, $\mathcal{D}$ is the set of all connected designs with t treatments and b blocks of size 3×2. In the following, each of the off-diagonal elements of Ω^* are considered, and conditions given, in terms of the correlation parameters, for when these elements are non-positive.

First consider the expression for $w_{1,2}$ given in Definition 7.7 (at the end of section 7.4), which can be re-written as

$$w_{1,2} = -\vartheta_4(x_{1,2} + \rho_3 z_{1,2})/\vartheta^*,$$

where

$$x_{1,2} = \lambda_{2,1}\vartheta_4 = (1-\rho_2)(1-\rho_1)$$

and $z_{1,2} = 2\vartheta_2\vartheta_5 - \lambda_{2,1}\vartheta_4 = 5 - \rho_1 + 3\rho_2 + \rho_1\rho_2 - 8\rho_1^2.$

Note that

$$z_{1,2} - (3 + \rho_1)\vartheta_1 = 2(1-\rho_1)^2(1+\rho_1),$$

which is positive. Therefore $z_{1,2} > 0$, since Λ is positive definite (i.e. $\vartheta_1 > 0$). It then follows that

$$w_{1,2} \leq 0 \quad \text{if} \quad \rho_3 \geq -\frac{x_{1,2}}{z_{1,2}}. \tag{7.6}$$

The expression for $w_{1,3}$ can be re-written as

$$w_{1,3} = -\lambda_{2,1}(x_{1,3} - \rho_3 z_{1,3})/\vartheta^*,$$

where

$$x_{1,3} = 2\rho_1\vartheta_2 + \vartheta_3\vartheta_4 = 1 + 3\rho_1 + \rho_2 + \rho_1\rho_2 - 6\rho_1^2$$

and $z_{1,3} = \vartheta_3\vartheta_4 = (1-\rho_1)(1-2\rho_1+\rho_2).$

When $z_{1,3} < 0$, $x_{1,3}/z_{1,3} < -1$, so $\rho_3 \geq x_{1,3}/z_{1,3}$ is true for all $|\rho_3| < 1$ here.

Hence,

$$w_{1,3} \leq 0 \quad \text{if} \quad \begin{cases} \rho_3 \leq \dfrac{x_{1,3}}{z_{1,3}} & \text{for } z_{1,3} > 0 \\ z_{1,3} < 0 \end{cases}. \tag{7.7}$$

The expression for $w_{1,4}$ can be written as

$$w_{1,4} = -\lambda_{2,1}(z_{1,3} - \rho_3 x_{1,3})/\vartheta^*.$$

When $x_{1,3} < 0$, $z_{1,3}/x_{1,3} < -1$, so

$$w_{1,4} \leq 0 \quad \text{if} \quad \begin{cases} \rho_3 \leq \dfrac{z_{1,3}}{x_{1,3}} & \text{for } x_{1,3} > 0 \\ x_{1,3} < 0 \end{cases}. \tag{7.8}$$

For $w_{1,5}$:

$$w_{1,5} = -(x_{1,5} - \rho_3 z_{1,5})/\vartheta^*,$$

where

$$x_{1,5} = 2(\rho_2 - \rho_1^2)\vartheta_2 + \lambda_{2,1}\vartheta_4^2$$

$$= 1 - 2\rho_1 + 5\rho_2 - 6\rho_1\rho_2 - 5\rho_1^2 + 2\rho_2^2 - 3\rho_1^2\rho_2 + 8\rho_1^3$$

and $z_{1,5} = \lambda_{2,1}\vartheta_4^2 = (1 - \rho_2)(1 - \rho_1)^2$.

Clearly, $z_{1,5} > 0$, so

$$w_{1,5} \leq 0 \quad \text{if} \quad \rho_3 \leq \dfrac{x_{1,5}}{z_{1,5}}. \tag{7.9}$$

Now consider $w_{1,6}$:

$$w_{1,6} = -(z_{1,5} - \rho_3 x_{1,5})/\vartheta^*,$$

and

$$w_{1,6} \leq 0 \quad \text{if} \quad \rho_3 x_{1,5} \leq z_{1,5}. \tag{7.10}$$

Finally consider $w_{3,4}$:

$$w_{3,4} = -\lambda_{2,1}(x_{3,4} + \rho_3 z_{3,4})/\vartheta^*,$$

where

$$x_{3,4} = \vartheta_3^2 = (1 - 2\rho_1 + \rho_2)^2$$

and $\quad z_{3,4} = 2(1 + \rho_2)\vartheta_2 - \vartheta_3^2 = 5 - 4\rho_1 + 6\rho_2 - 4\rho_1\rho_2 - 4\rho_1^2 + \rho_2^2.$

Lemma 7.2

When Λ is positive definite, $z_{3,4} > 0$.

<u>Proof</u>

First consider when

$$z_{3,4} > 0$$

i.e. $\quad (5 - 4\rho_1 - 4\rho_1^2) + 2(3 - 2\rho_1)\rho_2 + \rho_2^2 > 0,$

i.e. $\quad \rho_2 < q_1(\rho_1) \quad$ or $\quad \rho_2 > q_2(\rho_1),$

where

$$q_1(\rho_1) = -3 + 2\rho_1 - 2\sqrt{1 - 2\rho_1 + 2\rho_1^2}$$

and $\quad q_2(\rho_1) = -3 + 2\rho_1 + 2\sqrt{1 - 2\rho_1 + 2\rho_1^2}.$

Only $q_2(\rho_1)$ needs to be considered since $q_1(\rho_1) < -1$. Therefore $z_{3,4} > 0$ when $\rho_2 > q_2(\rho_1)$.

Note that

$$\rho_2 - q_2(\rho_1) - \vartheta_1 = 2\left\{(1 - \rho_1 + \rho_1^2) - \sqrt{1 - 2\rho_1 + 2\rho_1^2}\right\}$$

is positive, since the inequality

$$2\left\{(1 - \rho_1 + \rho_1^2) - \sqrt{1 - 2\rho_1 + 2\rho_1^2}\right\} > 0$$

simplifies to

$$\rho_1^2(1 - \rho_1)^2 > 0.$$

Since $\vartheta_1 > 0$ (for Λ positive definite), it follows that $\rho_2 - q_2(\rho_1) > 0$, which completes the proof. ∎

It follows from Lemma 7.2 that

$$w_{3,4} \leq 0 \quad \text{if} \quad \rho_3 \geq -\frac{x_{3,4}}{z_{3,4}}. \tag{7.11}$$

Theorem 7.3
For blocks of size 3×2 and $t \geq 6$ treatments under model IV, gls and a separable dependence structure, a design of type 117 is optimal if the conditions given by (7.6) to (7.11) are satisfied. ∎

The boundaries of the optimality regions for type 117 correspond to $w_{i,j} = 0$ for $i \neq j$. In Figure 7.3 and Figure 7.4, for example, the curves enclosing the optimality region for type 117 correspond to $w_{i,j} = 0$ ($i \neq j$). For each of the equations $w_{i,j} = 0$ ($i \neq j$), Table 7.2 lists the type which is equivalent to type 117 (i.e. the non-binary type which has $c_W = 4w_{1,1} + 2w_{3,3}$).

Table 7.2
For blocks of size 3×2 under a separable dependence structure, model IV and gls, type e is equivalent to type 117 when $w_{i,j} = 0$.

$w_{i,j} = 0$ ($i \neq j$)	e
$w_{1,2} = 0$	86
$w_{1,3} = 0$	87
$w_{1,4} = 0$	92
$w_{1,5} = 0$	99
$w_{1,6} = 0$	103
$w_{3,4} = 0$	116

Corollary 7.4
Type 117 cannot be optimal when $\rho_2 < 16\sqrt{2} - 23 \approx -0.37$. ∎

The proof of Corollary 7.4 is in Appendix A2.5. It means that type 117 is not optimal in Figure 7.1 and Figure 7.2, for $\rho_2 = -0.9$ and $\rho_2 = -0.5$, respectively.

7.5.2   Optimality of type 13

In order to specify the optimality region for type 13, c_W for type 13 is compared to c_W for the 17 types in $\Xi \setminus \{13\}$. It is shown in Appendix A2.6 that for the optimality of type 13 it is sufficient that type 13 is better than types 20, 60 and 67. Conditions, in terms of $\{\rho_i\}$, are now derived for type 13 to be better than types 20, 60 and 67.

First consider type 13 better than type 20. This is true when

$$w_{3,3} + 2w_{3,4} \geq 2w_{1,1} + 4w_{1,4} + 2w_{1,5}.$$

After some algebra, it can be shown that this inequality is equivalent to

$$x_{13,20} + \rho_3 z_{13,20} \leq 0,$$

where

$$x_{13,20} = 7 - 8\rho_1 + \rho_2^2$$

and $z_{13,20} = 23 - 8\rho_1 + 16\rho_2 - 31\rho_1^2$.

Note that $z_{13,20} - 16\vartheta_1 = (1 - \rho_1)(7 - \rho_1)$ is positive. Hence, $\vartheta_1 > 0 \implies z_{13,20} > 0$ (i.e. $z_{13,20} > 0$ for Λ positive definite). Therefore type 13 is better than type 20 when

$$\rho_3 \leq -\frac{x_{13,20}}{z_{13,20}}. \tag{7.12}$$

Type 13 is better than type 60 when

$$w_{3,3} + w_{3,4} \geq 2w_{1,1} + 2w_{1,2}.$$

After some algebra, it can be shown that this is equivalent to

$$1 - 2\rho_1 + \rho_2 \leq 0$$

i.e. $\vartheta_3 \leq 0$. $\tag{7.13}$

Type 13 is better than type 67 when

$$w_{3,3} + w_{3,4} \geq 2w_{1,1} + 2w_{1,5}.$$

This is equivalent to

$$x_{13,67} + \rho_3 z_{13,67} \leq 0,$$

where

$$x_{13,67} = \vartheta_4^2 = (1 - \rho_1)^2$$

and $z_{13,67} = 2 - 2\rho_1 + \rho_2 - \rho_1^2.$

Note that $z_{13,67} - \vartheta_1 = (1 - \rho_1)^2$ is positive. Hence, $z_{13,67} > 0$ for Λ positive definite. Therefore type 13 is better than type 67 when

$$\rho_3 \leq -\frac{x_{13,67}}{z_{13,67}}. \tag{7.14}$$

Theorem 7.5
For blocks of size 3×2 and $t \geq 6$ treatments under model IV, gls and a separable dependence structure, a design of type 13 is optimal if the conditions given by (7.12) to (7.14) are satisfied. ∎

The proof of Theorem 7.5 is given in Appendix A2.6.

7.5.3   Optimality of type 18

It is shown in Appendix A2.7 that for type 18 to be optimal, it is sufficient that type 18 is better than types 60, 61, 63, 67, 87, 99. It is now shown when type 18 is better than these types, in terms of $\{\rho_i\}$.

First consider when type 18 is better than type 99. This occurs when

$$w_{1,3} \geq 0.$$

From section 7.5.1 it can be seen that $w_{1,3} \geq 0$ is equivalent to

$$\rho_3 \geq \frac{x_{1,3}}{z_{1,3}}. \tag{7.15}$$

For $z_{1,3} < 0$, type 18 cannot be better than type 99, since $x_{1,3}/z_{1,3} < -1$, so $z_{1,3} > 0$ is assumed.

Type 18 is better than type 60 when

$$4w_{1,3} + 2w_{1,5} \geq 2w_{1,2} + w_{3,4}.$$

After some algebra, this inequality can be written as

$$\rho_3 z_{18,60} \geq x_{18,60},$$

where

$$x_{18,60} = 3 + 16\rho_1 + 11\rho_2 - 24\rho_1\rho_2 - 40\rho_1^2 + 24\rho_1^2\rho_2 + \rho_2^2 - 8\rho_1\rho_2^2 + 16\rho_1^3 + \rho_2^3$$

and

$$z_{18,60} = 21 - 32\rho_1 + 5\rho_2 + 8\rho_1\rho_2 - 8\rho_1^2 - 8\rho_1^2\rho_2 - 9\rho_2^2 + 8\rho_1\rho_2^2 + 16\rho_1^3 - \rho_2^3.$$

It is easy to show that when $z_{18,60} < 0$, $x_{18,60}/z_{18,60} < -1$. Hence, $z_{18,60} > 0$ is assumed, and type 18 is better than type 60 when

$$\rho_3 \geq \frac{x_{18,60}}{z_{18,60}}. \tag{7.16}$$

Now consider when type 18 is better than type 61:

$$2w_{1,3} + 2w_{1,5} \geq w_{1,2}.$$

After some algebra, this inequality can be shown to be equivalent to

$$\rho_3 z_{18,61} \geq x_{18,61},$$

where

$$x_{18,61} = 3 + 7\rho_1 + 11\rho_2 - 7\rho_1\rho_2 - 16\rho_1^2 + 2\rho_2^2$$

and $z_{18,61} = 9 - 7\rho_1 + \rho_2 + 7\rho_1\rho_2 - 8\rho_1^2 - 2\rho_2^2.$

When $z_{18,61} < 0$, $x_{18,61}/z_{18,61} < -1$. Hence, $z_{18,61} > 0$ is assumed, and type 18 is better than type 61 when

$$\rho_3 \geq \frac{x_{18,61}}{z_{18,61}}. \tag{7.17}$$

Type 18 is better than type 63 when

$$2w_{1,3} + 2w_{1,5} \geq w_{1,6}.$$

This is equivalent to

$$\rho_3 z_{18,63} \geq x_{18,63},$$

where

$$x_{18,63} = \vartheta_4 x_{18,61} = (1 - \rho_1)(3 + 7\rho_1 + 11\rho_2 - 7\rho_1\rho_2 - 16\rho_1^2 + 2\rho_2^2)$$

and $z_{18,63} = 3 - 8\rho_1 - 7\rho_2 + 14\rho_1\rho_2 + 11\rho_1^2 - 3\rho_1^2\rho_2 - 4\rho_2^2 + 2\rho_1\rho_2^2 - 8\rho_1^3.$

For $z_{18,63} < 0$, $x_{18,63}/z_{18,63} < -1$, therefore $z_{18,63} > 0$ is assumed. Hence, type 18 is better than type 63 when

$$\rho_3 \geq \frac{x_{18,63}}{z_{18,63}}. \tag{7.18}$$

Type 18 is better than type 67 when

$$4w_{1,3} \geq w_{3,4}.$$

This is equivalent to

$$\rho_3 z_{18,67} \geq x_{18,67},$$

where

$$x_{18,67} = 3 + 16\rho_1 + 2\rho_2 + 8\rho_1\rho_2 - 28\rho_1^2 - \rho_2^2$$

and $z_{18,67} = 9 - 16\rho_1 + 10\rho_2 - 8\rho_1\rho_2 + 4\rho_1^2 + \rho_2^2.$

For $z_{18,67} < 0$, type 18 cannot be better than type 67, since $x_{18,67}/z_{18,67} < -1$, so $z_{18,67} > 0$ is assumed. Hence, type 18 is better than type 67 when

$$\rho_3 \geq \frac{x_{18,67}}{z_{18,67}}. \tag{7.19}$$

Finally, type 18 is better than type 87 when

$$w_{1,3} + w_{1,5} \geq 0$$

i.e.　$\rho_3 z_{18,87} \geq x_{18,87},$

where

$$x_{18,87} = 2 + 3\rho_1 + 5\rho_2 - 3\rho_1\rho_2 - 8\rho_1^2 + \rho_2^2$$

and　$z_{18,87} = \lambda_{2,1}(2 - 3\rho_1 + \rho_2) = 2 - 3\rho_1 - \rho_2 + 3\rho_1\rho_2 - \rho_2^2.$

For $z_{18,87} < 0$, $x_{18,87} / z_{18,87} < -1$, so $z_{18,87} > 0$ is assumed. Hence, type 18 is better than type 87 when

$$\rho_3 \geq \frac{x_{18,87}}{z_{18,87}}. \tag{7.20}$$

Theorem 7.6
For blocks of size 3×2 and $t \geq 6$ treatments under model IV, gls and a separable dependence structure, a design of type 18 is optimal if the conditions given by (7.15) to (7.20) are satisfied. ■

This theorem is proved in Appendix A2.7.

7.5.4 Optimality of type 20

For type 20 to be optimal, it is sufficient that type 20 is better than types 65, 67, 92 and 99, as shown in Appendix A2.8. In terms of $\{\rho_i\}$, the conditions in (7.21) to (7.24), given below, need to be satisfied for type 20 to be optimal.

Type 20 is better than type 65 when

$$2w_{1,4} + 2w_{1,5} \geq w_{1,6}.$$

After some algebra, this inequality can be written as

$$\rho_3 z_{20,65} \geq x_{20,65},$$

where

$$x_{20,65} = 3 - 8\rho_1 + 11\rho_2 - 10\rho_1\rho_2 - 7\rho_1^2 - 9\rho_1^2\rho_2 + 2\rho_2^2 + 2\rho_1\rho_2^2 + 16\rho_1^3$$

and $z_{20,65} = 3 + 4\rho_1 - 7\rho_2 + 6\rho_1\rho_2 - 5\rho_1^2 + 13\rho_1^2\rho_2 - 4\rho_2^2 - 2\rho_1\rho_2^2 - 8\rho_1^3.$

It is assumed that $z_{20,65} > 0$, since $x_{20,65}/z_{20,65} < -1$ when $z_{20,65} < 0$.

Therefore, type 20 is better than type 65 when

$$\rho_3 \geq \frac{x_{20,65}}{z_{20,65}}. \tag{7.21}$$

Now consider when type 20 is better than type 67:

$$4w_{1,4} \geq w_{3,4}.$$

This can be written as

$$\rho_3 z_{20,67} \geq x_{20,67},$$

where

$$x_{20,67} = 3 - 8\rho_1 + 2\rho_2 + 4\rho_1^2 - \rho_2^2$$

and $z_{20,67} = 9 + 8\rho_1 + 10\rho_2 - 28\rho_1^2 + \rho_2^2.$

It is assumed that $z_{20,67} > 0$, since for $z_{20,67} < 0$, $x_{20,67}/z_{20,67} < -1$.

Therefore, type 20 is better than type 67 when

$$\rho_3 \geq \frac{x_{20,67}}{z_{20,67}}. \tag{7.22}$$

Type 20 is better than type 92 when

$$w_{1,4} + w_{1,5} \geq 0$$

i.e. $\rho_3 z_{20,92} \geq x_{20,92}$,

where

$$x_{20,92} = 2 - 5\rho_1 + 5\rho_2 - 4\rho_1\rho_2 - 3\rho_1^2 - 5\rho_1^2\rho_2 + \rho_2^2 + \rho_1\rho_2^2 + 8\rho_1^3$$

and $z_{20,92} = (1 - \rho_2)(2 + \rho_1 + \rho_2 + \rho_1\rho_2 - 5\rho_1^2)$.

Similarly to the above comparisons, $z_{20,92} > 0$ is assumed. Therefore, type 20 is better than type 92 when

$$\rho_3 \geq \frac{x_{20,92}}{z_{20,92}}. \tag{7.23}$$

Finally, type 20 is better than type 99 when

$$w_{1,4} \geq 0,$$

which is equivalent to

$$\rho_3 \geq \frac{z_{1,3}}{x_{1,3}}, \tag{7.24}$$

(see the condition in (7.8) in section 7.5.1).

A proof of the following theorem is given in Appendix A2.8.

Theorem 7.7
For blocks of size 3×2 and $t \geq 6$ treatments under model IV, gls and a separable dependence structure, a design of type 20 is optimal if the conditions given by (7.21) to (7.24) are satisfied. ∎

7.5.5 Optimality of type 60

For the optimality of type 60, it is sufficient that type 60 is better than types 13, 67, 86 and 116, as shown in Appendix A2.9.

From the condition (7.13) in section 7.5.2, it follows immediately that type 60 is better than type 13 when

$$\vartheta_3 \geq 0. \tag{7.25}$$

Type 60 is better than type 67 when

$$w_{1,2} \geq w_{1,5}$$

i.e. $\quad \rho_3 \leq \dfrac{(\rho_2 - \rho_1^2)}{(1 - \rho_1^2)},$ $\tag{7.26}$

(from part of the proof of Lemma A2.16 in Appendix A2.8).

Type 60 is better than type 86 when

$$w_{3,4} \geq 0.$$

From the inequality (7.11) in section 7.5.1, it follows immediately that this is equivalent to

$$\rho_3 \leq -\frac{x_{3,4}}{z_{3,4}}, \tag{7.27}$$

where

$$x_{3,4} = \vartheta_3^2$$

and $\quad z_{3,4} = 5 - 4\rho_1 + 6\rho_2 - 4\rho_1\rho_2 - 4\rho_1^2 + \rho_2^2 > 0.$

Finally, type 60 is better than type 116 when

$$w_{1,2} \geq 0$$

i.e. $\quad \rho_3 \leq -\dfrac{x_{1,2}}{z_{1,2}}$ $\hspace{4cm}$ (7.28)

This follows from the inequality (7.6) in section 7.5.1. Recall that

$$x_{1,2} = \lambda_{2,1} \vartheta_4$$

and $\quad z_{1,2} = 5 - \rho_1 + 3\rho_2 + \rho_1 \rho_2 - 8\rho_1^2 > 0.$

A proof of the following theorem is given in Appendix A2.9.

Theorem 7.8

For blocks of size 3×2 and $t \geq 6$ treatments under model IV, gls and a separable dependence structure, a design of type 60 is optimal if the conditions given by (7.25) to (7.28) are satisfied. $\hspace{2cm}$ ∎

7.5.6   Optimality of type 67

Appendix A2.10 shows that for the optimality of type 67, it is sufficient that type 67 is better than types 13, 18, 20, 60, 99 and 116. The conditions for type 67 to be better than types 13, 18, 20 and 60, follow immediately from the inequalities (7.14), (7.19), (7.22) and (7.26), respectively. Type 67 is better than type 99 when the condition in (7.27) is satisfied. The condition for type 67 to be better than type 116, follows from the inequality in (7.9). These conditions for the optimality of type 67, in terms of $\{w_{i,j}\}$ and $\{\rho_i\}$, are given in Table 7.3.

Table 7.3

For blocks of size 3×2 under a separable dependence structure, model IV and gls: optimality conditions for type 67, where type 67 is better than type e

e	In terms of		
	$\{w_{i,j}\}$	$\{\rho_i\}$	
13	$2w_{1,1} + 2w_{1,5} \geq w_{3,3} + w_{3,4}$	$\rho_3 \geq -\dfrac{x_{13,67}}{z_{13,67}}$	(7.29)
18	$w_{3,4} \geq 4w_{1,3}$	$\rho_3 \leq \dfrac{x_{18,67}}{z_{18,67}}$ for $z_{18,67} > 0$ or $z_{18,67} < 0$	(7.30)
20	$w_{3,4} \geq 4w_{1,4}$	$\rho_3 \leq \dfrac{x_{20,67}}{z_{20,67}}$ for $z_{20,67} > 0$ or $z_{20,67} < 0$	(7.31)
60	$w_{1,5} \geq w_{1,2}$	$\rho_3 \geq \dfrac{(\rho_2 - \rho_1^2)}{(1 - \rho_1^2)}$	(7.32)
99	$w_{3,4} \geq 0$	$\rho_3 \leq -\dfrac{x_{3,4}}{z_{3,4}}$	(7.33)
116	$w_{1,5} \geq 0$	$\rho_3 \geq \dfrac{x_{1,5}}{z_{1,5}}$	(7.34)

Recall that

$$x_{13,67} = \vartheta_4^2,$$

$$z_{13,67} = 2 - 2\rho_1 + \rho_2 - \rho_1^2 > 0,$$

$$x_{18,67} = 3 + 16\rho_1 + 2\rho_2 + 8\rho_1\rho_2 - 28\rho_1^2 - \rho_2^2,$$

$$z_{18,67} = 9 - 16\rho_1 + 10\rho_2 - 8\rho_1\rho_2 + 4\rho_1^2 + \rho_2^2,$$

$$x_{20,67} = 3 - 8\rho_1 + 2\rho_2 + 4\rho_1^2 - \rho_2^2,$$

$$z_{20,67} = 9 + 8\rho_1 + 10\rho_2 - 28\rho_1^2 + \rho_2^2,$$

$$x_{3,4} = \vartheta_3^2,$$

$$z_{3,4} = 5 - 4\rho_1 + 6\rho_2 - 4\rho_1\rho_2 - 4\rho_1^2 + \rho_2^2 > 0,$$

$$x_{1,5} = 1 - 2\rho_1 + 5\rho_2 - 6\rho_1\rho_2 - 5\rho_1^2 + 2\rho_2^2 - 3\rho_1^2\rho_2 + 8\rho_1^3,$$

and $z_{1,5} = \lambda_{2,1}\vartheta_4^2.$

This gives the following theorem, which is proved in Appendix A2.10.

Theorem 7.9
For blocks of size 3×2 and $t \geq 6$ treatments under model IV, gls and a
separable dependence structure, a design of type 67 is optimal if the conditions
given by (7.29) to (7.34) are satisfied. ∎

7.5.7   Plots and description of optimality regions

Plots of the exact optimality regions for the six types 117, 13, 18, 20, 63 and
67 are in Figure 7.1 to Figure 7.5 for ρ_2 fixed at $-0.9, -0.5, 0, 0.5, 0.9$,
respectively. Tentative optimality regions (see section 7.5) for other optimal
types are also shown. For $\rho_2 < 0$, the optimality regions in Figure 7.1 and
Figure 7.2 are fairly simple, with six possible optimal types. However, for
$\rho_2 \geq 0$, Figure 7.3 to Figure 7.5 are much more complicated, with many more
optimal types (up to 14 optimal types).

As in the results in chapters 5 and 6, the binary type (117) is optimal when the
correlation parameters are near to zero. For the NN1*NN1 process ($\rho_2 = 0$)
the optimality region of type 117 is larger than for $\rho_2 = 0.5, 0.9$. As ρ_2 nears
1, this region becomes very small. Note that three of the types in Ξ (types 29,
62 and 70) do not seem to be optimal, at least for the settings of ρ_2 considered
here.

When $\rho_1, \rho_3 \geq 0$, only types 20, 65, 92, 99, 103 or 117,

$$\begin{bmatrix} ab \\ ba \\ ab \end{bmatrix}, \quad \begin{bmatrix} ab \\ ca \\ bc \end{bmatrix}, \quad \begin{bmatrix} ab \\ ba \\ cd \end{bmatrix}, \quad \begin{bmatrix} ab \\ cd \\ ab \end{bmatrix}, \quad \begin{bmatrix} ab \\ cd \\ ba \end{bmatrix} \quad \text{or} \quad \begin{bmatrix} ab \\ cd \\ ef \end{bmatrix},$$

respectively, can be optimal. All these types have no self-adjacencies in either
rows or columns. As ρ_1 and ρ_3 increase, the number of diagonal self-
adjacencies in the optimal type increases. Note that types 20, 65 and 92,
which are only optimal when $\rho_1, \rho_3 > 0$, all have diagonal adjacencies.

Types 18, 61, 63 and 87,

$$\begin{bmatrix} ab \\ ab \\ ab \end{bmatrix}, \quad \begin{bmatrix} aa \\ bc \\ bc \end{bmatrix}, \quad \begin{bmatrix} ab \\ ac \\ bc \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} ab \\ ab \\ cd \end{bmatrix},$$

respectively, are only optimal when $\rho_1 < 0$, that is, when the correlation of adjacent plots within a column is negative. These types have column self-adjacencies and no diagonal self-adjacencies. As ρ_1 approaches $-\sqrt{\frac{1}{2}(1+\rho_2)}$, type 18, which has the maximal number of column self-adjacencies, is optimal. Types which can be optimal over both $\rho_1 \geq 0$ and $\rho_1 < 0$ are types 60, 67, 86, 99, 103 and 117, none of which have column self-adjacencies.

Types 13, 60, 61, 67, 86 and 116,

$$\begin{bmatrix} aa \\ bb \\ cc \end{bmatrix}, \quad \begin{bmatrix} aa \\ bb \\ cc \end{bmatrix}, \quad \begin{bmatrix} aa \\ bc \\ bc \end{bmatrix}, \quad \begin{bmatrix} ab \\ cc \\ ab \end{bmatrix}, \quad \begin{bmatrix} aa \\ cd \\ bb \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} bc \\ aa \\ de \end{bmatrix},$$

respectively, are only optimal when $\rho_3 < 0$, that is, when the within-row correlation is negative. These types have at least one non-binary row, with the number of non-binary rows increasing as ρ_1 increases and ρ_3 decreases. Types 18, 20, 87, 99 and 117 can be optimal for both $\rho_3 \geq 0$ and $\rho_3 < 0$. All these types have binary rows.

7.5.8 Optimality results for the AR(1)*AR(1) process

This section specifies the optimality regions for the six types considered in sections 7.5.1 to 7.5.6 under the AR(1)*AR(1) process, which is a special case of the separable process with $\rho_2 = \rho_1^2$. For the AR(1)*AR(1) process $w_{1,5} = w_{1,6}$, so more of the 117 types listed in Table 5.3 are equivalent than under reflection symmetry. That is, types 67 and 70 are equivalent, as are types 99 and 103. Optimality regions for types 117, 18, 20 and 60 are specified here, and it is shown that types 13 and 67 cannot be optimal here. A plot of the optimality regions (given as Figure 7.6) shows that the nine types, 18, 20, 60, 61, 86, 87, 92, 116 and 117, can be optimal here. For types 18, 20,

60 and 117, exact optimality regions are specified, and for the remaining five types, tentative optimality regions are shown.

Figure 7.6
Optimality regions for blocks of size 3×2 under the AR(1)*AR(1) process, model IV and gls.
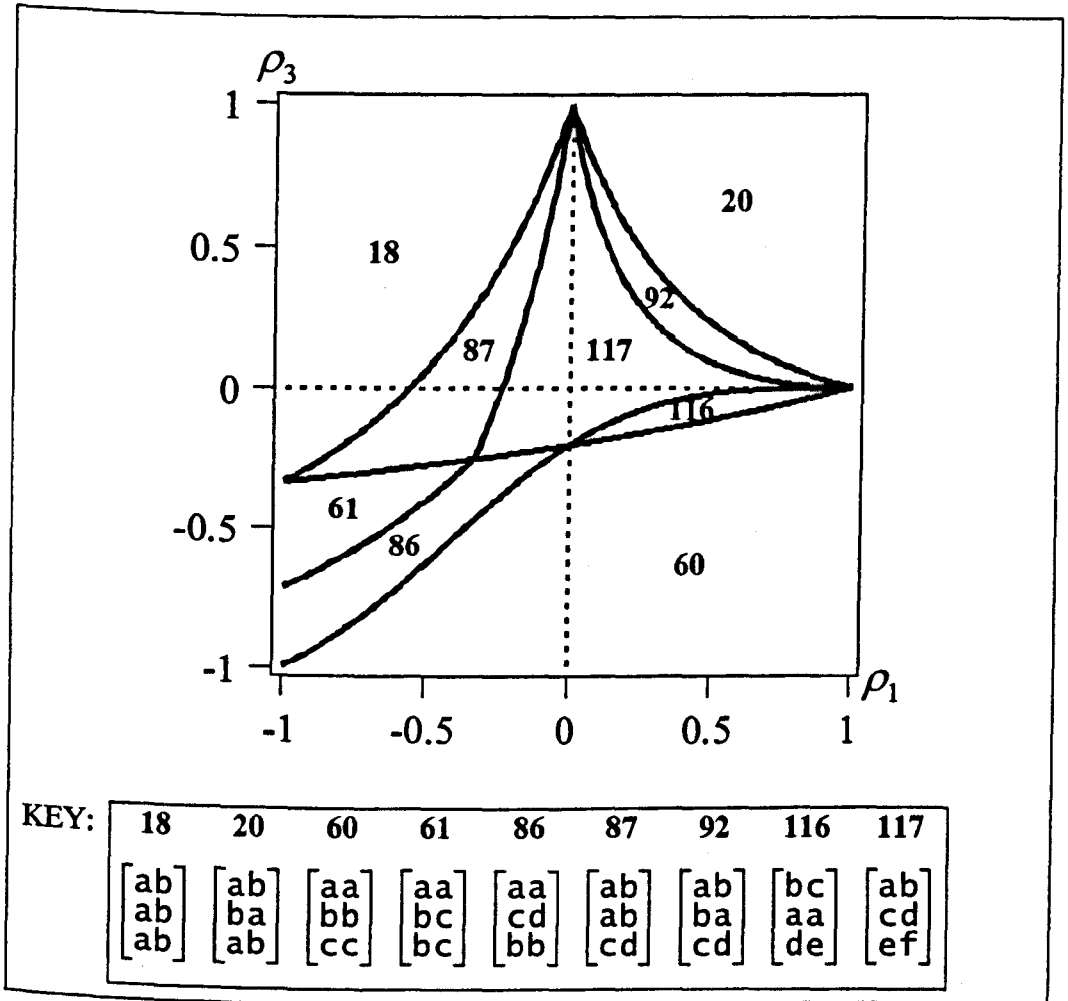
The conditions (7.6) to (7.11), for the optimality of the binary type (117) are simplified for the AR(1)*AR(1) process, and are given in Table 7.4. If ρ_1, $\rho_3 > 0$, the condition $w_{1,4} \leq 0$ in Table 7.4 for when $\rho_1 > 2 - \sqrt{5}$, is the optimality condition for type 117 given by Uddin and Morgan (1997a) (Theorem 5.18 in section 5.3.2.2.3). When ρ_1, $\rho_3 > 0$, clearly $w_{1,2} \leq 0$ and $w_{3,4} \leq 0$. It is also easy to show that $w_{1,4} \leq 0 \Rightarrow w_{1,3} \leq 0$ when ρ_1, $\rho_3 > 0$.

Table 7.4

For blocks of size 3×2 under the AR(1)*AR(1) process, model IV and gls: optimality conditions for type 117. † indicates that the condition is true.

$w_{1,2} \leq 0$	$\rho_3 \geq -\dfrac{(1-\rho_1)}{(5-\rho_1)}$
$w_{1,3} \leq 0$	$\rho_3 \leq \dfrac{(1+4\rho_1-\rho_1^2)}{(1-\rho_1)^2}$
$w_{1,4} \leq 0$	$\rho_3 \leq \dfrac{(1-\rho_1)^2}{(1+4\rho_1-\rho_1^2)}$ when $\rho_1 > 2-\sqrt{5}$ or $\rho_1 < 2-\sqrt{5}$
$w_{1,5} = w_{1,6} \leq 0$	$\rho_3 \leq 1$ †
$w_{3,4} \leq 0$	$\rho_3 \geq -\dfrac{(1-\rho_1)^3}{(5+\rho_1+3\rho_1^2-\rho_1^3)}$

For the optimality of type 18, conditions (7.15) to (7.20) need to be satisfied. However, under the AR(1)*AR(1) process it is sufficient that type 18 is better than type 87. That is, the condition (7.20), which simplifies to

$$\rho_3 \geq \frac{(2+3\rho_1-\rho_1^2)}{(1-\rho_1)(2-\rho_1)},$$

needs to be satisfied.

The four optimality conditions for the optimality of type 20, (7.21) to (7.24), are reduced to the one condition (7.23). This is the condition for type 20 to be better than type 92, and simplifies to

$$\rho_3 \geq \frac{(1-\rho_1)(2-\rho_1)}{(2+3\rho_1-\rho_1^2)}.$$

This is equivalent to the result in Uddin & Morgan (1997a), given here in Theorem 5.19 in section 5.3.2.2.3.

The two conditions (7.27) and (7.28) are sufficient for type 60 to be optimal. These conditions correspond to type 60 being better than types 86 and 116, and simplify, respectively, to:

$$\rho_3 \le -\frac{(1-\rho_1)^3}{(5+\rho_1+3\rho_1^2-\rho_1^3)}$$

and

$$\rho_3 \le -\frac{(1-\rho_1)}{(5-\rho_1)}.$$

Type 13 cannot be optimal here, since the condition, (7.13), for type 13 to be better than type 60, simplifies to $(1-\rho_1)^2 \le 0$. Also, type 67 cannot be optimal, since the condition (7.34) simplifies to $\rho_3 \ge 1$.

As mentioned previously, the binary type is optimal when the correlation is low (i.e. when (ρ_1,ρ_3) is near $(0,0)$). For $\rho_1,\rho_3 \ge 0$, only three types can be optimal. These are types 20, 92 and 117,

$$\begin{bmatrix} a & b \\ b & a \\ a & b \end{bmatrix}, \quad \begin{bmatrix} a & b \\ b & a \\ c & d \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} a & b \\ c & d \\ e & f \end{bmatrix},$$

respectively, which do not have any row or columns self-adjacencies, and the number of diagonal self-adjacencies increases as ρ_1 and ρ_3 increase.

When at least one of the correlation parameters are negative, optimal non-binary types have non-binary rows and/or columns, and no diagonal self-adjacencies. For $\rho_3 < 0$ and $\rho_1 > 0$ (positive within-column correlation) types 60, 116 and 117,

$$\begin{bmatrix} a & a \\ b & b \\ c & c \end{bmatrix}, \quad \begin{bmatrix} b & c \\ a & a \\ d & e \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} a & b \\ c & d \\ e & f \end{bmatrix},$$

respectively, which all have binary columns, are optimal. Also, as ρ_1 increases and ρ_3 decreases, the number of row self-adjacencies increases.

Similarly, when $\rho_1 < 0$ and $\rho_3 > 0$ (positive within-row correlation) types 18, 87 and 117,

$$\begin{bmatrix} ab \\ ab \\ ab \end{bmatrix}, \quad \begin{bmatrix} ab \\ ab \\ cd \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} ab \\ cd \\ ef \end{bmatrix},$$

respectively, which have binary rows, are optimal. Note that, as ρ_1 decreases and ρ_3 increases, the number of column self-adjacencies in the optimal type increases.

When $\rho_1, \rho_3 < 0$ six types can be optimal. These are types 18, 60, 61, 86, 87 and 117. All of these types, except type 117, have some column, row or diagonal self-adjacencies.

When $\rho_1 = \rho_3$, going from low ρ_1 to high ρ_1, types 86, 117, 92 and 20 are optimal. Type 86 is optimal when $\rho_1 \le -0.236$ (to 3 decimal places); type 117 is optimal when $-0.236 \le \rho_1 \le 0.268$; type 92 is optimal when $0.268 \le \rho_1 \le 0.358$; type 20 is optimal for $\rho_1 \ge 0.358$.

7.5.9   Discussion

It is clear that optimality regions are much more difficult to specify here than for the blocks of size 2×2 considered in chapter 6. For larger sized blocks, optimality results, are very difficult to obtain, unless the dependence structure is very simple. Even listing the different types for W centro-symmetric is computer intensive when blocks consist of $k \ge 8$ plots.

For large-sized blocks, given the dependence structure and its parameter values, optimising techniques, such as the simulated annealing algorithm of Martin & Eccleston (1997), could be used to try to solve the trace maximisation problem to find the optimal type. The design can then be constructed using SBAs. Another approach, for any number of blocks, is to use an optimisation technique to find a Φ_p-efficient design for a particular p. The former approach, although yielding a design with a large and restricted number of blocks, is likely to be much quicker at finding optimal designs since optimisation is over one block only.

8 Optimality results for the AR(1)*AR(1) process

8.1 Introduction

From the previous chapters, it is clear that optimality regions are very cumbersome to specify, unless the block size is very small, even if Λ has a simple structure. However, for the AR(1)*AR(1) process, which has a fairly simple structure for Λ^{-1}, optimality results have been derived by Uddin & Morgan (1997a, b) (see section 5.3) for blocks of size $p_1 \times 2$. In this chapter, further results are obtained for the AR(1)*AR(1) process under gls, using the SBA construction method. It is assumed here that $t \geq k$. For blocks of size $p_1 \times p_2$ ($p_1 \geq \max(2, p_2)$), the optimality region under model IV is specified in section 8.2 for the binary type, and it is shown that as p_1 and p_2 increase, the optimality region becomes smaller. The different off-diagonal elements of Ω^*, under model IV and gls, are listed. Although optimality conditions for non-binary designs, for general p_1, p_2, are extremely difficult to obtain, the results from Uddin & Morgan (1997a) for blocks of size $p_1 \times 2$ are extended, in section 8.3, for models III and IV under negative correlations. Also, optimality conditions for blocks of size 3×3 under model IV are derived in section 8.4.

8.2 Blocks of size $p_1 \times p_2$

The general blocksize $p_1 \times p_2$ for $p_1, p_2 \geq 2$, is considered in this section under model IV, gls and the AR(1)*AR(1) process.

Definition 8.1
In order to simplify the notation, the within-column and within-row correlation parameters, $\rho_{0,1}$ and $\rho_{1,0}$, are re-labelled as ρ_c and ρ_r, respectively. ∎

Recall from section 2.3.3.1 that, under the AR(1)*AR(1) process, the matrix

$$\Lambda = \Lambda_2 \otimes \Lambda_1,$$

where

$$\Lambda_1 = \begin{pmatrix} 1 & \rho_r & \rho_r^2 & \cdots & \rho_r^{p_2-1} \\ \rho_r & 1 & \rho_r & \cdots & \rho_r^{p_2-2} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \rho_r^{p_2-1} & \rho_r^{p_2-2} & \rho_r^{p_2-3} & \cdots & 1 \end{pmatrix}$$

and $\quad \Lambda_2 = \begin{pmatrix} 1 & \rho_c & \rho_c^2 & \cdots & \rho_c^{p_1-1} \\ \rho_c & 1 & \rho_c & \cdots & \rho_c^{p_1-2} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \rho_c^{p_1-1} & \rho_c^{p_1-2} & \rho_c^{p_1-3} & \cdots & 1 \end{pmatrix}$

for $|\rho_c|, |\rho_r| < 1$.

The elements of the matrix Ω^* are now derived. First consider

$$(1 - \rho_r^2)\Lambda_1^{-1} = (1 + \rho_r^2)I_{p_2} - \rho_r N_{p_2} - \rho_r^2 \Delta_{p_2},$$

where N_n and Δ_n are $n \times n$ matrices, such that

$$(N_n)_{i,j} = \begin{cases} 1 & \text{if } |i - j| = 1 \\ 0 & \text{otherwise} \end{cases}$$

and

$$(\Delta_n)_{i,j} = \begin{cases} 1 & \text{if } (i,j) = (1,1) \text{ or } (n,n) \\ 0 & \text{otherwise.} \end{cases}$$

It follows that

$$(1 - \rho_r^2)\Lambda_1^{-1}1_{p_2} = (1 - \rho_r)\big(1, (1-\rho_r), (1-\rho_r), \ldots, (1-\rho_r), 1 \big)',$$

and that

$$(1 - \rho_r^2)1_{p_2}'\Lambda_1^{-1}1_{p_2} = (1 - \rho_r)\{ 2 + (p_2 - 2)(1 - \rho_r) \}.$$

Similarly,

$$(1 - \rho_c^2)\Lambda_2^{-1}1_{p_1} = (1 - \rho_c)\big(1, (1-\rho_c), (1-\rho_c), \ldots, (1-\rho_c), 1 \big)',$$

and $\quad (1 - \rho_c^2)1_{p_1}'\Lambda_2^{-1}1_{p_1} = (1 - \rho_c)\{ 2 + (p_1 - 2)(1 - \rho_c) \}.$

The elements of Ω^* can be obtained from

$$\Omega^* = \Lambda_2^{-1} \otimes \Lambda_1^{-1} - \left(1_{p_1}'\Lambda_2^{-1}1_{p_1}\right)^{-1}\Lambda_2^{-1}1_{p_1}1_{p_1}'\Lambda_2^{-1} \otimes \left(1_{p_2}'\Lambda_1^{-1}1_{p_2}\right)^{-1}\Lambda_1^{-1}1_{p_2}1_{p_2}'\Lambda_1^{-1}.$$

When $p_1, p_2 \geq 5$, there are at most 25 distinct elements of Ω^*. In order to show which elements of Ω^* are equal, Ω^* is described in terms of the two classes of matrices described in Definition 8.2 and Definition 8.3.

Definition 8.2

Define a Class I $(n_1, n_2, U_1, U_2, U_3, U_4, U_5, U_6, U_7)$ matrix to be an $n_1n_2 \times n_1n_2$, symmetric and centro-symmetric matrix of the form

$$
\begin{pmatrix}
U_1 & U_2 & U_3 & U_3 & \cdots & U_3 & U_3 & U_4 \\
U_2 & U_5 & U_6 & U_7 & \cdots & U_7 & U_7 & U_3 \\
U_3 & U_6 & U_5 & U_6 & \ddots & U_7 & U_7 & U_3 \\
U_3 & U_7 & U_6 & U_5 & \ddots & U_7 & U_7 & U_3 \\
\vdots & \vdots & & \ddots & \ddots & & & \vdots \\
U_3 & U_7 & U_7 & U_7 & \ddots & U_5 & U_6 & U_3 \\
U_3 & U_7 & U_7 & U_7 & \cdots & U_6 & U_5 & U_2 \\
U_4 & U_3 & U_3 & U_3 & \cdots & U_3 & U_2 & U_1
\end{pmatrix}
\quad \text{for } n_1 \geq 5;
$$

$$
\begin{pmatrix}
U_1 & U_2 & U_3 & U_4 \\
U_2 & U_5 & U_6 & U_3 \\
U_3 & U_6 & U_5 & U_2 \\
U_4 & U_3 & U_2 & U_1
\end{pmatrix}
\quad \text{for } n_1 = 4;
$$

$$
\begin{pmatrix}
U_1 & U_2 & U_4 \\
U_2 & U_5 & U_2 \\
U_4 & U_2 & U_1
\end{pmatrix}
\quad \text{for } n_1 = 3;
$$

and
$$
\begin{pmatrix}
U_1 & U_2 \\
U_2 & U_1
\end{pmatrix}
\quad \text{for } n_1 = 2,
$$

where $U_1, U_2, U_3, U_4, U_5, U_6$ and U_7, are $n_2 \times n_2$ matrices for $n_2 \geq 1$. ∎

Definition 8.3

Define a Class $\mathrm{II}(n, u_1, u_2, u_3)$ matrix to be an $n \times n$ symmetric and centro-symmetric matrix of the form

$$
\begin{pmatrix}
u_1 & u_2 & u_2 & \cdots & u_2 & u_1 \\
u_2 & u_3 & u_3 & \cdots & u_3 & u_2 \\
u_2 & u_3 & u_3 & \cdots & u_3 & u_2 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
u_2 & u_3 & u_3 & \cdots & u_3 & u_2 \\
u_1 & u_2 & u_2 & \cdots & u_2 & u_1
\end{pmatrix} \quad \text{for } n \geq 3,
$$

and

$$
\begin{pmatrix}
u_1 & u_1 \\
u_1 & u_1
\end{pmatrix} \quad \text{for } n = 2,
$$

where u_1, u_2 and u_3 are scalars. ∎

Under model IV and gls, $\zeta_1 \Omega^*$ is a class I $(p_1, p_2, W_1, W_2, W_3, W_4, W_5, W_6, W_7)$ matrix, where ζ_1 is given in Definition 8.4 below. Let

$$
\zeta_1 \{\Omega^*\}_{j_1, j_2} = w_{j_1, j_2}.
$$

Before defining the matrices, $\{W_i\}$, note the functions of the correlation parameters given in Definition 8.4.

Definition 8.4

Let

$$
\zeta_1 = (1 - \rho_c^2)(1 - \rho_r^2)
$$

and

$$
\begin{aligned}
\zeta_2 &= \{2 + (p_1 - 2)(1 - \rho_c)\}\{2 + (p_2 - 2)(1 - \rho_r)\} \\
&= 4 + 2(p_1 - 2)(1 - \rho_c) + 2(p_2 - 2)(1 - \rho_r) + (p_1 - 2)(p_2 - 2)(1 - \rho_c)(1 - \rho_r)
\end{aligned}
$$

where $\zeta_i > 0$ for $i = 1, 2$. ∎

8.2.1 Elements of $\zeta_1 \Omega^*$

An element, w_{j_1,j_2}, from the matrix $\zeta_1 \Omega^*$ belongs to $\{s_1, s_2, ..., s_{31}\}$, where s_1 to s_{31} are defined in Definition 8.5. For $p_1, p_2 \geq 5$, $w_{j_1,j_2} \in \{s_1, s_2, ..., s_{25}\}$. Note that $s_1, ..., s_4 > 0$ and $s_{17}, ..., s_{25} < 0$.

Definition 8.5
Let

$$s_1 = 1 - (1 - \rho_c)(1 - \rho_r)/\zeta_2;$$

$$s_2 = (1 + \rho_r^2) - (1 - \rho_c)(1 - \rho_r)^3/\zeta_2;$$

$$s_3 = (1 + \rho_c^2) - (1 - \rho_c)^3(1 - \rho_r)/\zeta_2;$$

$$s_4 = (1 + \rho_c^2)(1 + \rho_r^2) - (1 - \rho_c)^3(1 - \rho_r)^3/\zeta_2;$$

$$s_5 = -\rho_r - (1 - \rho_c)(1 - \rho_r)^2/\zeta_2;$$

$$s_6 = -\rho_r - (1 - \rho_c)(1 - \rho_r)^3/\zeta_2;$$

$$s_7 = -\rho_r(1 + \rho_c^2) - (1 - \rho_c)^3(1 - \rho_r)^2/\zeta_2;$$

$$s_8 = -\rho_r(1 + \rho_c^2) - (1 - \rho_c)^3(1 - \rho_r)^3/\zeta_2;$$

$$s_9 = -\rho_c - (1 - \rho_c)^2(1 - \rho_r)/\zeta_2;$$

$$s_{10} = -\rho_c - (1 - \rho_c)^3(1 - \rho_r)/\zeta_2;$$

$$s_{11} = -\rho_c(1 + \rho_r^2) - (1 - \rho_c)^2(1 - \rho_r)^3/\zeta_2;$$

$$s_{12} = -\rho_c(1 + \rho_r^2) - (1 - \rho_c)^3(1 - \rho_r)^3/\zeta_2;$$

$$s_{13} = \rho_c\rho_r - (1 - \rho_c)^2(1 - \rho_r)^2/\zeta_2;$$

$$s_{14} = \rho_c\rho_r - (1 - \rho_c)^2(1 - \rho_r)^3/\zeta_2;$$

$$s_{15} = \rho_c\rho_r - (1 - \rho_c)^3(1 - \rho_r)^2/\zeta_2;$$

$$s_{16} = \rho_c\rho_r - (1 - \rho_c)^3(1 - \rho_r)^3/\zeta_2;$$

$$s_{17} = -(1 - \rho_c)(1 - \rho_r)/\zeta_2;$$

$$s_{18} = -(1 - \rho_c)(1 - \rho_r)^2/\zeta_2;$$

$$s_{19} = -(1 - \rho_c)(1 - \rho_r)^3/\zeta_2;$$

$$s_{20} = -(1-\rho_c)^2(1-\rho_r)/\zeta_2;$$

$$s_{21} = -(1-\rho_c)^3(1-\rho_r)/\zeta_2$$

$$s_{22} = -(1-\rho_c)^2(1-\rho_r)^2/\zeta_2;$$

$$s_{23} = -(1-\rho_c)^2(1-\rho_r)^3/\zeta_2;$$

$$s_{24} = -(1-\rho_c)^3(1-\rho_r)^2/\zeta_2;$$

$$s_{25} = -(1-\rho_c)^3(1-\rho_r)^3/\zeta_2;$$

$$s_{26} = -\rho_r - (1-\rho_c)(1-\rho_r)/\zeta_2;$$

$$s_{27} = -\rho_c - (1-\rho_c)(1-\rho_r)/\zeta_2;$$

$$s_{28} = \rho_c\rho_r - (1-\rho_c)(1-\rho_r)/\zeta_2;$$

$$s_{29} = \rho_c\rho_r - (1-\rho_c)^2(1-\rho_r)/\zeta_2;$$

$$s_{30} = \rho_c\rho_r - (1-\rho_c)^3(1-\rho_r)/\zeta_2;$$

$$s_{31} = -\rho_r(1+\rho_c^2) - (1-\rho_c)^3(1-\rho_r)/\zeta_2; \qquad \blacksquare$$

The elements of the matrices $\{W_i\}$ are now given in terms of the $\{s_i\}$.

The matrix W_1 is a class I ($p_2, 1, w_{1,1}, w_{1,2}, w_{1,3}, w_{1,p_2}, w_{2,2}, w_{2,3}, w_{2,4}$) matrix, where

$$w_{1,1} = s_1;$$

$$w_{1,2} = s_5 \quad \text{for } p_2 \geq 3;$$

$$w_{1,3} = s_{18} \quad \text{for } p_2 \geq 4;$$

$$w_{1,p_2} = \begin{cases} s_{26} & \text{for } p_2 = 2 \\ s_{17} & \text{for } p_2 \geq 3 \end{cases};$$

$$w_{2,2} = s_2 \quad \text{for } p_2 \geq 3;$$

$$w_{2,3} = s_6 \quad \text{for } p_2 \geq 4;$$

$$w_{2,4} = s_{19} \quad \text{for } p_2 \geq 5.$$

The matrix W_2 is a class I ($p_2, 1, w_{1,p_2+1}, w_{1,p_2+2}, w_{1,p_2+3}, w_{1,2p_2}, w_{2,p_2+2}, w_{2,p_2+3}, w_{2,p_2+4}$) matrix, where

$$w_{1,p_2+1} = \begin{cases} s_{27} & \text{for } p_1 = p_2 = 2 \\ s_9 & \text{otherwise} \end{cases};$$

$$w_{1,p_2+2} = s_{13} \quad \text{for } p_2 \geq 3;$$

$$w_{1,p_2+3} = s_{22} \quad \text{for } p_2 \geq 4;$$

$$w_{1,2p_2} = \begin{cases} s_{28} & \text{for } p_1 = p_2 = 2 \\ s_{29} & \text{for } p_1 \geq 3 \text{ and } p_2 = 2 \\ s_{20} & \text{for } p_2 \geq 3 \end{cases};$$

$$w_{2,p_2+2} = s_{11} \quad \text{for } p_2 \geq 3;$$

$$w_{2,p_2+3} = s_{14} \quad \text{for } p_2 \geq 4;$$

$$w_{2,p_2+4} = s_{23} \quad \text{for } p_2 \geq 5.$$

The matrix W_3 is a class II ($p_2, w_{1,2p_2+1}, w_{1,2p_2+2}, w_{2,2p_2+2}$) matrix, where, for $p_1 \geq 4$,

$$w_{1,2p_2+1} = s_{20};$$

$$w_{1,2p_2+2} = s_{22};$$

$$w_{2,2p_2+2} = s_{23}.$$

The matrix W_4 is a class II ($p_2, w_{1,(p_1-1)p_2+1}, w_{1,(p_1-1)p_2+2}, w_{2,(p_1-1)p_2+2}$) matrix, where, for $p_1 \geq 3$,

$$w_{1,(p_1-1)p_2+1} = s_{17};$$

$$w_{1,(p_1-1)p_2+2} = s_{18};$$

$$w_{2,(p_1-1)p_2+2} = s_{19}.$$

The matrix W_5 is a class I ($p_2, 1, w_{p_2+1, p_2+1}, w_{p_2+1, p_2+2}, w_{p_2+1, p_2+3}, w_{p_2+1, 2p_2}$, $w_{p_2+2, p_2+2}, w_{p_2+2, p_2+3}, w_{p_2+2, p_2+4}$) matrix, where, for $p_1 \geq 3$,

$$w_{p_2+1, p_2+1} = s_3;$$

$$w_{p_2+1, p_2+2} = s_7 \quad \text{for } p_2 \geq 3;$$

$$w_{p_2+1, p_2+3} = s_{24} \quad \text{for } p_2 \geq 4;$$

$$w_{p_2+1, 2p_2} = \begin{cases} s_{31} & \text{for } p_2 = 2 \\ s_{21} & \text{for } p_2 \geq 3 \end{cases};$$

$$w_{p_2+2, p_2+2} = s_4 \quad \text{for } p_2 \geq 3;$$

$$w_{p_2+2, p_2+3} = s_8 \quad \text{for } p_2 \geq 4;$$

$$w_{p_2+2, p_2+4} = s_{25} \quad \text{for } p_2 \geq 5.$$

The matrix W_6 is a class I ($p_2, 1, w_{p_2+1, 2p_2+1}, w_{p_2+1, 2p_2+2}, w_{p_2+1, 2p_2+3}, w_{p_2+1, 3p_2}$, $w_{p_2+2, 2p_2+2}, w_{p_2+2, 2p_2+3}, w_{p_2+2, 2p_2+4}$) matrix, where, for $p_1 \geq 4$,

$$w_{p_2+1, 2p_2+1} = s_{10};$$

$$w_{p_2+1, 2p_2+2} = s_{15} \quad \text{for } p_2 \geq 3;$$

$$w_{p_2+1, 2p_2+3} = s_{24} \quad \text{for } p_2 \geq 4;$$

$$w_{p_2+1, 3p_2} = \begin{cases} s_{30} & \text{for } p_2 = 2 \\ s_{21} & \text{for } p_2 \geq 3 \end{cases};$$

$$w_{p_2+2, 2p_2+2} = s_{12} \quad \text{for } p_2 \geq 3;$$

$$w_{p_2+2, 2p_2+3} = s_{16} \quad \text{for } p_2 \geq 4;$$

$$w_{p_2+2, 2p_2+4} = s_{25} \quad \text{for } p_2 \geq 5.$$

Finally, W_7 is a class II ($p_2, w_{p_2+1, 3p_2+1}, w_{p_2+1, 3p_2+2}, w_{p_2+2, 3p_2+2}$) matrix, where, for $p_1 \geq 5$,

$$w_{p_2+1, 3p_2+1} = s_{21};$$

$$w_{p_2+1, 3p_2+2} = s_{24};$$

$$w_{p_2+2, 3p_2+2} = s_{25}.$$

8.2.2   Optimality of the binary type

For a binary type to be optimal, all of the off-diagonal elements of Ω^* must be non-positive. By considering the elements of W_i, given in section 8.2.1, for $i = 1,2,...,7$, the optimality region for the binary type is specified.

First consider ρ_c, $\rho_r \geq 0$. Under this assumption, the $w_{j_1 j_2}$ ($j_1 \neq j_2$) which can be positive (and the corresponding s_i ($i \neq 1,2,3,4$)) are:

$$w_{1,p_2+2} = s_{13} = \rho_c \rho_r - (1-\rho_c)^2 (1-\rho_r)^2 / \zeta_2 \quad \text{for } p_2 \geq 3;$$

$$w_{1,2p_2} = \begin{cases} s_{28} = \rho_c \rho_r - (1-\rho_c)(1-\rho_r)/\zeta_2 & \text{for } p_1 = p_2 = 2 \\ s_{29} = \rho_c \rho_r - (1-\rho_c)^2 (1-\rho_r)/\zeta_2 & \text{for } p_1 \geq 3 \text{ and } p_2 = 2 \end{cases};$$

$$w_{2,p_2+3} = s_{14} = \rho_c \rho_r - (1-\rho_c)^2 (1-\rho_r)^3 / \zeta_2 \quad \text{for } p_2 \geq 4;$$

$$w_{p_2+1,2p_2+2} = s_{15} = \rho_c \rho_r - (1-\rho_c)^3 (1-\rho_r)^2 / \zeta_2 \quad \text{for } p_1 \geq 4 \text{ and } p_2 \geq 3;$$

$$w_{p_2+1,3p_2} = s_{30} = \rho_c \rho_r - (1-\rho_c)^3 (1-\rho_r)/\zeta_2 \quad \text{for } p_1 \geq 4 \text{ and } p_2 = 2;$$

$$w_{p_2+2,2p_2+3} = s_{16} = \rho_c \rho_r - (1-\rho_c)^3 (1-\rho_r)^3 / \zeta_2 \quad \text{for } p_1, p_2 \geq 4.$$

The following four cases, which include all valid values of p_1 and p_2 are considered:

i) $p_2 = 2$;

ii) $p_1 = p_2 = 3$;

iii) $p_1 \geq 4$ and $p_2 = 3$;

iv) $p_1, p_2 \geq 4$.

When $p_2 = 2$, there are three sub-cases that need to be examined:

i') $p_1 = 2$;

i") $p_1 = 3$;

i"') $p_1 \geq 4$.

For cases (i') and (i''), $s_{28} \leq 0$ and $s_{29} \leq 0$, respectively, are needed for the binary type to be optimal. For case (i'''), both $s_{29} \leq 0$ and $s_{30} \leq 0$ are needed. However, $s_{29} \leq s_{30}$, so a sufficient condition for the optimality of the binary type is $s_{30} \leq 0$. This gives exactly the conditions in Theorem 5.18 (Uddin & Morgan, 1997a). For case ii), $s_{13} \leq 0$ is required. For case (iii), $s_{15} \leq 0$ is sufficient, since $s_{13} \leq s_{15}$. For case (iv), the maximum of $\{s_{13}, s_{14}, s_{15}, s_{16}\}$ is s_{16}, so $s_{16} \leq 0$ is a sufficient condition for the optimality of the binary type.

Now assume that $\rho_c \geq 0$, $\rho_r < 0$. The $w_{j_1 j_2}$ $(j_1 \neq j_2)$ which can be positive (and the corresponding s_i $(i \neq 1,2,3,4)$) are:

$$w_{1,2} = s_5 = -\rho_r - (1-\rho_c)(1-\rho_r)^2 / \zeta_2 \quad \text{for } p_2 \geq 3;$$

$$w_{1,p_2} = s_{26} = -\rho_r - (1-\rho_c)(1-\rho_r) / \zeta_2 \quad \text{for } p_2 = 2;$$

$$w_{2,3} = s_6 = -\rho_r - (1-\rho_c)(1-\rho_r)^3 / \zeta_2 \quad \text{for } p_2 \geq 4;$$

$$w_{p_2+1,p_2+2} = s_7 = -\rho_r(1+\rho_c^2) - (1-\rho_c)^3(1-\rho_r)^2 / \zeta_2 \quad \text{for } p_1, p_2 \geq 3;$$

$$w_{p_2+1,2p_2} = s_{31} = -\rho_r(1+\rho_c^2) - (1-\rho_c)^3(1-\rho_r) / \zeta_2$$
$$\text{for } p_1 \geq 3 \text{ and } p_2 = 2;$$

$$w_{p_2+2,p_2+3} = s_8 = -\rho_r(1+\rho_c^2) - (1-\rho_c)^3(1-\rho_r)^3 / \zeta_2$$
$$\text{for } p_1 \geq 3 \text{ and } p_2 \geq 4.$$

The sufficient conditions for the optimality of the binary type are:

$s_{26} \leq 0$ for case (i');

$s_{31} \leq 0$ for cases (i'') and (i''');

$s_7 \leq 0$ for cases (ii), (iii) and (iv).

For $\rho_c < 0$, $\rho_r \geq 0$, the $w_{j_1 j_2}$ $(j_1 \neq j_2)$ which can be positive (and the corresponding s_i $(i \neq 1,2,3,4)$) are:

$$w_{1,p_2+1} = \begin{cases} s_{27} = -\rho_c - (1-\rho_c)(1-\rho_r)/\zeta_2 & \text{for } p_1 = p_2 = 2 \\ s_9 = -\rho_c - (1-\rho_c)^2(1-\rho_r)/\zeta_2 & \text{otherwise} \end{cases} ;$$

$$w_{2,p_2+2} = s_{11} = -\rho_c(1+\rho_r^2) - (1-\rho_c)^2(1-\rho_r)^3/\zeta_2 \quad \text{for } p_2 \geq 3;$$

$$w_{p_2+1,2p_2+1} = s_{10} = -\rho_c - (1-\rho_c)^3(1-\rho_r)/\zeta_2 \quad \text{for } p_1 \geq 4;$$

$$w_{p_2+2,2p_2+2} = s_{12} = -\rho_c(1+\rho_r^2) - (1-\rho_c)^3(1-\rho_r)^3/\zeta_2$$

$$\text{for } p_1 \geq 4 \text{ and } p_2 \geq 3.$$

The sufficient conditions for the optimality of the binary type are:

$s_{27} \leq 0$ for case (i');

$s_9 \leq 0$ for case (i");

$s_{10} \leq 0$ for case (i'");

$s_{11} \leq 0$ for cases (ii), (iii) and (iv).

Finally, assume that ρ_c, $\rho_r < 0$. The $w_{j_1 j_2}$ $(j_1 \neq j_2)$ which can be positive are the $w_{j_1 j_2}$ listed above for when $\rho_c \geq 0$ and/or $\rho_r \geq 0$. Sufficient conditions for the optimality of the binary type are:

$s_{26} \leq 0$ and $s_{27} \leq 0$ for case (i');

$s_{26} \leq 0$ and $s_9 \leq 0$ for cases (i") and (i'");

$s_5 \leq 0$ and $s_9 \leq 0$ for cases (ii), (iii) and (iv).

Figure 8.1 and Figure 8.2 show the optimality region for the binary type when $p_1 = p_2 = 4$ and $p_1 = p_2 = 10$, respectively. The curves corresponding to

$s_{16} = 0$ for ρ_c, $\rho_r \geq 0$;

$s_7 = 0$ for $\rho_c \geq 0$, $\rho_r < 0$;

$s_{11} = 0$ for $\rho_c < 0$, $\rho_r \geq 0$;

$s_5 = 0$ and $s_9 = 0$ for ρ_c, $\rho_r < 0$,

are the boundaries of the optimality region. Note that the curves given by $s_5 = 0$ and $s_7 = 0$ intersect at $\rho_c = 0$ and $\rho_r \approx -0.0690$ for $p_1 = p_2 = 4$, and they intersect at $\rho_c = 0$ and $\rho_r \approx -0.0101$ for $p_1 = p_2 = 10$. The curves given by $s_9 = 0$ and $s_{11} = 0$ intersect at $\rho_r = 0$ and $\rho_c \approx -0.0690$ for $p_1 = p_2 = 4$, and at $\rho_r = 0$ and $\rho_c \approx -0.0101$ for $p_1 = p_2 = 10$.

For ρ_c near 1, the binary design is optimal if ρ_r is near 0. Similarly, for ρ_r near 1, the binary design is optimal if ρ_c is near 0. If ρ_c or ρ_r are near -1, the binary design is not optimal, except when both ρ_c and ρ_r are near to -1 for $p_1 = p_2 = 2$ (see Figure 6.2d).

Figure 8.1
For the AR(1)*AR(1) process under model IV and gls: optimality region for binary type when $p_1 = p_2 = 4$.
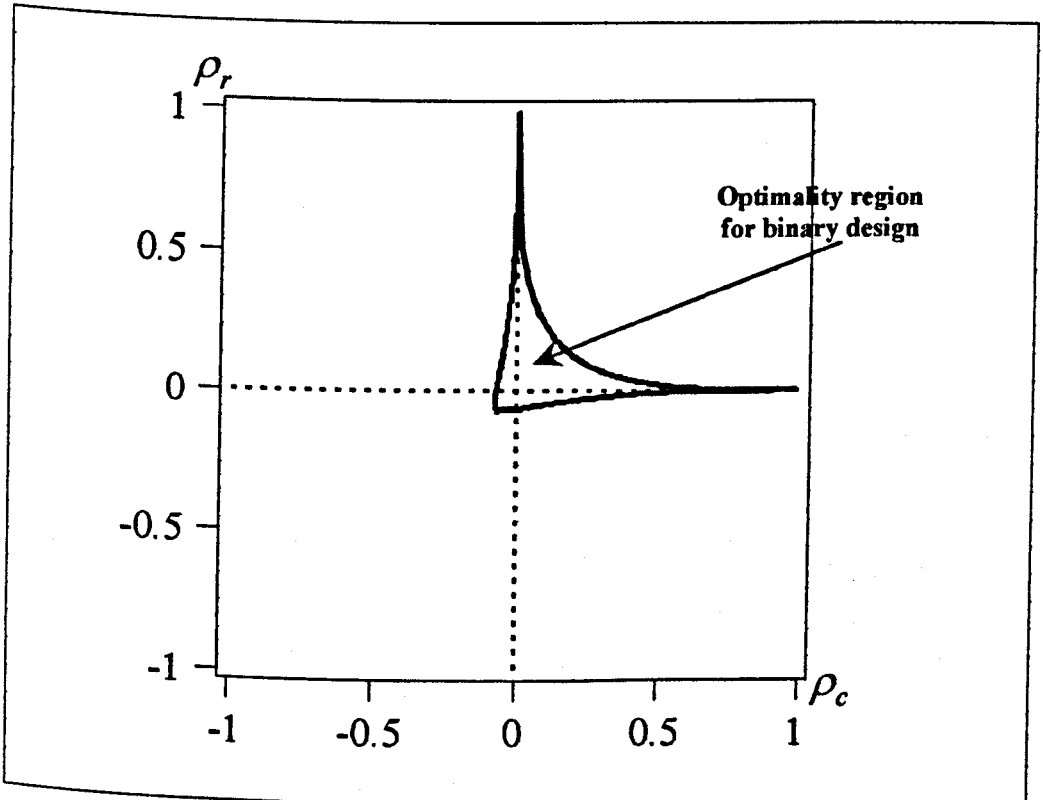
Figure 8.2

For the AR(1)*AR(1) process under model IV and gls: optimality region for binary type when $p_1 = p_2 = 10$.
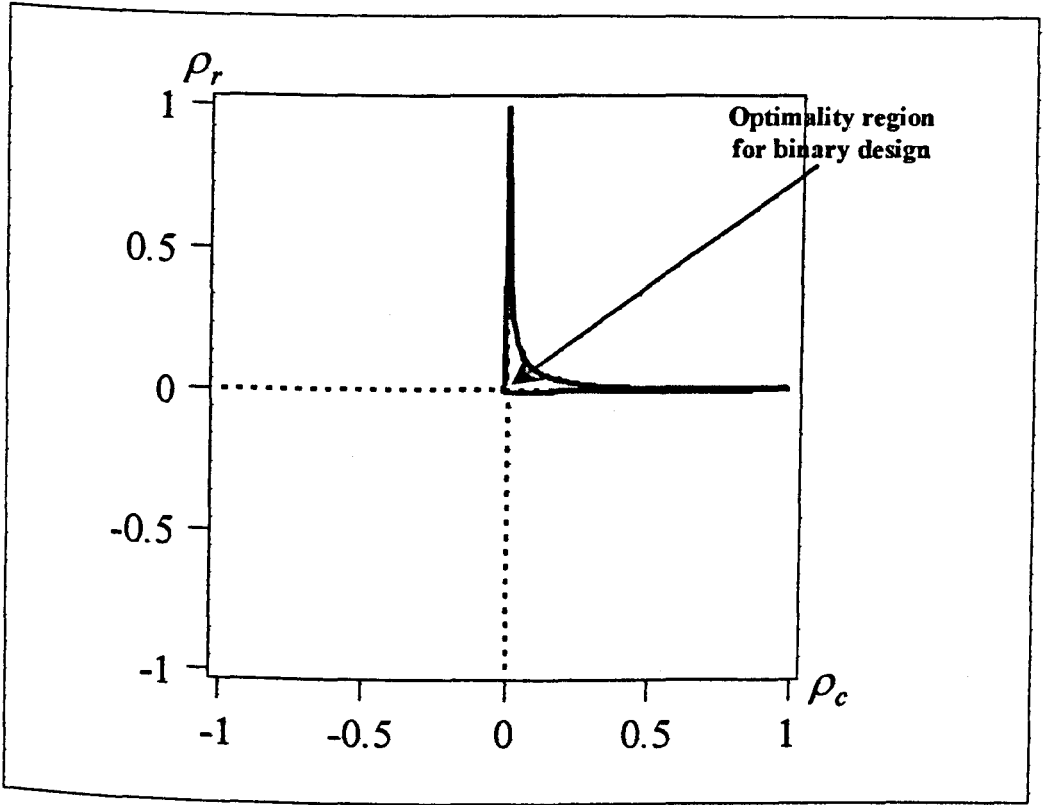
Notice that the size of the optimality region for the binary type is much smaller for $p_1 = p_2 = 10$ than for $p_1 = p_2 = 4$, with the binary type being optimal for a very small region when ρ_c, $\rho_r < 0$ for $p_1 = p_2 = 10$. For ρ_c, $\rho_r < 0$ the curves given by $s_5 = 0$ and $s_9 = 0$ intersect at $\rho_c = \rho_r \approx -0.0717$ and -0.0101 (to 4 decimal places) for $p_1 = p_2 = 4$ and $p_1 = p_2 = 10$, respectively.

For blocks of size 2×2 and 3×2 the optimality conditions derived here are precisely the optimality conditions from Theorem 6.1 (in section 6.2.1) and in Table 7.4 (in section 7.5.8), respectively. For other p_1 and p_2, optimality conditions are summarised in Theorem 8.1 to Theorem 8.3. Theorem 8.1 extends the results in Theorem 5.18 (Uddin & Morgan, 1997a) to negative correlations.

Theorem 8.1

For blocks of size $p_1 \times 2$ ($p_1 \geq 4$) and $t \geq k$ treatments under model IV, gls and an AR(1)*AR(1) process, a binary type design is optimal if and only if all the following conditions hold:

$$s_{10} \leq 0 \iff \rho_c + (1-\rho_c)^3(1-\rho_r)/\zeta_2 \geq 0,$$

$$s_{26} \leq 0 \iff \rho_r + (1-\rho_c)(1-\rho_r)/\zeta_2 \geq 0,$$

$$s_{30} \leq 0 \iff (1-\rho_c)^3(1-\rho_r)/\zeta_2 \geq \rho_c\rho_r,$$

$$s_{31} \leq 0 \iff \rho_r(1+\rho_c^2) + (1-\rho_c)^3(1-\rho_r)/\zeta_2 \geq 0. \qquad \blacksquare$$

Theorem 8.2

For blocks of size $p_1 \times 3$ ($p_1 \geq 3$) and $t \geq k$ treatments under model IV, gls and an AR(1)*AR(1) process, a binary type design is optimal if and only if all the following conditions hold:

$$s_5 \leq 0 \iff \rho_r + (1-\rho_c)(1-\rho_r)^2/\zeta_2 \geq 0,$$

$$s_7 \leq 0 \iff \rho_r(1+\rho_c^2) + (1-\rho_c)^3(1-\rho_r)^2/\zeta_2 \geq 0,$$

$$s_9 \leq 0 \iff \rho_c + (1-\rho_c)^2(1-\rho_r)/\zeta_2 \geq 0,$$

$$s_{11} \leq 0 \iff \rho_c(1+\rho_r^2) + (1-\rho_c)^2(1-\rho_r)^3/\zeta_2 \geq 0,$$

$$s_{13} \leq 0 \iff (1-\rho_c)^2(1-\rho_r)^2/\zeta_2 \geq \rho_c\rho_r \quad \text{for } p_1 = 3,$$

$$s_{15} \leq 0 \iff (1-\rho_c)^3(1-\rho_r)^2/\zeta_2 \geq \rho_c\rho_r \quad \text{for } p_1 \geq 4. \qquad \blacksquare$$

Theorem 8.3

For blocks of size $p_1 \times p_2$ ($p_1, p_2 \geq 4$) and $t \geq k$ treatments under model IV, gls and an AR(1)*AR(1) process, a binary type design is optimal if and only if all the following conditions hold:

$$s_5 \leq 0 \iff \rho_r + (1-\rho_c)(1-\rho_r)^2/\zeta_2 \geq 0,$$

$$s_7 \leq 0 \iff \rho_r(1+\rho_c^2) + (1-\rho_c)^3(1-\rho_r)^2/\zeta_2 \geq 0,$$

$$s_9 \leq 0 \iff \rho_c + (1-\rho_c)^2(1-\rho_r)/\zeta_2 \geq 0,$$

$$s_{11} \leq 0 \iff \rho_c(1+\rho_r^2) + (1-\rho_c)^2(1-\rho_r)^3/\zeta_2 \geq 0,$$

$$s_{16} \leq 0 \iff (1-\rho_c)^3(1-\rho_r)^3/\zeta_2 \geq \rho_c\rho_r. \qquad \blacksquare$$

For p_1 and p_2 not small, and $|\rho_c|, |\rho_r| < 1$.

$$s_5 \approx -\rho_r - (1-\rho_r)/(p_1 p_2);$$

$$s_7 \approx -\rho_r(1+\rho_c^2) - (1-\rho_c)^2(1-\rho_r)/(p_1 p_2);$$

$$s_9 \approx -\rho_c - (1-\rho_c)/(p_1 p_2);$$

$$s_{11} \approx -\rho_c(1+\rho_r^2) - (1-\rho_c)(1-\rho_r)^2/(p_1 p_2);$$

$$s_{16} \approx \rho_c \rho_r - (1-\rho_c)^2(1-\rho_r)^2/(p_1 p_2).$$

It follows that for fixed correlation parameters, as p_1 and p_2 increase, the optimality region for the binary type becomes smaller, as shown in Figure 8.1 and Figure 8.2. Also, when p_1 and p_2 are large, the binary type is optimal only for (ρ_c, ρ_r) very close to (0, 0).

That the optimality region for the binary type becomes smaller as p_1 and p_2 increase, is also shown by considering the optimality region for the binary type when $\rho_c = \rho_r$. For $\rho_c = \rho_r$, the binary type is optimal when $\rho_L \leq \rho_c \leq \rho_U$, where for $p_1 = p_2$, ρ_U and ρ_L can be obtained by solving

$$(1-\rho_U)^6 = \rho_U^2 \{p_1 - (p_1 - 2)\rho_U\}^2$$

and $(1-\rho_L)^3 = -\rho_L\{p_1 - (p_1 - 2)\rho_L\}^2,$

respectively. For $p_1 = p_2 = 2, 3, \ldots, 10, 50, 100$, the values of ρ_L and ρ_U are listed in Table 8.1.

Table 8.1

ρ_L and ρ_U

(to 3 decimal places, except that exact values are given for $p_1 = p_2 = 2$, and ρ_L and ρ_U are given to 4 decimal places for $p_1 = p_2 = 50, 100$).

$p_1 = p_2$	ρ_L	ρ_U
2	-1	$\frac{1}{3}$
3	-0.155	0.219
4	-0.072	0.161
5	-0.043	0.139
6	-0.029	0.123
7	-0.021	0.110
8	-0.016	0.099
9	-0.013	0.090
10	-0.010	0.083
50	-0.0004	0.0192
100	-0.0001	0.0098

For $p_1 = p_2$ not small, approximations for ρ_U and ρ_L can be obtained by solving

$$(1 - \rho_U)^2 = p_1 \rho_U \qquad (8.1)$$

and $\quad 1 - \rho_L = -p_1^2 \rho_L, \qquad (8.2)$

respectively. An approximate solution to the equation in (8.1) gives

$$\rho_U \approx 1/(p_1 + 2),$$

and the solution to the equation in (8.2) gives

$$\rho_L \approx -1/(p_1^2 - 1).$$

These approximations for ρ_U and ρ_L are reasonably close to the exact values in Table 8.1 for $p_1 \geq 4$ and $p_1 \geq 5$, respectively (for $p_1 = 4$, the approximation for ρ_U is $\frac{1}{6} \approx 0.167$, and for $p_1 = 5$, the approximation for ρ_L is $-1/24 \approx 0.042$). For $p_1 \geq 4$, $\rho_U < 1/(p_1 + 2)$ and $\rho_L > -1/(p_1^2 - 3)$. This means that $\rho_U - \rho_L < 1/(p_1 + 2) + 1/(p_1^2 - 3)$. Hence, as suggested by the values in Table 8.1, as $p_1 = p_2$ increases, the size of the optimality region for the binary type decreases.

8.3 Blocks of size $p_1 \times 2$

Uddin & Morgan (1997a) (see section 5.3.2) gave results for blocks of size $p_1 \times 2$ under the AR(1)*AR(1) process and gls. However, for models III and IV, they only considered ρ_c, $\rho_r \geq 0$. In this section, these results of Uddin & Morgan (1997a) are extended for either ρ_c or ρ_r negative. Models IV and III are considered, respectively, in sections 8.3.1 and 8.3.2. When both ρ_c and ρ_r are negative, deriving optimality results is much more difficult, and so attention is restricted here to $\rho_c \geq 0$ and $\rho_r < 0$, and to $\rho_c < 0$ and $\rho_r \geq 0$.

8.3.1 Model IV

Model IV is assumed in this section. For $\rho_c \geq 0$ and $\rho_r < 0$, optimality results follow easily from an examination of the off-diagonal elements of Ω^* which can be positive. This is described in section 8.3.1.1. In section 8.3.1.2, the method used by Uddin & Morgan (1997a) to obtain optimal types for positive correlations is adapted here for $\rho_c < 0$ and $\rho_r \geq 0$.

8.3.1.1 When $\rho_c \geq 0$ and $\rho_r < 0$

Under the assumption that $\rho_c \geq 0$ and $\rho_r < 0$, only the elements

$$w_{1,p_2} = w_{1,2} = -\rho_r - (1-\rho_c)(1-\rho_r)/\zeta_2$$

and $w_{p_2+1,2p_2} = w_{3,4} = -\rho_r(1+\rho_c^2) - (1-\rho_c)^3(1-\rho_r)/\zeta_2$ for $p_1 \geq 3$,

can be positive. Inclusion of the element $w_{1,2}$ in c_{Ω^*} corresponds to non-binary top and bottom (end) rows, and the inclusion of $w_{3,4}$ in c_{Ω^*} corresponds to the other (interior) rows being non-binary. The results in chapter 6 considered $p_1 = 2$, and hence attention is restricted to $p_1 \geq 3$ here.

Lemma 8.4

$$w_{3,4} \geq w_{1,2} \quad \text{for } \rho_c \geq 0 \text{ and } \rho_r < 0.$$

Proof

Note that

$$w_{3,4} - w_{1,2} = -\rho_r \rho_c^2 + (1 - \rho_c)(1 - \rho_r)\{1 - (1 - \rho_c)^2\}/\zeta_2.$$

It follows that for $\rho_c \geq 0$ and $\rho_r < 0$, $w_{3,4} \geq w_{1,2}$, since

$$1 - (1 - \rho_c)^2 = \rho_c(2 - \rho_c) \geq 0 \text{ and } \rho_r \rho_c^2 < 0. \qquad \blacksquare$$

It is clear from Lemma 8.4 that $w_{3,4} \leq 0 \Rightarrow w_{1,2} \leq 0$, and hence $w_{3,4} \leq 0$ (i.e. $s_{31} \leq 0$) is a sufficient condition for the optimality of the binary type (as shown in section 8.2.2, cases (i") and (i'")). This means that non-binary designs are optimal when $w_{3,4} \geq 0$. It follows immediately that designs D8.1 and D8.2, described below, are then optimal for $w_{1,2} \leq 0$ and $w_{3,4} \geq 0$, and $w_{1,2} \geq 0 (\Rightarrow w_{3,4} \geq 0)$, respectively.

Definition 8.6

Design D8.1 consists of blocks where the type has binary columns, binary end rows and non-binary interior rows. Design D8.2 consists of blocks where the type has binary columns and has all rows non-binary. $\qquad \blacksquare$

For example, when $p_1 = 5$, designs D8.1 and D8.2 have blocks of type

$$\begin{bmatrix} d\,e \\ a\,a \\ b\,b \\ c\,c \\ f\,g \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} a\,a \\ b\,b \\ c\,c \\ d\,d \\ e\,e \end{bmatrix},$$

respectively.

Now consider the following theorem.

Theorem 8.5
For blocks of size $p_1 \times 2$ ($p_1 \geq 3$) and $t \geq k$ under model IV, gls and an

AR(1)*AR(1) process, design D8.1 is optimal, for $\rho_c \geq 0$ and $\rho_r < 0$, if

$$w_{1,2} \leq 0 \text{ and } w_{3,4} \geq 0,$$

and design D8.2 is optimal if

$$w_{1,2} \geq 0,$$

otherwise the binary design is optimal. ■

As seen in the results in chapters 6 and 7 for the AR(1)*AR(1) process, when

$\rho_c \geq 0$, $\rho_r < 0$ and $p_2 = 2$ at most three types can be optimal, and as ρ_c

increases and/or ρ_r decreases the number of non-binary rows in the optimal

type increases. For $p_1 = 3$ (see Figure 7.6) D8.2 (called a design of type 60 in

chapter 7) is optimal for most of the region under consideration, including for

all $\rho_c \geq 0$ when $\rho_r < -\frac{1}{3}$. In general for $p_1 \geq 3$, D8.2 is optimal for all

$\rho_c \geq 0$ when $\rho_r < -1/(2p_1 - 1)$. Therefore, the size of the optimality region

for D8.2 increases as p_1 increases, and the size of the optimality regions for

the binary type and design D8.1 decreases.

8.3.1.2   When $\rho_c < 0$ and $\rho_r \geq 0$

For $\rho_c < 0$ and $\rho_r \geq 0$, the elements

$$w_{1,p_2+1} = w_{1,3} \quad \text{and} \quad w_{p_2+1,2p_2+1} = w_{3,5} \text{ for } p_1 \geq 4$$

can be positive. The inclusion of the element $w_{1,3}$ in $c_{\Omega^\bullet}$ corresponds to

column neighbours to the corner plots, and the inclusion of $w_{3,5}$ in $c_{\Omega^\bullet}$

corresponds to column neighbours for the other (interior) plots. Unlike in

section 8.3.1.1, optimality results cannot be easily obtained here by examining

the elements of $\Omega^\bullet$ which can be positive. Instead, optimal designs are

identified by the method used by Uddin & Morgan (1997a) to obtain

optimality results for $\rho_c, \rho_r \geq 0$. They made a close examination of *diagonal strings* in a type (see Uddin & Morgan, 1997a, for further details). Here, *column strings*, which are defined as a set of consecutive plots in a column containing the same treatment, are examined. The *column pattern* is the list of string lengths in a column, and a *column-type* (n, q_1, q_2) has n disjoint column strings, where the lengths of the strings containing the end plots are q_1 and q_2, such that $q_1 \geq q_2$. If there is only one column string, the column-type is $(1, p_1, 0)$. For example, for $p_1 = 7$, consider the type

$$
\begin{bmatrix}
a\,d \\
a\,d \\
b\,e \\
b\,e \\
g\,h \\
c\,f \\
c\,f
\end{bmatrix},
$$

which has disjoint columns of column-type (4,2,2), with column patterns (2,2,1,2).

The C-matrix under model IV, is given in section 5.3.2.2 as equation (5.20). It follows from this that

$$
\mathrm{tr}(C) = (1 + \rho_c^2)\mathrm{tr}(X'X) - \rho_c^2\mathrm{tr}(R_E) + \rho_c\rho_r\mathrm{tr}(N^D) - \rho_c\mathrm{tr}(N^C)
$$

$$
- \rho_r\mathrm{tr}(N^R) - \rho_c^2\rho_r\mathrm{tr}(N_I^R) - \{(1 - \rho_c)(1 - \rho_r)/\zeta_2\}\sum_{i=1}^{b} V_i'V_i ,
$$

where R_E, N^D, N^C, N^R, N_I^R and V_i are as defined in section 5.3.2.2. Clearly $\mathrm{tr}(X'X)$ is the number of plots in the design, and $\mathrm{tr}(R_E)$ is the number of corner plots in a design. Hence, an upper bound for $\mathrm{tr}(C)$ is given by $\mathrm{tr}(C) \leq 2p_1 b(1 + \rho_c^2) - 4b\rho_c^2 + H$, where

$$
H = -\rho_c\mathrm{tr}(N^C) - \{(1 - \rho_c)(1 - \rho_r)/\zeta_2\}\sum_{i=1}^{b} V_i'V_i ,
$$

with equality if

i) all the rows are binary (i.e. $\operatorname{tr}(N^R) = \operatorname{tr}(N_I^R) = 0$);

ii) there are no diagonal self-adjacencies (i.e. $\operatorname{tr}(N^D) = 0$).

It is assumed that columns 1 and 2 contain disjoint sets of treatments, so that (i) and (ii) are satisfied.

As well as assuming that all blocks are of the same type, it is assumed that both columns are of the same column-type. This means that H can be written as

$$H = -2bH^*,$$

where

$$H^* = \rho_c \operatorname{tr}(N_{ih}^C) + \{(1-\rho_c)(1-\rho_r)/\zeta_2\}V_{ih}{}'V_{ih},$$

and for any column h in any block i, $\operatorname{tr}(N_{ih}^C)$ and $V_{ih} = \underline{r}_{Eih} + (1-\rho_c)\underline{r}_{Iih}$ are the contributions of that column to $\operatorname{tr}(N^C)$ and V_i, respectively, and $\underline{r}_{Eih}$ and $\underline{r}_{Iih}$ are defined in section 5.3.2.2. Therefore, the optimal type can be found by minimising H^*.

Given any column h in any block i, it is always possible to make the column strings be composed of separate sets of treatments, without changing $\operatorname{tr}(N_{ih}^C)$. For example, consider the following two columns for $p_1 = 8$ and $t = 5$, called C1 and C2, respectively:

$$\begin{bmatrix} 1 \\ 1 \\ 2 \\ 3 \\ 3 \\ 1 \\ 1 \\ 4 \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} 1 \\ 1 \\ 2 \\ 3 \\ 3 \\ 4 \\ 4 \\ 5 \end{bmatrix}.$$

Column C1 has two strings containing treatment 1, and C2 has disjoint sets of strings. However, both C1 and C2 have $\operatorname{tr}(N_{ih}^C) = 6$.

Given two columns with the same value for $tr(N_{ih}^C)$, where only one of the two columns is composed of disjoint sets of strings, the column with the disjoint sets of strings will have a lower value for $V_{ih}'V_{ih}$ than the other column. Therefore the column with the disjoint sets of strings has a lower value for H^*. For example, C1 has

$$V_{ih}'V_{ih} = 2\{1 + 3(1 - \rho_c) + 7(1 - \rho_c)^2\},$$

and C2, which has disjoint sets of column strings, has a lower value for $V_{ih}'V_{ih}$ of

$$V_{ih}'V_{ih} = 2\{1 + (1 - \rho_c) + 5(1 - \rho_c)^2\}.$$

Hence, it is assumed that the column strings are composed of separate treatment sets, and the column-type which minimises H^* is the optimal column-type.

A column-type (n, q_1, q_2) with column pattern $(q_1, t_1, t_2, ..., t_{n-2}, q_2)$ and $q_2 \geq 1$ (i.e. $n > 1$) has

$$V_{ih}'V_{ih} = (1 - \rho_c)^2 \left\{ (q_1 - 1)^2 + (q_2 - 1)^2 + \sum_{l=1}^{n-2} t_l^2 \right\}$$

$$+ 2(1 - \rho_c)(q_1 + q_2 - 2) + 2 \qquad \text{for } n > 1.$$

For $n = 1$ (i.e. when $q_1 = p_1$ and $q_2 = 0$), $V_{ih}'V_{ih} = \frac{1}{4}\varsigma_2^2$.

For $n > 1$, $V_{ih}'V_{ih}$ is minimised over all column-types (n, q_1, q_2) by minimising $\sum_{l=1}^{n-2} t_l^2$ such that $\sum_{l=1}^{n-2} t_l = p_1 - q_1 - q_2$. Let the minimum value of $V_{ih}'V_{ih}$ over all column-types (n, q_1, q_2) be denoted by $w(n, q_1, q_2)$, then

$$w(n, q_1, q_2) = (1-\rho_c)^2 \left\{ (q_1 - 1)^2 + (q_2 - 1)^2 + k(p_1 - q_1 - q_2, n-2) \right\}$$
$$+ 2(1 - \rho_c)(q_1 + q_2 - 2) + 2 \qquad \text{for } n > 1,$$

where

$$k(x, y) = \min \sum_{i=1}^{y} t_i^2$$

for $\{t_1, t_2, ..., t_y\}$ a set of y non-negative integers, such that $\sum_{i=1}^{y} t_i = x$.

Uddin & Morgan (1997a) gave the value of $k(x, y)$ as

$$k(x, y) = x + (2x - y)\text{int}\left(\frac{x}{y}\right) - y\left\{\text{int}^2\left(\frac{x}{y}\right)\right\}.$$

For $n = 1$, it is clear that $w(1, p_1, 0) = \frac{1}{4}\zeta_2^2$. For a column-type (n, q_1, q_2), $\text{tr}(N_{ih}^C) = 2(p_1 - n)$.

Therefore, the optimal type consists of two disjoint columns, both of column-type (n, q_1, q_2), which minimise

$$2(p_1 - n)\rho_c + \{(1 - \rho_c)(1 - \rho_r)/\zeta_2\}w(n, q_1, q_2).$$

Given (p_1, ρ_c, ρ_r), this is an integer programming problem that can easily be solved on a computer. Similarly to Uddin & Morgan (1997a), this problem is solved for $p_1 = 3, 4, ..., 10, 15, 20$ and $\rho_r = 0.1, 0.2, ..., 0.9$, with $\rho_c = -\rho_r$. The optimal column types are given in Table 8.2. Recall that for $p_1 = 3$, column-types $(3,1,1)$, $(2,2,1)$ and $(1,3,0)$ correspond to types 117, 87 and 18, respectively, in chapter 7 (see Figure 7.6).

Table 8.2

For blocks of size $p_1 \times 2$ under the AR(1)*AR(1) process, model IV and gls: optimal column-types for $\rho_c = -\rho_r$.

p_1	— ρ_r								
	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9
3	(3,1,1)	(2,2,1)		(1,3,0)					
4	(4,1,1)	(2,2,2)			(1,4,0)				
5	(5,1,1)	(3,2,2)	(2,3,2)			(1,5,0)			
6	(3,2,2)		(2,3,3)				(1,6,0)		
7	(4,2,2)	(3,3,2)		(2,4,3)			(1,7,0)		
8	(4,2,2)		(3,3,3)	(2,4,4)				(1,8,0)	
9	(5,2,2)	(3,3,3)		(2,5,4)				(1,9,0)	
10	(5,2,2)	(4,3,3)	(3,4,3)		(2,5,5)			(1,10,0)	
15	(7,3,2)	(5,3,3)	(4,4,4)	(3,5,5)			(2,8,7)		(1,15,0)
20	(7,3,3)	(5,4,4)	(4,5,5)		(3,7,7)		(2,10,10)		(1,20,0)

Optimality conditions for the binary type have been given in section 8.2.2. Hence, attention is restricted here to $1 \le n \le p_1 - 1$. Optimality conditions for the column-type $(1, p_1, 0)$ are derived next, for which the following Lemma, from Uddin & Morgan (1997a, page 1199), is required.

Lemma 8.6 (Uddin & Morgan, 1997a)
For $2 \le n \le p_1$,

$$w(1,p_1,0) - w(n,q_1,q_2) \le \begin{cases} \tfrac{1}{8}(n-1)\zeta_2^2 & \text{for } p_1 \text{ even} \\ \tfrac{1}{8}(n-1)\{\zeta_2^2 - 4(1-\rho_c)^2\} & \text{for } p_1 \text{ odd} \end{cases},$$

with equality for $n = 2$ and $q_1 = \text{int}\{\tfrac{1}{2}(p_1 + 1)\}$.   ∎

Let D8.3 be a design with blocks that have disjoint columns of column-type $(1, p_1, 0)$. That is, D8.3 has blocks of type

$$\begin{bmatrix} ab \\ ab \\ \vdots \\ ab \end{bmatrix}.$$ D8.3

Theorem 8.7

For blocks of size $p_1 \times 2$ ($p_1 \geq 2$) and $t \geq k$ under model IV, gls and an

AR(1)*AR(1) process, design D8.3 is optimal, for $\rho_c < 0$ and $\rho_r \geq 0$, if

$$16\rho_c + (1-\rho_c)(1-\rho_r)\zeta_2 \leq 0 \quad \text{for } p_1 \text{ even;}$$

$$16\rho_c + (1-\rho_c)(1-\rho_r)\zeta_2 - 4(1-\rho_c)^3(1-\rho_r)/\zeta_2 \leq 0 \quad \text{for } p_1 \text{ odd.}$$

<u>Proof</u>

For a design of column-type $(1, p_1, 0)$, let H^* be called H_1^*, where

$$H_1^* = 2(p_1 - 1)\rho_c + \{(1-\rho_c)(1-\rho_r)/\zeta_2\}w(1, p_1, 0).$$

For any other column-type, let H^* be called H_2^*, where

$$H_2^* \geq 2(p_1 - n)\rho_c + \{(1-\rho_c)(1-\rho_r)/\zeta_2\}w(n, q_1, q_2) \quad \text{for } 2 \leq n \leq p_1 - 1.$$

Column-type $(1, p_1, 0)$ is then optimal if

$$H_1^* \leq H_2^*.$$

This is true if

$$H_1^* \leq 2(p_1 - n)\rho_c + \{(1-\rho_c)(1-\rho_r)/\zeta_2\}w(n, q_1, q_2),$$

i.e. $\quad 2(n-1)\rho_c + \{(1-\rho_c)(1-\rho_r)/\zeta_2\}\{w(1, p_1, 0) - w(n, q_1, q_2)\} \leq 0.$ (8.3)

By Lemma 8.6, the inequality in (8.3) is true for p_1 even when

$$2(n-1)\rho_c + \tfrac{1}{8}(n-1)(1-\rho_c)(1-\rho_r)\zeta_2 \leq 0,$$

i.e. $\quad 16\rho_c + (1-\rho_c)(1-\rho_r)\zeta_2 \leq 0,$

and similarly for p_1 odd. ∎

It is clear from Table 8.2 and from Theorem 8.7 that as ρ_c decreases and/or ρ_r increases, the number of column self-adjacencies in the optimal type increases. This is illustrated in Figure 7.6 for $p_1 = 3$, where type 18 corresponds to design D8.3. Note also that the size of the optimality region for design D8.3 becomes smaller as p_1 increases.

8.3.2 Model III

Assuming model III in this section, recall from Table 4.1 that $B = 1_{p_1} \otimes I_{p_2}$. Only blocks of size $p_1 \times 2$ are considered here. By a careful examination of the off-diagonal elements of Ω^* (given in section 8.3.2.1) some optimality results are derived for $p_1 \geq 3$ in section 8.3.2.2. For $p_1 = 3$, the problem of finding optimal types is completely solved for $|\rho_c|$, $|\rho_r| < 1$. For $p_1 \geq 4$, optimality results are much more difficult, in general, to derive. However, some results, which were fairly easily be obtained, are given.

8.3.2.1 *Elements of* $\zeta_1 \Omega^*$

Here the elements of $\Omega^* = \Lambda^{-1} - \Lambda^{-1}B(B'\Lambda^{-1}B)^{-1}B'\Lambda^{-1}$ are derived. Recall that $\Lambda = \Lambda_2 \otimes \Lambda_1$, where Λ_1 and Λ_2 are defined in section 2.3.3.1. Consider

$$\Lambda^{-1}B = \left(\Lambda_2^{-1} \otimes \Lambda_1^{-1}\right)\left(1_{p_1} \otimes I_{p_2}\right) = \Lambda_2^{-1}1_{p_1} \otimes \Lambda_1^{-1}.$$

If follows that

$$B'\Lambda^{-1}B = \left(1_{p_1}'\Lambda_2^{-1}1_{p_1}\right)\Lambda_1^{-1},$$

so then

$$\left(B'\Lambda^{-1}B\right)^{-1} = \left(1_{p_1}'\Lambda_2^{-1}1_{p_1}\right)^{-1}\Lambda_1.$$

Therefore,

$$\Lambda^{-1}B(B'\Lambda^{-1}B)^{-1}B'\Lambda^{-1} = \left(1_{p_1}'\Lambda_2^{-1}1_{p_1}\right)^{-1}\Lambda_2^{-1}J_{p_1}\Lambda_2^{-1} \otimes \Lambda_1^{-1}$$

$$= \{2(1+\rho_c)/\zeta_2\}\Lambda_2^{-1}J_{p_1}\Lambda_2^{-1} \otimes \Lambda_1^{-1},$$

since $1_{p_1}'\Lambda_2^{-1}1_{p_1} = \tfrac{1}{2}\zeta_2(1-\rho_c)/(1-\rho_c^2) = \tfrac{1}{2}\zeta_2/(1+\rho_c)$.

Note that $(1+\rho_c)^2\Lambda_2^{-1}J_{p_1}\Lambda_2^{-1}$ is a class II ($p_1, 1, (1-\rho_c), (1-\rho_c)^2$) matrix.

Now consider

$$\Omega^* = \left(\Lambda_2^{-1} - \{2(1+\rho_c)/\zeta_2\}\Lambda_2^{-1} J_{p_1} \Lambda_2^{-1} \right) \otimes \Lambda_1^{-1}.$$

This means that, for $p_2 = 2$ under model III and gls, $\zeta_1\Omega^*$ is a

class I $(p_1, 2, W_1, W_2, W_3, W_4, W_5, W_6, W_7)$ matrix. As for model IV, let

$$\zeta_1 \{\Omega^*\}_{j_1, j_2} = w_{j_1, j_2}.$$

The 2×2 matrices $\{W_i\}$ are of class I $(2, 1, w_{j_1, j_2}, w_{j_1, j_2+1})$, such that

$$w_{j_1, j_2+1} = -\rho_r w_{j_1, j_2} \text{ for } j_2 \text{ odd.}$$

The elements w_{j_1, j_2} for j_2 odd, are defined in Table 8.3.

Table 8.3
For blocks of size $p_1 \times 2$ under the AR(1)*AR(1) process, model III and gls: element w_{j_1, j_2} of the matrix W_i for j_2 odd $(i = 1, 2, ..., 7)$.

i	(j_1, j_2)	w_{j_1, j_2}
1	$(1,1)$	$1 - 2(1-\rho_c)/\zeta_2 > 0$
2	$(1,3)$	$\begin{cases} -\rho_c - 2(1-\rho_c)/\zeta_2 < 0 & \text{for } p_1 = 2 \\ -\rho_c - 2(1-\rho_c)^2/\zeta_2 & \text{for } p_1 \geq 3 \end{cases}$
3	$(1,5)$	$-2(1-\rho_c)^2/\zeta_2 < 0 \qquad \text{for } p_1 \geq 4$
4	$(1, 2p_1 - 1)$	$-2(1-\rho_c)/\zeta_2 < 0 \qquad \text{for } p_1 \geq 3$
5	$(3,3)$	$(1+\rho_c^2) - 2(1-\rho_c)^3/\zeta_2 > 0 \quad \text{for } p_1 \geq 3$
6	$(3,5)$	$-\rho_c - 2(1-\rho_c)^3/\zeta_2 \qquad \text{for } p_1 \geq 4$
7	$(3,7)$	$-2(1-\rho_c)^3/\zeta_2 < 0 \qquad \text{for } p_1 \geq 5$

8.3.2.2   *Optimality results*

Optimality results are now obtained by considering the off-diagonal elements of Ω^*. The binary type is never optimal for model III, since $w_{1,2\,p_1} > 0$ for $\rho_r \geq 0$, otherwise $w_{1,2} > 0$.

First consider $\rho_c, \rho_r \geq 0$. Recall from section 5.3.2.2 that an optimal type under model IV is optimal under model III if the treatment labels in the end (interior) plots of the first column of the type are a permutation of the treatment labels in the end (interior) plots of the second column. Theorem 5.20 in section 5.3.2.2.4 uses this relationship between models III and IV to show that a design of type

$$\begin{bmatrix} ab \\ ba \\ ab \\ ba \\ \vdots\ \vdots \end{bmatrix}$$

is optimal for $\rho_c, \rho_r \geq 0$ and p_1 even if

$$16\rho_c\rho_r \geq (1 - \rho_c)(1 - \rho_r)\zeta_2.$$

From the off-diagonal elements of Ω^* in Table 8.3, it is clear that

$$w_{1,4}, w_{1,6}, w_{1,2\,p_1}, w_{3,6} > 0 \quad \text{for } p_1 \geq 4,$$

and also $w_{3,8} > 0$ for $p_1 \geq 5$. Hence, it is difficult to determine optimal types for $p_1 \geq 4$.

However, for $p_1 = 3$, which is not included in Theorem 5.20, only $w_{1,4}$ and $w_{1,2\,p_1} = w_{1,6}$ are positive. It is assumed, until the end of Theorem 8.8, that $p_1 = 3$. Inclusion of the element $w_{1,4}$ in $\zeta_1 c_{\Omega^*}$ corresponds to diagonal self-adjacencies in the type, as illustrated in Figure 8.3a. Note that a pair of like treatments, which are diagonal neighbours, contribute 2 to the total number of diagonal self-adjacencies in a type.

For a given type, the expression for $\zeta_1 c_{\Omega}\cdot$ is taken to be of the form

$$\zeta_1 c_{\Omega}\cdot = 4w_{1,1} + 2w_{3,3} + 2\sum_{j=2}^{6} x_{1,j}w_{1,j} + 2x_{3,4}w_{3,4}, \tag{8.4}$$

where x_{j_1,j_2} is the coefficient of $2w_{j_1,j_2}$ $(j_1 \neq j_2)$ in $\zeta_1 c_{\Omega}\cdot$. This means that $2x_{1,4}$ is the number of diagonal self-adjacencies in a type, where $x_{1,4} \in \{0,1,2,3,4\}$. The element $w_{1,6}$ in $\zeta_1 c_{\Omega}\cdot$ corresponds to like treatments on the corner plots (see Figure 8.3b), and $x_{1,6} \in \{0,1,2\}$. For some $(x_{1,4}, x_{1,6})$ combinations, $c_{\Omega}\cdot$ includes the negative off-diagonal elements $w_{1,2}$, $w_{1,3}$ and $w_{1,5}$. The pairs of plots corresponding to these elements are also illustrated in Figure 8.3.

Figure 8.3
Pairs of plots corresponding to $w_{1,4}$, $w_{1,6}$, $w_{1,2}$, $w_{1,3}$ and $w_{1,5}$ for blocks of size 3×2.

a) $w_{1,4}$ b) $w_{1,6}$ c) $w_{1,2}$ d) $w_{1,3}$ e) $w_{1,5}$
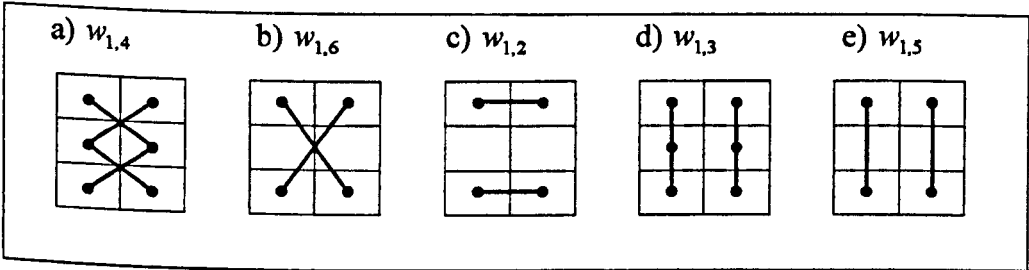
The different types corresponding to valid combinations of $(x_{1,4}, x_{1,6})$ are listed in Table 8.4. The type numbers are those used in chapter 7. Expressions for $c_{\Omega}\cdot$ follow immediately from the $\{x_{j_1,j_2}\}$ terms, since

$$\zeta_1 c_{\Omega}\cdot = 4w_{1,1} + 2w_{3,3} + 2(x_{1,4}w_{1,4} + x_{1,6}w_{1,6}) + 2(x_{1,2}w_{1,2} + x_{1,3}w_{1,3} + x_{1,5}w_{1,5}),$$

where $4w_{1,1} + 2w_{3,3} + 2(x_{1,4}w_{1,4} + x_{1,6}w_{1,6}) > 0$ and $x_{1,2}w_{1,2} + x_{1,3}w_{1,3} + x_{1,5}w_{1,5} < 0$. This means that the type with maximal

$$(x_{1,4}w_{1,4} + x_{1,6}w_{1,6}) + (x_{1,2}w_{1,2} + x_{1,3}w_{1,3} + x_{1,5}w_{1,5})$$

is the optimal type.

Table 8.4

List of types for blocks of size 3×2 under the AR(1)*AR(1) process ($\rho_r \geq 0$), model III and gls, with corresponding values of $x_{1,4}, x_{1,6}$, and of $x_{1,2}, x_{1,3}$, and $x_{1,5}$ (see equation (8.4)), where $w_{1,4}, w_{1,6} > 0$ and $w_{1,2}, w_{1,3}, w_{1,5} < 0$.

When $\rho_c \geq 0$ ($\rho_c < 0$), inadmissible types are marked by + (-), and a type which is better is given.

Type no.	Type	Better type when $\rho_c \geq 0$	Better type when $\rho_c < 0$	$x_{1,4}$	$x_{1,6}$	$x_{1,2}$	$x_{1,3}$	$x_{1,5}$
117 +-	$\begin{bmatrix} ab \\ cd \\ ef \end{bmatrix}$	92	92	0	0	0	0	0
112 +-	$\begin{bmatrix} ab \\ cd \\ ea \end{bmatrix}$	103	103	0	1	0	0	0
103 +	$\begin{bmatrix} ab \\ cd \\ ba \end{bmatrix}$	92 †		0	2	0	0	0
110 +-	$\begin{bmatrix} ab \\ ca \\ de \end{bmatrix}$	92	92	1	0	0	0	0
93 +-	$\begin{bmatrix} ab \\ ca \\ bd \end{bmatrix}$	92 †	103 ‡	1	1	0	0	0
53 +-	$\begin{bmatrix} ba \\ ac \\ ab \end{bmatrix}$	36 †	103 †	1	2	0	1	0
92 -	$\begin{bmatrix} ab \\ ba \\ cd \end{bmatrix}$		103 ‡	2	0	0	0	0
36 +-	$\begin{bmatrix} ba \\ ab \\ ac \end{bmatrix}$	37 ‡	53 ‡	2	1	0	1	0
19 +-	$\begin{bmatrix} ab \\ ab \\ ba \end{bmatrix}$	20 ‡	103 †	2	2	0	2	0

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Table 8.4 continued.

Type no.	Type	Better type when		$x_{1,4}$	$x_{1,6}$	$x_{1,2}$	$x_{1,3}$	$x_{1,5}$
37 +-	$\begin{bmatrix} ab \\ ba \\ ac \end{bmatrix}$	20 or 92 @	36 #	3	0	0	0	1
7 +-	$\begin{bmatrix} aa \\ ba \\ ab \end{bmatrix}$	92 #	103@	3	1	1	1	1
20 -	$\begin{bmatrix} ab \\ ba \\ ab \end{bmatrix}$		19 #	4	0	0	0	2

Notes for Table 8.4:

When $\rho_c \geq 0$: † since $w_{1,4} > w_{1,6}$;

‡ since $w_{1,4} + w_{1,5} > w_{1,3} + w_{1,6}$;

since $w_{1,2} + w_{1,3} + w_{1,4} + w_{1,5} + w_{1,6} < 0$;

@ since type 20 is better than type 37 if $w_{1,4} + w_{1,5} \geq 0$,

otherwise type 92 is better than type 37.

When $\rho_c < 0$: † since $w_{1,3} + w_{1,4} < 0$;

‡ since $w_{1,4} < w_{1,6}$;

since $w_{1,3} + w_{1,6} > w_{1,4} + w_{1,5}$;

@ since $w_{1,6} > w_{1,2} + w_{1,3} + 3w_{1,4} + w_{1,5}$

When $\rho_c, \rho_r \geq 0$, the two types 20 and 92 are admissible. This leads to the following theorem. Figure 8.4 shows the optimality regions for these two types.

Theorem 8.8
For blocks of size 3×2 and $t \geq 6$ under model III, gls and an AR(1)*AR(1) process, a design of type 20 is optimal for $\rho_c, \rho_r \geq 0$ if

$$w_{1,4} + w_{1,5} \geq 0 \iff (1 + \rho_c)(1 + \rho_r) \geq 2,$$

otherwise a design of type 92 is optimal. ■

Figure 8.4
Optimality regions for blocks of size 3×2 under the AR(1)*AR(1) process, model III and gls.
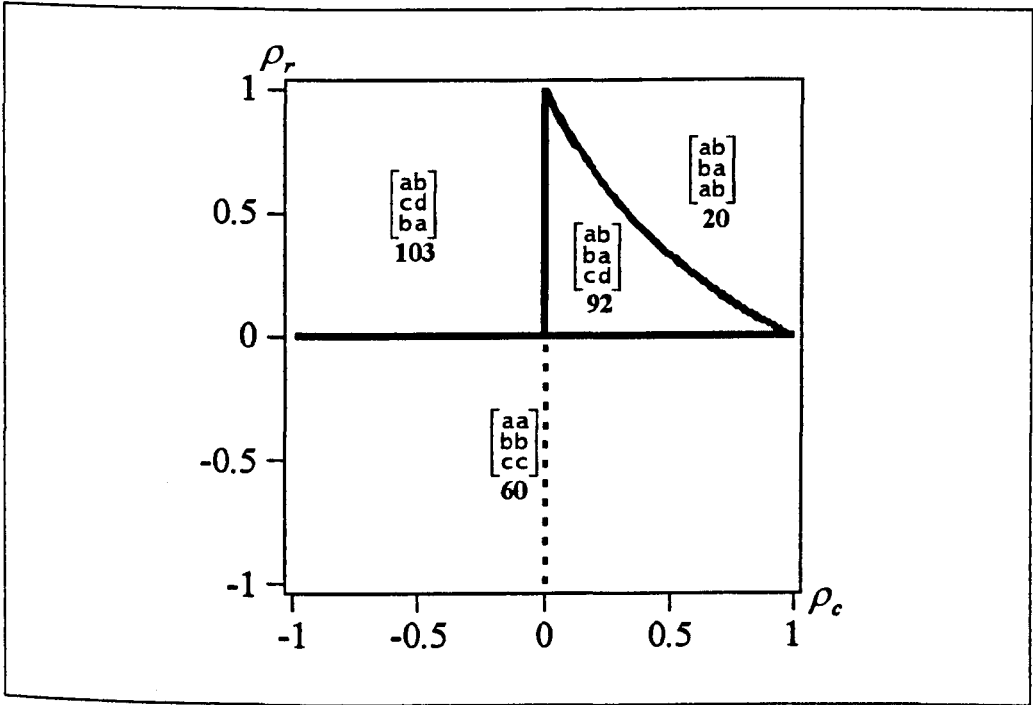
Now assume that $\rho_c \geq 0$ and $\rho_r < 0$. Only $w_{1,2}$ and $w_{3,4}$ are positive for $p_1 \geq 3$. Hence, design D8.2 (defined in section 8.3.1.1) which has blocks of type

$$\begin{bmatrix} a\,a \\ b\,b \\ c\,c \\ d\,d \\ \vdots\;\vdots \end{bmatrix}$$

is optimal, giving the following theorem.

Theorem 8.9
For blocks of size $p_1 \times 2$ ($p_1 \geq 3$) and $t \geq k$ under model III, gls and an AR(1)*AR(1) process, design D8.2 is optimal for $\rho_c \geq 0$ and $\rho_r < 0$. ∎

For $\rho_c, \rho_r < 0$, $w_{1,2}$ and $w_{3,4}$ are positive, and $w_{1,3}$ and $w_{1,4}$ can be positive for $p_1 \geq 3$. For $p_1 \geq 4$, as well as $w_{1,3}$ and $w_{1,4}$, $w_{3,5}$ and $w_{3,6}$ can also be positive. However, if $w_{1,3} \leq 0$ then $w_{3,5} \leq 0$ since $w_{3,5} < w_{1,3}$, and so $w_{1,4}, w_{3,6} \leq 0$. This means that if $w_{1,3} \leq 0$, only $w_{1,2}$ and $w_{3,4}$ are positive, so design D8.2 is optimal. The condition $w_{1,3} \leq 0$ is equivalent to

$$1 + (p_1 - 2)\rho_c - (p_1 - 3)\rho_c^2 \geq 0,$$

which can be written as

$$\rho_c \geq \tfrac{1}{2}\left((p_1 - 2) - \sqrt{(p_1^2 - 8)}\right)/(p_1 - 3) \quad \text{for } p_1 \geq 4. \tag{8.5}$$

Note that if $w_{1,3} \geq 0$ then $w_{1,4} \geq 0$, and $w_{3,5}$ and $w_{3,6}$ can also be positive. Hence, optimal types are difficult to determine when $w_{1,3} \geq 0$.

Theorem 8.10
For blocks of size $p_1 \times 2$ ($p_1 \geq 3$) and $t \geq k$ under model III, gls and an AR(1)*AR(1) process, design D8.2 is optimal for $\rho_c, \rho_r < 0$ if

$$w_{1,3} \leq 0 \Leftrightarrow 1 + (p_1 - 2)\rho_c - (p_1 - 3)\rho_c^2 \geq 0. \qquad \blacksquare$$

For $p_1 = 3$, $w_{1,3} \leq 0 \Leftrightarrow 1 + \rho_c \geq 0$. This gives the following corollary.

Corollary 8.11
For blocks of size 3×2 and $t \geq 6$ under model III, gls and an AR(1)*AR(1) process, design D8.2 is optimal for all $\rho_c, \rho_r < 0$ $\qquad \blacksquare$

When $\rho_c, \rho_r < 0$, it is clear from the inequality in (8.5) that as p_1 increases, the size of the optimality region for D8.2 decreases.

Finally, consider $\rho_c < 0$ and $\rho_r \geq 0$. Here $w_{1,6}$, $w_{1,2p_1}$, $w_{3,8}$ are positive for $p_1 \geq 5$, and $w_{1,3}$, $w_{1,4}$, $w_{3,5}$, $w_{3,6}$ can be positive for $p_1 \geq 4$. As for when $\rho_c, \rho_r \geq 0$, it is complicated to determine optimality conditions for general p_1. However, for $p_1 = 3$, only $w_{1,4}$ and $w_{1,2p_1} = w_{1,6}$ are positive. Recall that $w_{1,3} < 0 \iff 1 + \rho_c > 0$, and so $w_{1,4} > 0$. From the list of types in Table 8.4, it is clear that type 103 is optimal, since all other types are inadmissible.

Theorem 8.12
For blocks of size 3×2 and $t \geq 6$ under model III, gls and an AR(1)*AR(1) process, a design of type 103 is optimal for $\rho_c < 0$ and $\rho_r \geq 0$.   ∎

Figure 8.4 gives a plot of the optimality regions for $p_1 = 3$. As mentioned in the discussion of Uddin & Morgan (1997a) (see section 5.3.2.4), the optimal type for small $\rho_c, \rho_r \geq 0$ has binary columns under model III. For $\rho_c, \rho_r \geq 0$, as ρ_c and/or ρ_r increase the number of diagonal self-adjacencies in the optimal type increases. For $\rho_r < 0$, the optimal type (type 60) has binary columns and non-binary rows. Recall that for model IV (see Figure 7.6), type 60 is optimal for most of the region when $\rho_c < 0$.

8.4 Blocks of size 3×3

In this section, optimal non-binary types are considered for blocks of size 3×3 under model IV and gls. It is difficult to obtain optimality conditions for $\rho_c, \rho_r < 0$. However, when at least one of (ρ_c, ρ_r) is positive, optimality conditions have been derived here. As for the blocks of size 2×2 considered in chapter 6, the optimality regions for a type and its diagonal reflection are symmetric about $\rho_c = \rho_r$. This means that optimality results for $\rho_c < 0$ and $\rho_r \geq 0$ follow immediately from the results for $\rho_c \geq 0$ and $\rho_r < 0$.

The matrix $\zeta_1\Omega^*$ is a class I $(3,3,W_1,W_2,W_4,W_5)$ matrix,

i.e. $\quad \zeta_1\Omega^* = \begin{pmatrix} W_1 & W_2 & W_4 \\ W_2 & W_5 & W_2 \\ W_4 & W_2 & W_1 \end{pmatrix}$.

The matrices W_1, W_2, W_4 and W_5 are of the form:

$$W_1 = \begin{pmatrix} w_{1,1} & w_{1,2} & w_{1,3} \\ w_{1,2} & w_{2,2} & w_{1,2} \\ w_{1,3} & w_{1,2} & w_{1,1} \end{pmatrix}, \quad W_2 = \begin{pmatrix} w_{1,4} & w_{1,5} & w_{1,6} \\ w_{1,5} & w_{2,5} & w_{1,5} \\ w_{1,6} & w_{1,5} & w_{1,4} \end{pmatrix},$$

$$W_4 = \begin{pmatrix} w_{1,7} & w_{1,8} & w_{1,7} \\ w_{1,8} & w_{2,8} & w_{1,8} \\ w_{1,7} & w_{1,8} & w_{1,7} \end{pmatrix}, \quad W_5 = \begin{pmatrix} w_{4,4} & w_{4,5} & w_{4,6} \\ w_{4,5} & w_{5,5} & w_{4,5} \\ w_{4,6} & w_{4,5} & w_{4,4} \end{pmatrix}.$$

From section 8.2.2, the off-diagonal elements of $\zeta_1\Omega^*$ that can be positive are

$$w_{1,2} = -\rho_r - (1-\rho_c)(1-\rho_r)^2/\zeta_2,$$

$$w_{1,p_2+1} = w_{1,4} = -\rho_c - (1-\rho_c)^2(1-\rho_r)/\zeta_2,$$

$$w_{1,p_2+2} = w_{1,5} = \rho_c\rho_r - (1-\rho_c)^2(1-\rho_r)^2/\zeta_2,$$

$$w_{2,p_2+2} = w_{2,5} = -\rho_c(1+\rho_r^2) - (1-\rho_c)^2(1-\rho_r)^3/\zeta_2$$

and $\quad w_{p_2+1,p_2+2} = w_{4,5} = -\rho_r(1+\rho_c^2) - (1-\rho_c)^3(1-\rho_r)^2/\zeta_2,$

where

$$\zeta_2 = (3-\rho_c)(3-\rho_r).$$

All other off-diagonal elements of $\zeta_1\Omega^*$ are negative.

For a given type, the expression for $\zeta_1 c_{\Omega^*}$ is taken to be of the form

$$\zeta_1 c_{\Omega^*} = 4w_{1,1} + 2w_{2,2} + 2w_{4,4} + w_{5,5} + 2\sum_{j=2}^{8} x_{1,j}w_{1,j}$$

$$+ 2\left(x_{2,5}w_{2,5} + x_{2,8}w_{2,8} + x_{4,5}w_{4,5} + x_{4,6}w_{4,6}\right), \tag{8.6}$$

where x_{j_1,j_2} is the coefficient of $2w_{j_1,j_2}$ $(j_1 \neq j_2)$ in $\zeta_1 c_{\Omega^*}$.

8.4.1 When $\rho_c, \rho_r \geq 0$

It is assumed here that $\rho_c, \rho_r \geq 0$. Recall from section 8.2.2 that the binary type is optimal for blocks of size 3×3 if $w_{1,p_2+2} = w_{1,5} \leq 0$ (case (ii)). It follows that if $w_{1,5} \geq 0$, non-binary types are optimal. Inclusion of the element $w_{1,5}$ in c_{Ω^*} corresponds to diagonal self-adjacencies in the type, as illustrated by the pairs of diagonally adjacent connected nodes in Figure 8.5a. If the number of diagonal self-adjacencies is greater than or equal to eight (i.e. if $x_{1,5} \geq 4$), then c_{Ω^*} must include at least one of the negative off-diagonal elements: $w_{1,3}, w_{2,8}, w_{4,6}$. Inclusion of the element $w_{1,3}$ in c_{Ω^*} corresponds to like treatments on the corner plots. Figure 8.5 illustrates the pairs of plots corresponding to these elements. Note that $x_{1,5} \in \{0,1,...,8\}$, $x_{1,3} \in \{0,1,3,6\}$ and $x_{2,8}, x_{4,6} \in \{0,1\}$.

Figure 8.5
Pairs of plots corresponding to $w_{1,5}$, $w_{1,3}$, $w_{2,8}$ and $w_{4,6}$ for blocks of size 3×3.
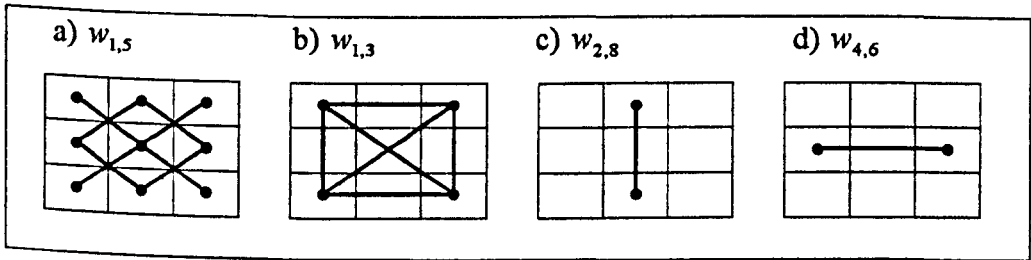
When $x_{1,3} = x_{2,8} = x_{4,6} = 0$, the highest value of $x_{1,5}$ that is possible is $x_{1,5} = 3$. Let the corresponding type be called type 1. To ensure that all the types which can be optimal are considered, Table 8.5 lists all the 80 combinations of $x_{1,5} \geq 4$, $x_{1,3}$, $x_{2,8}$ and $x_{4,6}$. A type exists for only 19 of these 80 combinations (called *valid* combinations). These 19 types are given in Table 8.6.

Vertical and horizontal reflections of a type will result in an equivalent type with respect to c_{Ω^*}. For some of the types listed in Table 8.6 other equivalent types are also possible. For brevity, these are not all listed, however, they can be easily obtained given the values of $x_{1,5}$, $x_{1,3}$, $x_{2,8}$ and $x_{4,6}$. For example, for type 3, which has $(x_{1,5}, x_{1,3}, x_{2,8}, x_{4,6}) = (4,1,0,0)$, the types in Figure 8.6 are equivalent. The three rows in Figure 8.6 show the different arrangements of the treatment label a, such that $x_{1,3} = 1$, and the two columns show the arrangements of the treatment labels b and c.

Figure 8.6
For blocks of size 3×3 under the AR(1)*AR(1) process, model IV and gls: equivalent types to type 2.

$$
\begin{bmatrix} a b a \\ b a c \\ d c e \end{bmatrix}, \quad
\begin{bmatrix} a b a \\ c a b \\ d c e \end{bmatrix},
$$

$$
\begin{bmatrix} a b d \\ b a c \\ e c a \end{bmatrix}, \quad
\begin{bmatrix} a b d \\ c a b \\ e c a \end{bmatrix},
$$

$$
\begin{bmatrix} a b d \\ b a c \\ a c e \end{bmatrix}, \quad
\begin{bmatrix} a b d \\ c a b \\ a c e \end{bmatrix}.
$$
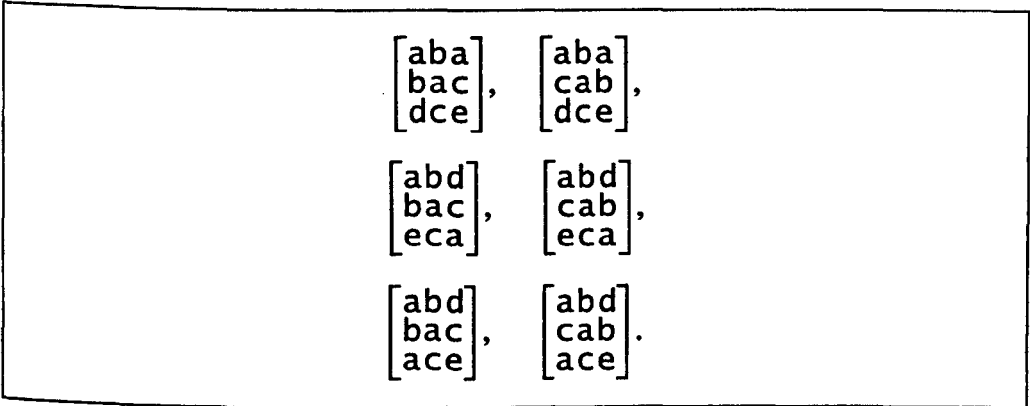
Table 8.5

List of all combinations of $x_{1,5} \in \{4,5,...,8\}$, $x_{1,3} \in \{0,1,3,6\}$ and $x_{2,8}$, $x_{4,6} \in \{0,1\}$ (see equation (8.6)).

✓ indicates that the combination is valid (i.e. a type with the $\{x_{i,j}\}$ values exists); ✗ indicates that the combination is invalid.

$x_{1,5}$	$x_{1,3}$	$x_{2,8}$	$x_{4,6}$		$x_{1,5}$	$x_{1,3}$	$x_{2,8}$	$x_{4,6}$		$x_{1,5}$	$x_{1,3}$	$x_{2,8}$	$x_{4,6}$	
4	0	0	0	✗	6	0	0	0	✗	8	0	0	0	✗
4	0	0	1	✗	6	0	0	1	✗	8	0	0	1	✗
4	0	1	0	✗	6	0	1	0	✗	8	0	1	0	✗
4	0	1	1	✓	6	0	1	1	✗	8	0	1	1	✗
4	1	0	0	✓	6	1	0	0	✗	8	1	0	0	✗
4	1	0	1	✓	6	1	0	1	✗	8	1	0	1	✗
4	1	1	0	✓	6	1	1	0	✗	8	1	1	0	✗
4	1	1	1	✗	6	1	1	1	✓	8	1	1	1	✗
4	3	0	0	✓	6	3	0	0	✗	8	3	0	0	✗
4	3	0	1	✗	6	3	0	1	✗	8	3	0	1	✗
4	3	1	0	✗	6	3	1	0	✗	8	3	1	0	✗
4	3	1	1	✗	6	3	1	1	✗	8	3	1	1	✗
4	6	0	0	✓	6	6	0	0	✓	8	6	0	0	✗
4	6	0	1	✓	6	6	0	1	✓	8	6	0	1	✗
4	6	1	0	✓	6	6	1	0	✓	8	6	1	0	✗
4	6	1	1	✗	6	6	1	1	✗	8	6	1	1	✓
5	0	0	0	✗	7	0	0	0	✗					
5	0	0	1	✗	7	0	0	1	✗					
5	0	1	0	✗	7	0	1	0	✗					
5	0	1	1	✓	7	0	1	1	✗					
5	1	0	0	✗	7	1	0	0	✗					
5	1	0	1	✗	7	1	0	1	✗					
5	1	1	0	✗	7	1	1	0	✗					
5	1	1	1	✗	7	1	1	1	✗					
5	3	0	0	✓	7	3	0	0	✗					
5	3	0	1	✓	7	3	0	1	✗					
5	3	1	0	✓	7	3	1	0	✗					
5	3	1	1	✗	7	3	1	1	✓					
5	6	0	0	✓	7	6	0	0	✗					
5	6	0	1	✗	7	6	0	1	✗					
5	6	1	0	✗	7	6	1	0	✗					
5	6	1	1	✗	7	6	1	1	✗					

Table 8.6

List of valid types for blocks of size 3×3 under the AR(1)*AR(1) process ($\rho_c, \rho_r \geq 0$), model IV and gls, with corresponding values of $x_{1,5} \geq 4$, $x_{1,3}$, $x_{2,8}$ and $x_{4,6}$ (see equation (8.6)). The binary type (type 0), and the type with $x_{1,5} = 3$, $x_{1,3} = x_{2,8} = x_{4,6} = 0$ (type 1) are also included. Assume $w_{1,5} \geq 0$ and $w_{1,3}, w_{2,8}, w_{4,6} < 0$. For inadmissible types, type numbers are in brackets, and a type which is better is given.

Type no.	Type	Better type(s)	$x_{1,5}$	$x_{1,3}$	$x_{2,8}$	$x_{4,6}$
(0)	$\begin{bmatrix} abc \\ def \\ ghi \end{bmatrix}$	1	0	0	0	0
1	$\begin{bmatrix} abd \\ bac \\ ecf \end{bmatrix}$		3	0	0	0
(2)	$\begin{bmatrix} bac \\ ada \\ eaf \end{bmatrix}$	10	4	0	1	1
(3)	$\begin{bmatrix} aba \\ bac \\ dce \end{bmatrix}$	1 or 10	4	1	0	0
(4)	$\begin{bmatrix} abc \\ bab \\ ade \end{bmatrix}$	3	4	1	0	1
(5)	$\begin{bmatrix} abc \\ bad \\ abe \end{bmatrix}$	3	4	1	1	0
(6)	$\begin{bmatrix} aba \\ bac \\ ade \end{bmatrix}$	3	4	3	0	0
(7)	$\begin{bmatrix} aba \\ cad \\ aea \end{bmatrix}$	3	4	6	0	0
(8)	$\begin{bmatrix} aca \\ bab \\ ada \end{bmatrix}$	3	4	6	0	1
(9)	$\begin{bmatrix} aba \\ cad \\ aba \end{bmatrix}$	3	4	6	1	0
10	$\begin{bmatrix} bac \\ aba \\ dae \end{bmatrix}$		5	0	1	1

Table 8.6 continued.

Type no.	Type	Better type(s)	$x_{1,5}$	$x_{1,3}$	$x_{2,8}$	$x_{4,6}$
(11)	$\begin{bmatrix} aba \\ bac \\ acd \end{bmatrix}$	10	5	3	0	0
(12)	$\begin{bmatrix} aba \\ bab \\ acd \end{bmatrix}$	11	5	3	0	1
(13)	$\begin{bmatrix} aba \\ bac \\ abd \end{bmatrix}$	11	5	3	1	0
(14)	$\begin{bmatrix} aba \\ bac \\ ada \end{bmatrix}$	11	5	6	0	0
15	$\begin{bmatrix} aba \\ bab \\ cbd \end{bmatrix}$		6	1	1	1
(16)	$\begin{bmatrix} aba \\ bac \\ aca \end{bmatrix}$	15	6	6	0	0
(17)	$\begin{bmatrix} aba \\ bab \\ aca \end{bmatrix}$	16	6	6	0	1
(18)	$\begin{bmatrix} aba \\ bac \\ aba \end{bmatrix}$	16	6	6	1	0
19	$\begin{bmatrix} aba \\ bab \\ abc \end{bmatrix}$		7	3	1	1
20	$\begin{bmatrix} aba \\ bab \\ aba \end{bmatrix}$		8	6	1	1

Twenty-one types are listed in Table 8.6. The type with maximal

$$x_{1,5}w_{1,5} + x_{1,3}w_{1,3} + x_{2,8}w_{2,8} + x_{4,6}w_{4,6}$$

is the optimal type, under the assumption that $w_{1,5} \geq 0$.

Recall from section 8.2.1 that,

$$w_{1,p_2} = w_{1,3} = -(1-\rho_c)(1-\rho_r)/\zeta_2 < 0;$$

$$w_{1,p_2+2} = w_{1,5} = \rho_c\rho_r - (1-\rho_c)^2(1-\rho_r)^2/\zeta_2;$$

$$w_{2,(p_1-1)p_2+2} = w_{2,8} = -(1-\rho_c)(1-\rho_r)^3/\zeta_2 < 0;$$

$$w_{p_2+1,2p_2} = w_{4,6} = -(1-\rho_c)^3(1-\rho_r)/\zeta_2 < 0.$$

Sixteen types are inadmissible when $w_{1,5} \geq 0$ (marked by brackets in Table 8.6). That type $e \in \{0, 2, 4, 5, 6, 7, 8, 9, 12, 13, 14, 17, 18\}$ is inadmissible, follows immediately from a comparison of $(x_{1,5}, x_{1,3}, x_{2,8}, x_{4,6})$ for type e and the type which is better (given in Table 8.6). The inadmissibility of types 3, 11 and 16 follows from Lemma 8.13 and Lemma 8.14, as shown below.

Lemma 8.13
     $w_{2,8} \geq w_{1,3}$ for $\rho_r \geq 0$.

Proof

Note that

$$w_{2,8} - w_{1,3} = (1-\rho_c)(1-\rho_r)\{1-(1-\rho_r)^2\}/\zeta_2.$$

It follows that for $\rho_r \geq 0$, $w_{2,8} \geq w_{1,3}$, since $\{1-(1-\rho_r)^2\} = \rho_r(2-\rho_r) \geq 0$.

    ■

Lemma 8.14
     $w_{4,6} \geq w_{1,3}$ for $\rho_c \geq 0$.

Proof

The proof is similar to the proof for Lemma 8.13.   ■

The inadmissibility of types 3, 11 and 16 is now shown. First consider type 3. Type 1 is better than type 3 if

$$w_{1,3} + w_{1,5} \leq 0, \tag{8.7}$$

and type 10 is better than type 3 if

$$w_{1,3} \leq w_{1,5} + w_{2,8} + w_{4,6}. \tag{8.8}$$

When the inequality (8.7) does not hold (i.e. when $w_{1,3} + w_{1,5} \geq 0$), the inequality (8.8) is true if

$$2w_{1,3} \leq w_{2,8} + w_{4,6},$$

which clearly holds by Lemma 8.13 and Lemma 8.14. Hence, either type 1 or type 10 is better than type 3.

The conditions for type 10 to be better than type 11, and for type 15 to be better than type 16 are

$$3w_{1,3} \leq w_{2,8} + w_{4,6}$$

and $5w_{1,3} \leq w_{2,8} + w_{4,6}$,

respectively, which are clearly true by Lemma 8.13 and Lemma 8.14 (and since $w_{1,3} < 0$).

Therefore, only the five types 1, 10, 15, 19 and 20, remain to be considered. Theorem 8.15 to Theorem 8.19 show that these five types are the only non-binary types that can be optimal for $\rho_c, \rho_r \geq 0$.

For each optimal type, e^*, Theorem 8.15 to Theorem 8.19 give sufficient optimality conditions. These conditions correspond to type e^* being better than the type number in parentheses, which is given after each condition. For example, in Theorem 8.15, type $e^* = 1$ is optimal when type 1 is better than types 0 and 10. In terms of $\{w_{i,j}\}$, type 1 is better than types 0 and 10 when $w_{1,5} \geq 0$ and $2w_{1,5} + w_{2,8} + w_{4,6} \leq 0$, respectively.

Theorem 8.15 to Theorem 8.19 can be proved by showing that under the optimality conditions given, type e^* is better than the remaining admissible types. A detailed proof is given for Theorem 8.15. The proofs for Theorem 8.16 to Theorem 8.19 follow in a similar way. A plot of the optimality regions for $\rho_c, \rho_r \geq 0$ is given as Figure 8.7.

Figure 8.7
For blocks of size 3×3 under the AR(1)*AR(1) process, model IV and gls: optimality regions for $\rho_c, \rho_r \geq 0$
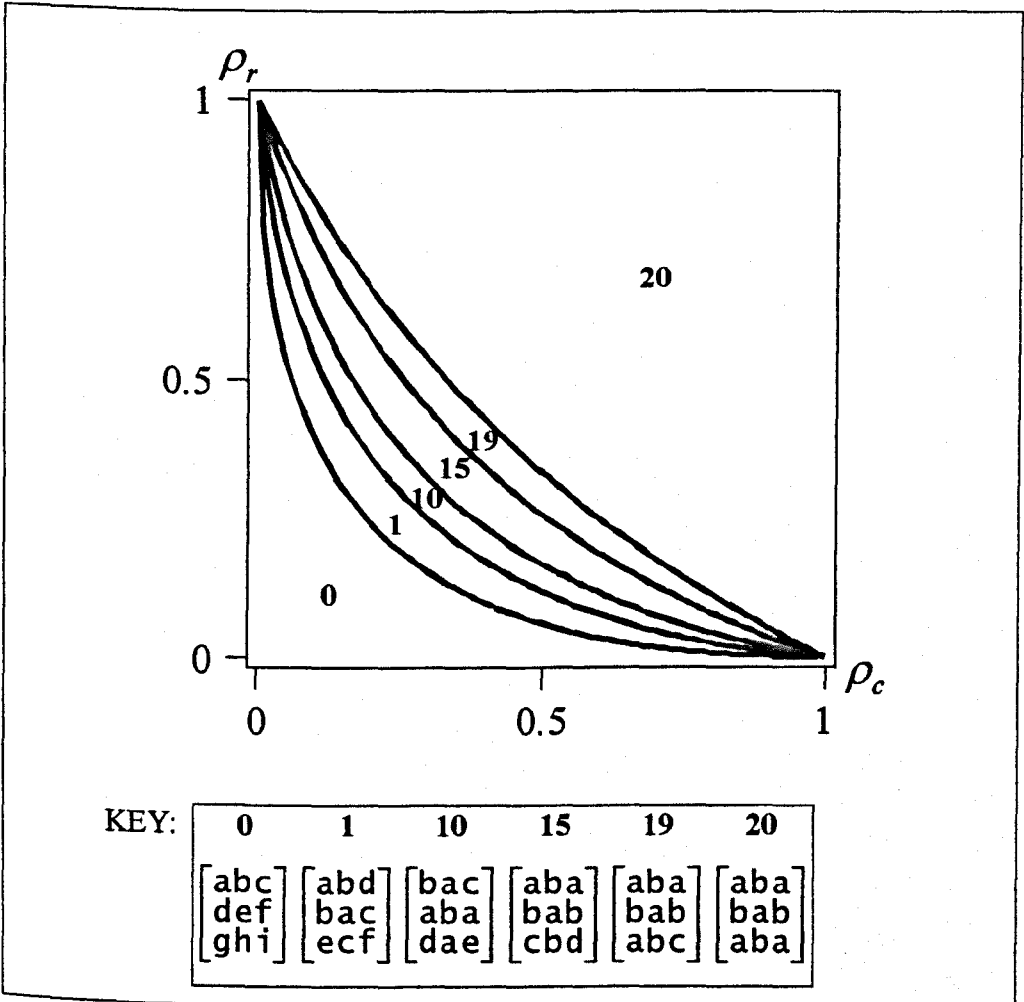
Theorem 8.15

For blocks of size 3×3 and $t \geq 9$ treatments under model IV, gls and an AR(1)*AR(1) process, a design of type 1 is optimal for $\rho_c, \rho_r \geq 0$, when

$$w_{1,5} \geq 0 \quad \text{(type 0);}$$

and $\quad 2w_{1,5} + w_{2,8} + w_{4,6} \leq 0 \quad \text{(type 10).}$

Proof

Assume that type 1 is better than types 0 and 10. Table 8.7 gives the conditions for type 1 to be better than the three remaining admissible types. It follows from Lemma 8.13 and Lemma 8.14 that when type 1 is better than type 10,

$$w_{1,3} + w_{1,5} \leq 0.$$

The inequalities in Table 8.7 are clearly satisfied when $w_{1,5} \geq 0$,

$2w_{1,5} + w_{2,8} + w_{4,6} \leq 0$ and $w_{1,3} + w_{1,5} \leq 0$.

Table 8.7

For blocks of size 3×3 under the AR(1)*AR(1) process, model IV and gls: condition for type 1 to be better than type e.

e	Type 3 better than type e when:
15	$3w_{1,5} + w_{1,3} + w_{2,8} + w_{4,6} \leq 0$
19	$4w_{1,5} + 3w_{1,3} + w_{2,8} + w_{4,6} \leq 0$
20	$5w_{1,5} + 6w_{1,3} + w_{2,8} + w_{4,6} \leq 0$

∎

Theorem 8.16

For blocks of size 3×3 and $t \geq 9$ treatments under model IV, gls and an AR(1)*AR(1) process, a design of type 10 is optimal for $\rho_c, \rho_r \geq 0$, when

$$2w_{1,5} + w_{2,8} + w_{4,6} \geq 0 \quad \text{(type 1);}$$

and $\quad w_{1,5} + w_{1,3} \leq 0 \quad \text{(type 15).}$ ∎

Theorem 8.17

For blocks of size 3×3 and $t \geq 9$ treatments under model IV, gls and an AR(1)*AR(1) process, a design of type 15 is optimal for $\rho_c, \rho_r \geq 0$, when

$$w_{1,5} + w_{1,3} \geq 0 \quad \text{(type 10)}$$

and $\quad w_{1,5} + 2w_{1,3} \leq 0 \quad \text{(type 19)}.$ ■

Theorem 8.18

For blocks of size 3×3 and $t \geq 9$ treatments under model IV, gls and an AR(1)*AR(1) process, a design of type 19 is optimal for $\rho_c, \rho_r \geq 0$, when

$$w_{1,5} + 2w_{1,3} \geq 0 \quad \text{(type 15)}$$

and $\quad w_{1,5} + 3w_{1,3} \leq 0 \quad \text{(type 20)}.$ ■

Theorem 8.19

For blocks of size 3×3 and $t \geq 9$ treatments under model IV, gls and an AR(1)*AR(1) process, a design of type 20 is optimal for $\rho_c, \rho_r \geq 0$, when

$$w_{1,5} + 3w_{1,3} \geq 0 \quad \text{(type 19)}.$$ ■

Although only two of the optimal types for $\rho_c, \rho_r \geq 0$ have binary rows and columns, none of the six optimal types have any row or column self-adjacencies. As for the blocks of size 2×2 and 3×2 under the AR(1)*AR(1) process in chapters 6 and 7, respectively (see Figure 6.2d and Figure 7.6, respectively), it is clear from Figure 8.7 that for $\rho_c, \rho_r \geq 0$, as ρ_c and ρ_r increase, the number of diagonal self-adjacencies in the optimal type increases. Notice that, type 20, which has the maximal number of diagonal self-adjacencies over the types which can be optimal, is optimal for more than half of the region under consideration. When $\rho_c = \rho_r$, as $\rho_c = \rho_r$ increases from zero, the optimal type changes from:

- type 0 (binary type) to type 1 at $\rho_c \approx 0.219$,

- type 1 to type 10 at $\rho_c \approx 0.274$,

- type 10 to type 15 at $\rho_c \approx 0.311$,

- type 15 to type 19 at $\rho_c \approx 0.371$,

- type 19 to type 20 at $\rho_c \approx 0.414$.

8.4.2 When $\rho_c \geq 0$ and $\rho_r < 0$

Under the assumption that $\rho_c \geq 0$ and $\rho_r < 0$, only the off-diagonal elements $w_{1,2}$ and $w_{p_2+1,p_2+2} = w_{4,5}$ can be positive. Note that $w_{4,5} \geq w_{1,2}$. Therefore the following three cases need to be considered here:

a) $w_{4,5} \leq 0$ ($\Rightarrow w_{1,2} \leq 0$),

b) $w_{1,2} \leq 0$ and $w_{4,5} \geq 0$,

c) $w_{1,2} \geq 0$ ($\Rightarrow w_{4,5} \geq 0$).

Recall from section 8.2.2 that a sufficient condition for the binary type to be optimal is $w_{4,5} \leq 0$ (case (ii)). As illustrated in Figure 8.8, inclusion of $w_{1,2}$ in c_{Ω^*} corresponds to row self-adjacencies in the top and bottom rows, and the inclusion of $w_{4,5}$ in c_{Ω^*} corresponds to row self-adjacencies in the middle row. Here $x_{1,2} \in \{0,1,...,4\}$ and $x_{4,5} \in \{0,1,2\}$.

Figure 8.8
Pairs of plots corresponding to $w_{1,2}$, $w_{4,5}$, $w_{1,3}$ and $w_{4,6}$ for blocks of size 3×3.
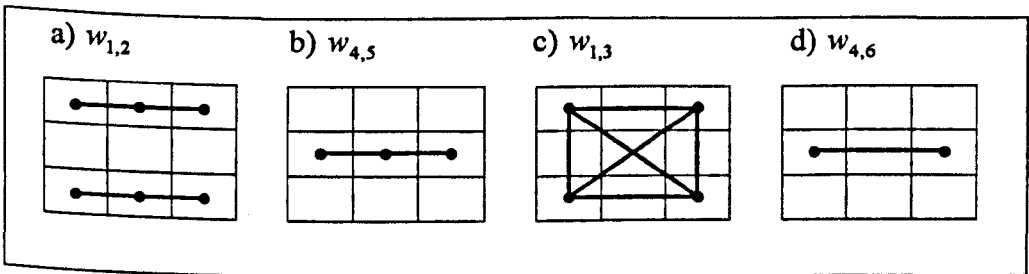
For $x_{1,2} > 1$, $x_{1,3}$ may be positive, and Figure 8.8c illustrates the pairs of plots corresponding to the inclusion of the negative $w_{1,3}$ in c_{Ω^*}. If the plots in both the top and bottom rows contain the same treatment, i.e.

$$\begin{bmatrix} a\,a\,a \\ b\,c\,d \\ a\,a\,a \end{bmatrix},$$

then $x_{1,2} = 4$ and $x_{1,3} = 6$. However, if the plots in the top and bottom rows have different treatments, i.e.

$$\begin{bmatrix} a\,a\,a \\ c\,d\,e \\ b\,b\,b \end{bmatrix},$$

then $x_{1,2}$ is still equal to 4, but $x_{1,3}$ is reduced to 2. The latter type is better, and hence $x_{1,3}$ is taken to belong to $\{0,1,2\}$. If the middle row contains the same treatment, i.e.

$$\begin{bmatrix} b\,c\,d \\ a\,a\,a \\ e\,f\,g \end{bmatrix},$$

then $x_{4,5} = 2$ and $x_{4,6} = 1$. The pair of plots corresponding to the inclusion of the negative $w_{4,6}$ in c_{Ω^*} is illustrated in Figure 8.8d.

Similarly to section 8.4.1, the 18 different types with $x_{1,2} \in \{0,1,...,4\}$, $x_{4,5} \in \{0,1,2\}$ and the possible valid combinations of $x_{1,3}$ and $x_{4,6}$ are listed in Table 8.8. As in section 8.4.1, equivalent types, to those listed in Table 8.8, can easily be obtained for given values of $(x_{1,2}, x_{4,5}, x_{1,3}, x_{4,6})$. Recall from section 8.2.1 that

$$w_{1,2} = -\rho_r - (1-\rho_c)(1-\rho_r)^2 / \zeta_2,$$

$$w_{p_2+1,p_2+2} = w_{4,5} = -\rho_r(1+\rho_c^2) - (1-\rho_c)^3(1-\rho_r)^2 / \zeta_2,$$

$$w_{1,p_2} = w_{1,3} = -(1-\rho_c)(1-\rho_r)/\zeta_2 < 0,$$

and $w_{p_2+1,2p_2} = w_{4,6} = -(1-\rho_c)^3(1-\rho_r)/\zeta_2 < 0.$

When $w_{1,2} \leq 0$ and $w_{4,5} \geq 0$, (case b) only types with $x_{1,2} = 0$ need to be considered, i.e. types 0, 21 and 22. Clearly, type 21 is better than type 0, so only types 21 and 22 need to be compared, and the type with maximal

$$x_{4,5}w_{4,5} + x_{4,6}w_{4,6}$$

is optimal. This gives Theorem 8.20 and Theorem 8.21. In the theorems given in this section, as in section 8.4.1, the sufficient optimality conditions for type e^* correspond to type e^* being better than the type number in parentheses.

Theorem 8.20

For blocks of size 3×3 and $t \geq 9$ treatments under model IV, gls and an AR(1)*AR(1) process, a design of type 21 is optimal for $\rho_c \geq 0$ and $\rho_r < 0$

when $\qquad w_{1,2} \leq 0 \qquad$ (type 27);

$\qquad\qquad w_{4,5} \geq 0 \qquad$ (type 0);

and $\quad w_{4,5} + w_{4,6} \leq 0 \qquad$ (type 22). ∎

Theorem 8.21

For blocks of size 3×3 and $t \geq 9$ treatments under model IV, gls and an AR(1)*AR(1) process, a design of type 22 is optimal for $\rho_c \geq 0$ and $\rho_r < 0$

when $\qquad w_{1,2} \leq 0 \qquad$ (type 28)

and $\quad w_{4,5} + w_{4,6} \geq 0 \qquad$ (type 21). ∎

Table 8.8

List of types for blocks of size 3×3 under the AR(1)*AR(1) process, ($\rho_c \geq 0$, $\rho_r < 0$), model IV and gls, with corresponding values of ($x_{1,2}, x_{4,5}, x_{1,3}, x_{4,6}$) (see equation (8.6)). Under the assumption that $w_{1,2}, w_{4,5} \geq 0$ and $w_{1,3}, w_{4,6} < 0$, inadmissible types have type numbers in brackets, and a better type is given.

Type no.	Type	Better type	$x_{1,2}$	$x_{4,5}$	$x_{1,3}$	$x_{4,6}$
(0)	$\begin{bmatrix} abc \\ def \\ ghi \end{bmatrix}$	21	0	0	0	0
(21)	$\begin{bmatrix} bcd \\ aae \\ fgh \end{bmatrix}$	27	0	1	0	0
(22)	$\begin{bmatrix} bcd \\ aaa \\ efg \end{bmatrix}$	28	0	2	0	1
(23)	$\begin{bmatrix} aab \\ cde \\ fgh \end{bmatrix}$	27	1	0	0	0
(24)	$\begin{bmatrix} aac \\ bbd \\ efg \end{bmatrix}$	27	1	1	0	0
(25)	$\begin{bmatrix} aac \\ bbb \\ def \end{bmatrix}$	28	1	2	0	1
(26)	$\begin{bmatrix} aac \\ def \\ bbg \end{bmatrix}$	27	2	0	0	0
27	$\begin{bmatrix} aad \\ bbe \\ ccf \end{bmatrix}$		2	1	0	0
28	$\begin{bmatrix} aad \\ bbb \\ cce \end{bmatrix}$		2	2	0	1
(29)	$\begin{bmatrix} aaa \\ bcd \\ efg \end{bmatrix}$	26	2	0	1	0
(30)	$\begin{bmatrix} aaa \\ bbc \\ def \end{bmatrix}$	27	2	1	1	0

Table 8.8 continued.

Type no.	Type	Better type	$x_{1,2}$	$x_{4,5}$	$x_{1,3}$	$x_{4,6}$
(31)	$\begin{bmatrix} aaa \\ bbb \\ cde \end{bmatrix}$	28	2	2	1	1
(32)	$\begin{bmatrix} aaa \\ cde \\ bbf \end{bmatrix}$	33	3	0	1	0
(33)	$\begin{bmatrix} aaa \\ bbd \\ cce \end{bmatrix}$	27 or 36	3	1	1	0
(34)	$\begin{bmatrix} aaa \\ bbb \\ ccd \end{bmatrix}$	28 or 37	3	2	1	1
(35)	$\begin{bmatrix} aaa \\ cde \\ bbb \end{bmatrix}$	36	4	0	2	0
36	$\begin{bmatrix} aaa \\ bbd \\ ccc \end{bmatrix}$		4	1	2	0
37	$\begin{bmatrix} aaa \\ bbb \\ ccc \end{bmatrix}$		4	2	2	1

Note: To avoid confusion with the types in Table 8.6, the types here are numbered from 21 onwards, except for type 0, which is also in Table 8.6.

When $w_{1,2} \geq 0$ ($\Rightarrow w_{4,5} \geq 0$) (case c), the type with maximal

$$x_{1,2}w_{1,2} + x_{4,5}w_{4,5} + x_{1,3}w_{1,3} + x_{4,6}w_{4,6}$$

is optimal. From the 18 types listed in Table 8.8, only the four types, 27, 28, 36 and 37 need to be considered, since the other types are inadmissible. Type 33 is inadmissible since type 27 is better if $w_{1,2} + w_{1,3} \leq 0$, otherwise type 36 is better. The inadmissibility of type 34 can be shown similarly.

Lemma 8.22

$$w_{4,5} + w_{4,6} \geq w_{1,2} + w_{1,3} \quad \text{when } \rho_c \geq 0 \text{ and } \rho_r < 0.$$

<u>Proof</u>

From the expressions for $w_{1,2}$, $w_{1,3}$, $w_{4,5}$ and $w_{4,6}$ given earlier in this section,

$$(w_{4,5} + w_{4,6}) - (w_{1,2} + w_{1,3}) =$$

$$-\rho_r \rho_c^2 + (1 - \rho_c)(1 - \rho_r)(2 - \rho_r)\{1 - (1 - \rho_c)^2\}/\zeta_2.$$

It follows that when $\rho_c \geq 0$ and $\rho_r < 0$, $w_{4,5} + w_{4,6} \geq w_{1,2} + w_{1,3}$, since

$1 - (1 - \rho_c)^2 = \rho_c(2 - \rho_c) \geq 0$ for $\rho_c \geq 0$, and $-\rho_r \rho_c^2 > 0$ for $\rho_r < 0$. ∎

Lemma 8.22 means that $w_{4,5} + w_{4,6} \leq 0 \Rightarrow w_{1,2} + w_{1,3} \leq 0$, and so type 36

cannot be optimal since both $w_{4,5} + w_{4,6} \leq 0$ and $w_{1,2} + w_{1,3} \geq 0$ are required

for type 36 to be better than types 37 and 27, respectively. Therefore, a

comparison of the three remaining types, 27, 28 and 37, leads to Theorem 8.23

to Theorem 8.25.

Theorem 8.23

For blocks of size 3×3 and $t \geq 9$ treatments under model IV, gls and an

AR(1)*AR(1) process, a design of type 27 is optimal for $\rho_c \geq 0$ and $\rho_r < 0$

when $\qquad w_{1,2} \geq 0 \quad$ (type 21)

and $\quad w_{4,5} + w_{4,6} \leq 0 \quad$ (type 28).

<u>Proof</u>

Type 27 is better than type 37 when $2w_{1,2} + w_{4,5} + 2w_{1,3} + w_{4,6} \leq 0$, which is

clearly true when type 27 is better than type 28. This completes the proof.

∎

Theorem 8.24

For blocks of size 3×3 and $t \geq 9$ treatments under model IV, gls and an AR(1)*AR(1) process, a design of type 28 is optimal for $\rho_c \geq 0$ and $\rho_r < 0$

when $\quad\quad w_{1,2} \geq 0 \quad$ (type 22);

$\quad\quad w_{4,5} + w_{4,6} \geq 0 \quad$ (type 27);

and $\quad w_{1,2} + w_{1,3} \leq 0 \quad$ (type 37). ■

Theorem 8.25

For blocks of size 3×3 and $t \geq 9$ treatments under model IV, gls and an AR(1)*AR(1) process, a design of type 37 is optimal for $\rho_c \geq 0$ and $\rho_r < 0$

when $\quad w_{1,2} + w_{1,3} \geq 0 \quad$ (type 28). ■

Figure 8.9 illustrates the optimality regions for types 0, 21, 22, 27, 28, and 37, which all have binary columns. As for the blocks of size 2×2 and 3×2 under the AR(1)*AR(1) process (see Figure 6.2d and Figure 7.6, respectively), as ρ_c increases and/or ρ_r decreases, the number of row self-adjacencies in the optimal type increases. Type 37, which has the maximum number of row self-adjacencies, is the optimal type for approximately 85% of the region under consideration.

Figure 8.9

For blocks of size 3×3 under the AR(1)*AR(1) process, model IV and gls: optimality regions for $\rho_c \geq 0$ and $\rho_r < 0$.

KEY:

0	21	22	27	28	37
$\begin{bmatrix} abc \\ def \\ ghi \end{bmatrix}$	$\begin{bmatrix} bcd \\ aae \\ fgh \end{bmatrix}$	$\begin{bmatrix} bcd \\ aaa \\ efg \end{bmatrix}$	$\begin{bmatrix} aad \\ bbe \\ ccf \end{bmatrix}$	$\begin{bmatrix} aad \\ bbb \\ cce \end{bmatrix}$	$\begin{bmatrix} aaa \\ bbb \\ ccc \end{bmatrix}$
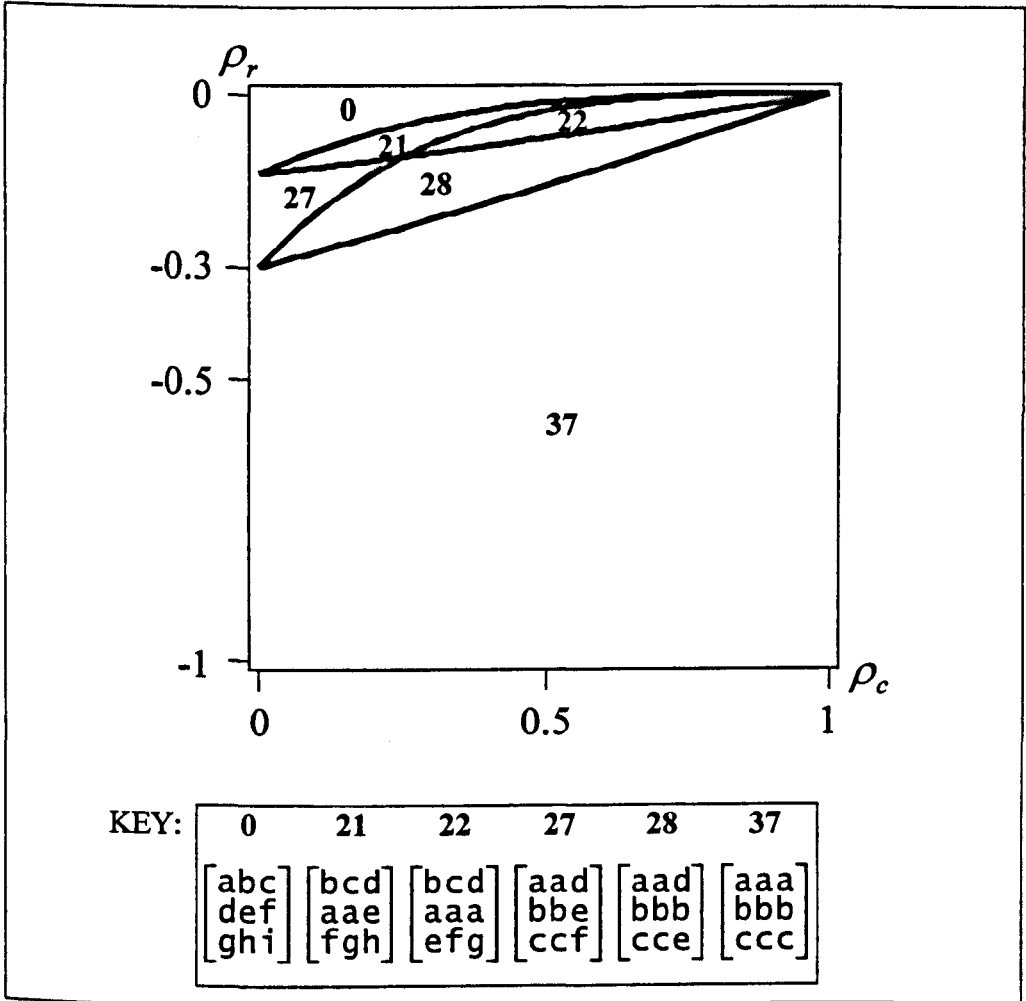
8.4.3   When $\rho_c < 0$ and $\rho_r \geq 0$

Optimality results for $\rho_c < 0$ and $\rho_r \geq 0$ follow immediately from the results, in section 8.4.2 by interchanging ρ_c and ρ_r in the optimality conditions in section 8.4.2 (i.e. swapping $w_{1,2}$ and $w_{1,4}$; $w_{4,5}$ and $w_{2,5}$; $w_{4,6}$ and $w_{2,8}$) and interchanging types 21, 22, 27, 28 and 37 with types 21', 22', 27', 28' and 37', which are given in Definition 8.7 below.

Definition 8.7
Let the types

$$\begin{bmatrix} bac \\ dae \\ fgh \end{bmatrix}, \begin{bmatrix} bac \\ dae \\ fag \end{bmatrix}, \begin{bmatrix} abc \\ abc \\ def \end{bmatrix}, \begin{bmatrix} abc \\ abc \\ dbe \end{bmatrix} \text{ and } \begin{bmatrix} abc \\ abc \\ abc \end{bmatrix},$$

be called types 21', 22', 27', 28' and 37', respectively.   ∎

8.4.4   When $\rho_c, \rho_r < 0$

When $\rho_c, \rho_r < 0$, the $w_{i,j}$ which can be positive are $w_{1,2}$, $w_{1,4}$, $w_{1,5}$, $w_{2,5}$ and $w_{4,5}$. Recall from section 7.5.8 (Figure 7.6) that for blocks of size 3×2 under the AR(1)*AR(1) process and model IV, 3 types can be optimal in each of the regions specified by $\{\rho_c, \rho_r : \rho_c, \rho_r \geq 0\}$, $\{\rho_c, \rho_r : \rho_c \geq 0, \rho_r < 0\}$ and $\{\rho_c, \rho_r : \rho_c < 0, \rho_r \geq 0\}$. For blocks of size 3×3, double the number of types (i.e. 6 types) can be optimal in each of these 3 regions. For $\rho_c, \rho_r < 0$, 6 types can be optimal for blocks of size 3×2. Therefore, it is likely that for blocks of size 3×3, more than 10 types could be optimal when $\rho_c, \rho_r < 0$. Hence, it is difficult to specify optimality regions for non-binary types here. However, the binary type is optimal for $\rho_c, \rho_r < 0$ when $w_{1,2} \leq 0$ and $w_{1,4} \leq 0$ (see Theorem 8.2). Figure 8.10 shows the optimality regions for all the types which can be optimal when at least one of (ρ_c, ρ_r) is positive, as well as the optimality region for the binary type for $|\rho_c|, |\rho_r| < 1$.

Figure 8.10
Optimality regions for blocks of size 3×3 under the AR(1)*AR(1) process, model IV and gls.

KEY:

0	20	37	37'
$\begin{bmatrix} abc \\ def \\ ghi \end{bmatrix}$	$\begin{bmatrix} aba \\ bab \\ aba \end{bmatrix}$	$\begin{bmatrix} aaa \\ bbb \\ ccc \end{bmatrix}$	$\begin{bmatrix} abc \\ abc \\ abc \end{bmatrix}$

? indicates the region for which optimal types are not known.

Note: the types corresponding to the optimality regions which are not labelled can be seen in Figure 8.7 and Figure 8.9.
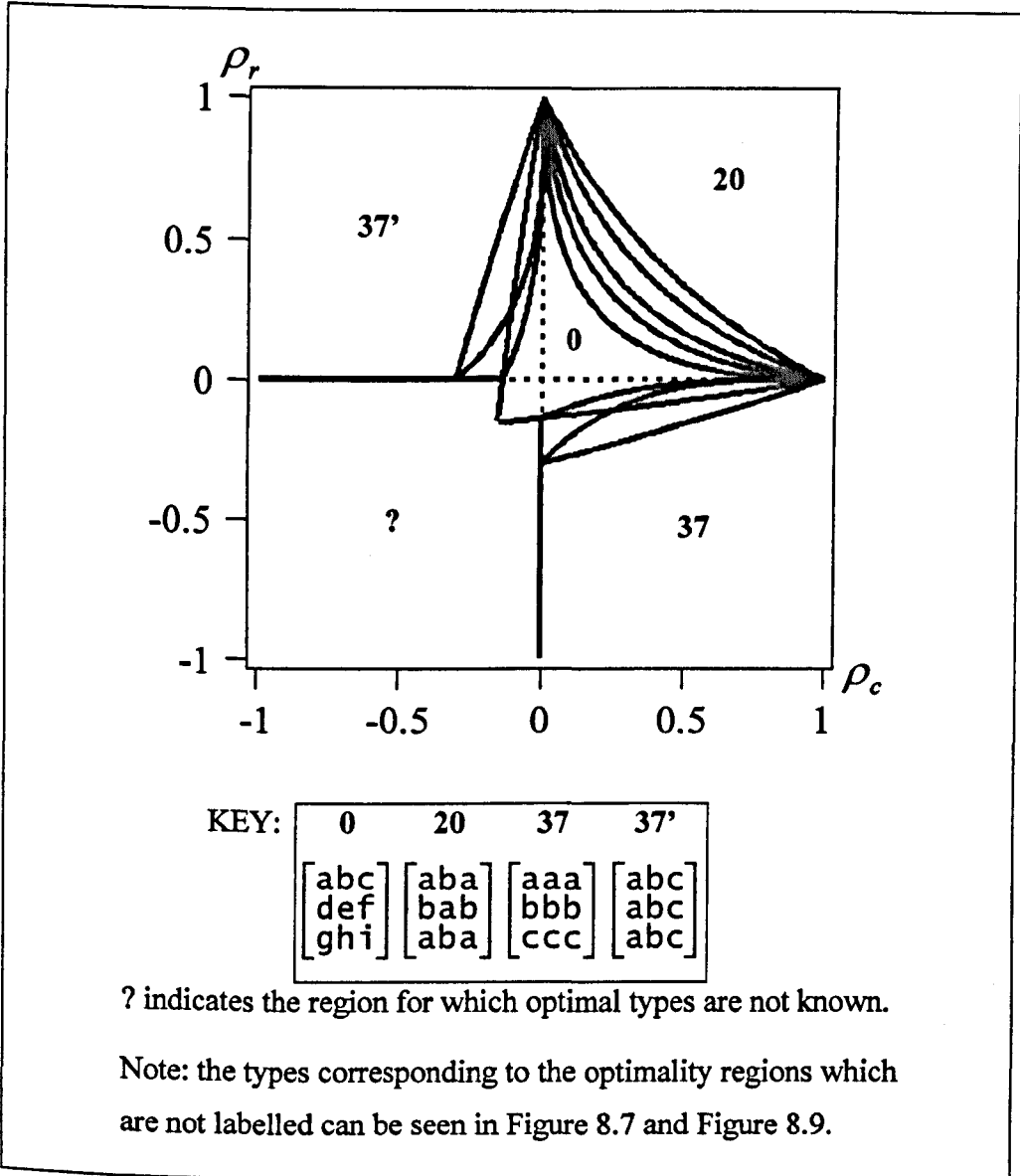
The plots of the optimality regions for blocks of size 2×2 and 3×2, given as Figure 6.2d and Figure 7.6, respectively, show that designs with the maximum number of row self-adjacencies and binary columns, and designs with the maximum number of column self-adjacencies and binary rows, can be optimal for $\rho_c, \rho_r < 0$. For blocks of size 3×2, a design of type 61

$$\begin{bmatrix} a\,a \\ b\,c \\ b\,c \end{bmatrix},$$

which has both row and column self-adjacencies, can also be optimal for $\rho_c, \rho_r < 0$.

These results for blocks of size 2×2 and 3×2, suggest that for blocks of size 3×3, type 37 is likely to be optimal for part of the region given by $\rho_r < \rho_c < 0$, and type 37' is likely to be optimal for part of the region given by $\rho_c < \rho_r < 0$. Also, types which have both row and column self-adjacencies, such as

$$\begin{bmatrix} a\,a\,d \\ b\,e\,c \\ b\,f\,c \end{bmatrix}, \quad \begin{bmatrix} a\,a\,e \\ b\,c\,d \\ b\,c\,d \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} a\,a\,b \\ c\,e\,b \\ c\,d\,d \end{bmatrix},$$

(and diagonal reflections of these types) are likely to be optimal when $\rho_c, \rho_r < 0$.

8.5   Discussion

A brief summary of the optimality results obtained in this chapter is given here.

Sufficient optimality conditions for the binary type, for blocks of size $p_1 \times p_2$ under model IV, have been derived in terms of (ρ_c, ρ_r). These show that for large-sized blocks, the optimality region of the binary type is small. The optimality of non-binary types is very difficult to ascertain for general (p_1, p_2) and also for $\rho_c, \rho_r < 0$. However, when at least one of (ρ_c, ρ_r) is positive:

- the results of Uddin & Morgan (1997a) have been extended for $p_2 = 2$;
- all the optimal types have been derived for $p_1 = p_2 = 3$.

Results obtained for the AR(1)*AR(1) process under model IV show that:

- for $\rho_c, \rho_r \geq 0$, as ρ_c and/or ρ_r increase,

  the number of **diagonal** self-adjacencies in the optimal type increases;

- for $\rho_c \geq 0$ and $\rho_r < 0$, as ρ_c increases and/or ρ_r decreases,

  the number of **row** self-adjacencies in the optimal type increases;

- for $\rho_c < 0$ and $\rho_r \geq 0$, as ρ_c decreases and/or ρ_r increases,

  the number of **column** self-adjacencies in the optimal type increases.

Note that for $\rho_c, \rho_r < 0$, optimal designs are likely to include those designs with both row and column self-adjacencies, as well as designs with the maximum number of row self-adjacencies and binary columns ($\rho_c > \rho_r$), and designs with the maximum number of column self-adjacencies and binary rows ($\rho_c < \rho_r$).

Under model III, some optimality results for blocks of size $p_1 \times 2$ have been obtained, and all the optimal types have been determined for blocks of size 3×2. It is expected that some results could also easily be derived for general (p_1, p_2) under model III.

9 Background material for early generation variety trial designs

Background material for statistical aspects of early generation variety trials is provided in this chapter. Section 9.1 gives an introduction to early generation variety trials. Model definitions and derivation of estimators and efficiency criteria are given in section 9.2. Algorithmic methods to obtain efficient designs for early generation variety trials under spatial dependence are discussed in section 9.3.

9.1 Introduction

For crops such as wheat, barley and sugar cane, plant breeders are continually developing new varieties, which are submitted for extensive testing before being used commercially (Patterson & Silvey, 1980). This testing includes a selection programme, where top performing varieties are identified. Performance is usually assessed with respect to several factors, such as yield, grain quality, disease resistance and processing quality.

At the early stages of a selection programme, there are usually a large number of new varieties to be tested – usually greater than 200 new varieties, sometimes many more. The field trials used to select the top performing new varieties at the early stages are called *early generation variety trials* (EGVTs). The top performers are then tested further in the later stages of the selection programme. The importance of accurately selecting the top performers from an EGVT is highlighted by Cullis *et al.* (1998), who state that, *"The accurate estimation of the genetic merit of breeding lines in early stage variety trials is crucial to the success of the entire breeding programme. Furthermore, incorrect selection at this stage can also result in serious cost inefficiencies."*

EGVTs are often called *unreplicated trials*, since the new varieties (also called test varieties) are unreplicated at a given site, usually due to the limited amount of seed available. Replicated standard varieties (also called check or control varieties) are included for comparative purposes and to detect the existence of trends. Variety trials in which the new varieties are replicated are often called *replicated variety trials*.

Several papers advocating spatial analyses of variety trials are briefly summarised in section 9.1.1. Some of the papers considered in section 9.1.1 include examples of designs for unreplicated trials. These designs, as well as others, are considered in section 9.1.2.

9.1.1   Spatial analyses of variety trials

The likely association between neighbouring plots in agricultural field trials has long been recognised. For example, regarding the layout of field trials, Fisher (1960, chapter IV, part 29) wrote, "*After choosing the area we usually have no guidance beyond the widely veritable fact that patches in close proximity are commonly more alike, as judged by the yield of crops, than those which are further apart.*" A commonly used approach (mainly for replicated trials) to take account of this association between neighbouring plots has been the use of incomplete block designs with a valid randomisation of treatments to plots. A method of analysis used for these designs is outlined in Cochran & Cox (1957, chapter 9), and is called an *incomplete block analysis* here.

Recently, the rapid increase in computing power has made it feasible to analyse agricultural field experiments by taking the spatial dependence of adjoining plots into account. Such analyses are called *spatial analyses*.

Besag & Kempton (1986) considered several different applications where neighbouring plot values can be used in the analysis of replicated agricultural field experiments. They consider the use of spatial models based on first differences to take account of fertility effects in replicated trials.

Gleeson & Cullis (1987) proposed a one-dimensional spatial analysis for replicated field experiments with long narrow plots. They consider a model for plot yield, which as well as having independent local errors, includes *random trend* effects. For long narrow plots, the correlation of the yield of adjacent plots is likely to be much higher within the direction of the shorter side, and so it may be reasonable to model spatial correlation only in this direction. For example, if $\rho_{1,0}$ and $\rho_{0,1}$ are the lag 1 correlations of plot yields within-rows and within-columns, respectively, and the short side of the plots is along the rows of the trial layout, as illustrated in Figure 9.1, then $\rho_{0,1} \gg \rho_{1,0}$ is likely. Hence the within-row correlation is assumed to be negligible (i.e. $\rho_{1,0} = 0$ is modelled). Gleeson & Cullis (1987) modelled trend effects to be from a one-dimensional process (a low-order ARIMA process), and hence the analysis they proposed is described as a one-dimensional analysis. They proposed the use of the residual maximum likelihood (REML) method of Patterson & Thompson (1971) to estimate the parameters of the model.

Figure 9.1
Layout of long thin plots with short side of plots within rows.
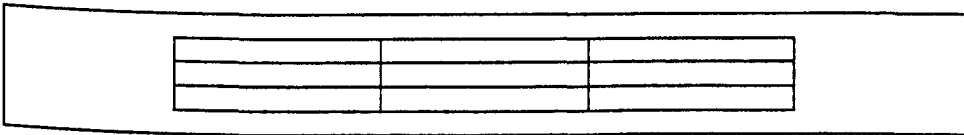
Cullis & Gleeson (1989) investigated the spatial analysis proposed by Gleeson & Cullis (1987) on 1019 Australian replicated variety trials, and obtained an average reduction of 42% in the variances of varietal yield differences, compared with conventional randomised *complete block analyses*. For incomplete block analyses (see Cullis & Gleeson, 1989, for details) on 219 of

these trials, the average reduction in variances was 33%, compared with the complete block analyses. These results therefore provide evidence to support the use of spatial analyses.

For the situation where plots are approximately square, substantial spatial correlation may exist in both directions (rows and columns) and so the method of Gleeson & Cullis (1987) was extended to a two-dimensional analysis by Cullis & Gleeson (1991). Cullis & Gleeson (1991) modelled the random trend effects to be from a separable process, with row and column correlation structures taken as ARIMA processes (let this separable process be called an ARIMA*ARIMA process).

To assess the benefits of taking account of two-dimensional spatial variation, Kempton *et al.* (1994) studied a two-dimensional version of the spatial analysis proposed by Besag & Kempton (1986) on 224 UK replicated cereal trials. They demonstrated that a two-dimensional spatial analysis was appreciably better than a one-dimensional spatial analysis.

As well as using the conventional complete block and incomplete block analyses, Grondona *et al.* (1996) used the methods of Cullis & Gleeson (1987, 1991) to analyse 35 replicated cereal yield trials. The one-dimensional analysis of Cullis & Gleeson (1987) was used when the random trend was modelled as low-order ARIMA processes, and when the random trend was modelled as two-dimensional ARIMA*ARIMA processes, the analysis method of Cullis & Gleeson (1991) was used. The average estimated standard error of the pairwise varietal yield differences was used to assess model adequacy. It was shown that the spatial analyses were generally better than the complete block and incomplete block analyses, and that modelling two-dimensional spatial correlation was generally better than modelling one-dimensional spatial correlation. Moreover, the AR(1)*AR(1) process outperformed the other processes considered in 21 of the 35 trials.

Gilmour *et al.* (1997) identified three major components of spatial variation in plot errors from field experiments, and extended the two-dimensional spatial method of Cullis & Gleeson (1991) to account for them. These components are:

- non-stationary, global variation across the field;
- stationary, local variation within the trial;
- extraneous variation, often induced by the experimental procedures.

For a $p_1 \times p_2$ array of plots, they propose the model

$$\underline{y} = X\underline{\tau} + Z\underline{\alpha} + \underline{\xi} + \underline{\eta}, \qquad (9.1)$$

where

$\underline{y}$ is the m-vector of plot data (usually yield);

$\underline{\tau}$ is a vector of fixed effects (such as treatment effects);

$\underline{\alpha}$ is a vector of random effects (such as row and column effects);

X and Z are the design matrices corresponding to $\underline{\tau}$ and $\underline{\alpha}$, respectively;

$\underline{\eta}$ is the vector of zero mean random errors;

$\underline{\xi}$ represents the spatial trend effect.

Henceforth, the spatial trend effect will be called the *additional spatial component*. Large scale variation may be taken into account by differencing of the data (as in, for example, Besag & Kempton, 1986). However, Gilmour *et al.* (1997) point out that the need for differencing has been questioned by several authors and that it can lead to the need for more complex modelling of the variance structure for the plot errors. Therefore, they include, if deemed appropriate, polynomial functions of the spatial co-ordinates in the matrix X as an alternative to differencing. Smoothing splines may also be used by including the appropriate terms in X and Z (see Gilmour *et al.*, 1997, for details). The additional spatial component is intended to take account of the local variation, and models for $\underline{\xi}$ are chosen from a class of separable processes. The restriction to separable processes is justified by the "*significant savings in computer time for the analysis of larger trials,*" resulting from the separability assumption. The AR(1)*AR(1) process is

recommended as an initial model for $\underline{\xi}$ due to its *"general superiority over the incomplete block model."* Also, Gilmour *et al.* (1997) state that the AR(1)*AR(1) process facilitates a more accurate assessment of the presence of global and extraneous variation than the incomplete block model. Also, they note that the extraneous variation is often well described by design factors such as rows and columns.

Most of the literature on the spatial analysis of field trials employs a frequentist analysis. However, Besag & Higdon (1999) have described a Bayesian spatial methodology for the analysis of agricultural field trials.

Now consider EGVTs. Various methods for ranking the new varieties in EGVTs have been used. Early methods calculated a fertility index, from the yields of the control varieties, for every plot in the experiment. These indices were used to adjust the yields of the new varieties for local variation in fertility (see Cochran & Cox, 1957, section 9.51).

Methods that take spatial dependencies into account for EGVTs have been investigated by Kempton (1984), Besag & Kempton (1986), Cullis *et al.* (1989), and more recently by Cullis *et al.* (1998).

Cullis *et al.* (1989) extended the method of Gleeson & Cullis (1987) to the analysis of EGVTs with long narrow plots. Cullis *et al.* (1998) gave a method for the spatial analysis of *multi-environment* EGVTs, that is EGVTs that are carried out across several sites. They state that *"it is now generally accepted that spatial models of analysis provide more accurate and precise estimates of genotype effects than either complete or incomplete blocks analysis."* They suggest that the AR(1)*AR(1) process be used as an initial model for the additional spatial component.

Federer (1998) proposed a method of analysis for designs called *augmented row-column* designs, which could be used for unreplicated trials. He considered a mixed effects model with random new variety effects and fixed control variety effects, and included uncorrelated errors. Polynomial regression values of row and column positions and their interactions were used, and were considered to be random effects (see Federer, 1998, sections 8 and 9, for further details).

9.1.2   Designs for unreplicated trials

Assume here a two-dimensional layout of plots in a $p_1 \times p_2$ array. Assume further that there are c control varieties and t new varieties. Then the total number of varieties is $v = c + t$. Let $r_i > 0$ denote the number of times that control variety i is replicated ($i = 1, \ldots, c$), and under equi-replication of the control varieties, let $r_i = r \; \forall \; i$.

The experimental designs most frequently employed for EGVTs have had replicated plots of control varieties, which are called *check plots*, systematically distributed among the unreplicated plots of new varieties, with the new varieties randomly allocated to the non-check plots.

For unreplicated trials, Federer & Raghavarao (1975) give $r \times r$ *augmented designs* (ADs) for a fixed effects model, which includes row and column effects. These designs are constructed from Youden designs (see Federer & Raghavarao, 1975, for details), and have each control variety occurring once in each row and column. As an example, they consider the following representation of a 7×7 AD with $c = 3$ controls and $t = 28$ test varieties. The symbol • represents the new varieties, and 1, 2 and 3 represent the control varieties. In practice, the rows and columns of this representation would be randomised.

1	•	•	•	3	•	2
2	1	•	•	•	3	•
•	2	1	•	•	•	3
3	•	2	1	•	•	•
•	3	•	2	1	•	•
•	•	3	•	2	1	•
•	•	•	3	•	2	1

Note that this design has a high proportion of check plots (check plots taking up about 42% of the plots).

Federer & Raghavarao (1975) suggested four ways to assess the efficiency of unreplicated designs, with respect to the average variance of all pairwise comparisons

  i)   among control varieties,

 ii)   among new varieties,

iii)   between control and new varieties,

iv)   among all varieties.

Federer *et al.* (1975) proposed ADs for $p_1 = p_2$, which have roughly half the plots for the control varieties with the unreplicated new varieties neighboured by 2, 3, or 4 control varieties. The ADs in Federer *et al.* (1975) were compared with respect to the average variance of all pairwise comparisons among new varieties, although Federer *et al.* (1975) suggested that the average variance of all pairwise comparisons between control and new varieties be used in screening experiments.

Usually a high proportion of check plots would not be possible for EGVTs since, typically, there are a large number of new varieties and a limited number of plots that can be used. Therefore, the ADs proposed by Federer & Raghavarao (1975) and Federer *et al.* (1975), which have a high proportion of check plots, cannot usually be used in EGVTs. For this reason (and some other reasons discussed by them), split-plot designs, called modified ADs (MADs) were proposed by Lin & Poushinsky (1983) for square or nearly

square plots. A description of these designs, and an outline of the proposed method of analysis, is now given.

The MADs have 9 sub-plots within a whole-plot, arranged in a 3×3 square. The outer dimensions of the experimental area are therefore multiples of 3 times the sub-plot dimensions. The restriction to square or nearly square sub-plots "*ensures an approximately equal distance between a centre sub-plot and its surrounding eight sub-plots*". The importance of this property is discussed in Lin & Poushinsky (1983, section 5). For illustration purposes, they consider designs with $p_1 = p_2 = 3c$ and $r = c + 2$, where the centre of each whole-plot has one of the c control varieties allocated to it, according to a $c \times c$ Latin square design. Also, for each control variety, x, two whole-plots are arbitrarily chosen from the c whole-plots which already contain control variety x, and control variety x is then arbitrarily allocated to one of the eight remaining sub-plots (called *outer* sub-plots). This means that $t = 2c(4c - 1)$. For $c = 2$ to $c = 12$, 22% to 13% of the plots are check plots. After allocating the control varieties, the test varieties are allocated randomly to the remaining sub-plots.

They give the following design with $p_1 = p_2 = 12$, $t = 120$, $c = 4$ and $r = 6$, as an example, where 1 to 4 represent the control varieties.

They assume the following model:

$$y_{i,j} = \tau_{T(i,j)} + \beta_i + \varepsilon_{i,j},$$

with $\mathrm{var}(y_{i,j}) = \sigma_\beta^2 + \sigma_\varepsilon^2$

and $\mathrm{cov}(y_{i,j}, y_{i,j'}) = \sigma_\beta^2$ for $j \neq j'$,

where

$y_{i,j}$ is the yield of the variety in whole-plot i and sub-plot j;

$\tau_{T(i,j)}$ is the fixed effect of the variety in whole-plot i and sub-plot j;

β_i is the effect of whole-plot i ;

$\varepsilon_{i,j}$ is the error.

The yields from the centre sub-plots provide an estimate of $\sigma_\beta^2 + \sigma_\varepsilon^2$, and the additional check plots allow σ_ε^2 to be estimated. The estimated yields for the test varieties can then be adjusted for estimated row and column effects. Two other methods of adjusting the estimated yields are also given (see Lin & Poushinsky, 1983, for details). The new varieties corresponding to a pre-assigned proportion of the best adjusted values are then selected for further testing.

Since the above MADs are intended for approximately square plots, MADs for long and narrow plots were given by Lin & Poushinsky (1985). These MADs have the whole-plots arranged as in the MADs of Lin & Poushinsky (1983), but the sub-plots are laid out in rows within whole-plots. There are 5 sub-plots in each whole-plot, with the centre sub-plot being a check plot.

In separate work, Kempton (1984) considers the use of replicated standard varieties for unreplicated trials. He recommends that the frequency of check plots should be less than 1 in 5. This holds for the MADs of Lin & Poushinsky (1983) for $c = 3$ to $c = 12$, but clearly not for the ADs of Federer et al. (1975).

A set of plots, $\mathcal{X}$, is defined to be *in a diagonal* if for any plot $x \in \mathcal{X}$,

- either all the lag (1, 1), (2, 2), (3, 3), …
- or all the lag (1, -1), (2, -2), (3, -3), …

neighbouring plots of x (see Figure 3.1 in section 3.1.1.4) are the plots in $\mathcal{X} \setminus \{x\}$.

Kempton (1984) gives several examples of systematic designs, one of which (from 1905) has the check plots in several diagonals with check plots three plots apart in rows and columns, as in the following design which has $p_1 = 4$, $p_2 = 6$, $t = 16$, $c = 1$ and $r = 8$.

•	•	1	•	•	1
•	1	•	•	1	•
1	•	•	1	•	•
•	•	1	•	•	1

Recently, designs with the check plots in diagonals have been used in EGVTs by New South Wales (NSW) Agriculture, Australia. Also, an example of an EGVT, conducted by the Centro Internacional de Mejoramiento de Maiz y Trigo (International Maize and Wheat Improvement Center), Mexico, was considered by Federer (1998). The augmented row-column design in Federer (1998), which had $p_1 = 15$, $p_2 = 12$, $t = 120$, $c = 2$ and $r = 30$, with one-third of the plots being check plots, is given as:

1	•	•	2	•	•	1	•	•	2	•	•
•	1	•	•	2	•	•	1	•	•	2	•
•	•	1	•	•	2	•	•	1	•	•	2
2	•	•	1	•	•	2	•	•	1	•	•
•	2	•	•	1	•	•	2	•	•	1	•
•	•	2	•	•	1	•	•	2	•	•	1
1	•	•	2	•	•	1	•	•	2	•	•
•	1	•	•	2	•	•	1	•	•	2	•
•	•	1	•	•	2	•	•	1	•	•	2
2	•	•	1	•	•	2	•	•	1	•	•
•	2	•	•	1	•	•	2	•	•	1	•
•	•	2	•	•	1	•	•	2	•	•	1
1	•	•	2	•	•	1	•	•	2	•	•
•	2	•	•	1	•	•	2	•	•	1	•
•	•	2	•	•	1	•	•	2	•	•	1

The check plots are three plots apart in rows and columns (i.e. in diagonals, as in the above example design from Kempton, 1984) with 2 or 3 replicates of each control variety appearing in each column and twice in each row. Each of the diagonals containing the check plots has the same control variety allocated to them, except for the check plots in the bottom two rows.

Another example design in Kempton (1984) and also in Besag & Kempton (1986) has $c = 2$, with the control varieties allocated to every sixth row so that the two control varieties alternate within the rows and columns, as in the transpose of the following design.

```
1 • • • • • 2 • • • • • 1 • • • • • 2 • • • • • 1 • • •
2 • • • • • 1 • • • • • 2 • • • • • 1 • • • • • 2 • • •
1 • • • • • 2 • • • • • 1 • • • • • 2 • • • • • 1 • • •
2 • • • • • 1 • • • • • 2 • • • • • 1 • • • • • 2 • • •
1 • • • • • 2 • • • • • 1 • • • • • 2 • • • • • 1 • • •
```

This type of design is recommended by Kempton (1984) for long and narrow plots, and has been used for winter wheat trials at the Plant Breeding Institute, Cambridge, UK. Besag & Kempton (1986) give an example of such a design, that was used in an EGVT from 1980, where the plots are of size $1.5\text{m} \times 4.5\text{m}$, and $p_1 = 52$, $p_2 = 37$, $t = 1560$, $c = 2$ and $r = 182$. The short side of the plots is within rows, as shown in Figure 9.1. The check plots take up about 19% of the plots.

Cullis *et al.* (1989) state that long narrow plots are generally used in cereal testing programmes in Australia, and that a common layout has the control varieties allocated at a given (within row) frequency with additional check plots placed throughout the trial. They give an example of a NSW wheat trial from 1988, with plots of size $15\text{m} \times 1.8\text{m}$, and $p_1 = 10$, $p_2 = 67$, $t = 525$, $c = 7$ and $(r_1, \ldots, r_7) = (121, 3, 4, 5, 4, 4, 4)$, with the long side of the plots within rows. Control variety 1 was allocated to the ten plots in each of the columns 1, 7, 13, ..., 67, (every sixth plot within each row), and the remaining plots of this control variety and the other 6 control varieties were allocated randomly over the trial. The check plots constitute about 22% of the plots.

Another example of a systematic design is the following design, given by Kempton & Talbot (1988), for roughly square plots with $c = 4$.

```
1 • • • • • 2 • • • • • 3 • • • • • 4 • • • • • 1 • • •
• • • 3 • • • • • 4 • • • • • 1 • • • • • 2 • • • • • 3
4 • • • • • 1 • • • • • 2 • • • • • 3 • • • • • 4 • • •
• • • 2 • • • • • 3 • • • • • 4 • • • • • 1 • • • • • 2
3 • • • • • 4 • • • • • 1 • • • • • 2 • • • • • 3 • • •
```

The check plots for this design are 6 plots apart in rows, and 2 plots apart in columns, with every third column containing check plots. Note also that the columns are binary.

Cullis *et al.* (1998) consider a multi-site EGVT from 1991 for wheat in South Australia. This trial had plots of size $1.33\text{m} \times 3\text{m}$, and $p_1 = 34$, $p_2 = 12$, $t = 330$, $c = 6$ and $r = 12$, with the short side of the plots within rows. The six control varieties were allocated at random to six plots within each column, except for the first column, where they were allocated to the top six plots. A *"filler variety"* was replicated six times in the bottom six plots of the last column to *"maintain a rectangular layout"*, since $t + cr = 402$ is less than $p_1 p_1 = 408$. The check plots constitute about 18% of the plots for this trial.

9.2 Models, estimators, predictors and criteria

For an EGVT on a $p_1 \times p_2$ array of plots, the general form of the models assumed here is:

$$\underline{y} = \underline{1}_m \mu + X_s \underline{\tau}_s + X_n \underline{\tau}_n + Z_r \underline{\gamma} + Z_c \underline{\delta} + \underline{\xi} + \underline{\eta} \tag{9.2}$$

and

$$\text{var}(\underline{y}) = V,$$

where

$\underline{y}$ is the m-vector of observations in lexicographic order;

$\underline{\tau}_s$, $\underline{\tau}_n$, $\underline{\gamma}$, $\underline{\delta}$, $\underline{\eta}$ and $\underline{\xi}$ are control variety effects, new variety effects, random row effects, random column effects, random error and additional spatial component, respectively;

X_s, X_n, $Z_r = I_{P_1} \otimes 1_{P_2}$ and $Z_c = 1_{P_1} \otimes I_{P_2}$ are the design matrices corresponding to $\underline{\tau}_s$, $\underline{\tau}_n$, $\underline{\gamma}$ and $\underline{\delta}$, respectively;

V is a $m \times m$ positive definite matrix.

The model in (9.2) is a special case of the initial model given by Gilmour *et al.* (1997), but here large scale variation is assumed to be adequately modelled by $\text{var}(\underline{y}) = V$. Therefore polynomial functions of the spatial co-ordinates and smoothing splines are not included.

Definition 9.1
Let

$$\underline{\tau} = (\underline{\tau}_s', \underline{\tau}_n')' \quad \text{and} \quad X = [X_s \mid X_n].$$ ∎

In this thesis, three special cases of the model in (9.2), which are defined in Definition 9.2, are considered.

Definition 9.2
Models 1, 2 and 3 are special cases of the model in (9.2), such that,

- for model 1: $\underline{\tau}$ is a vector of fixed effects;
- for model 2: $\underline{\tau}_s$, and $\underline{\tau}_n$ are vectors of fixed and random effects, respectively;
- for model 3: $\underline{\tau}$ is a vector of random effects. ∎

Definition 9.3

For model i ($i = 1,2,3$) let

$$\text{var}(\underline{y}) = V_i,$$

and let

$$V_i^* = V_i^{-1} - (\underline{1}_m ' V_i^{-1} \underline{1}_m)^{-1} V_i^{-1} J_m V_i^{-1}. \qquad \blacksquare$$

For unreplicated trials, Federer & Raghavarao (1975), Lin & Poushinsky (1983, 1985), Kempton (1984) and Besag & Kempton (1986) modelled both control and new variety effects as fixed effects, as in model 1. In Cullis *et al.* (1989) and Federer (1998), fixed control effects and random new variety effects were modelled, as in model 2. For multi-environment EGVTs, Cullis *et al.* (1998), modelled both control and new varieties as random effects, as in model 3.

It is assumed that $\underline{\theta} = (\underline{\gamma}', \underline{\delta}', \underline{\xi}', \underline{\eta}')'$ has zero mean, and variance matrix

$$\text{var}(\underline{\theta}) = \begin{pmatrix} \sigma_\gamma^2 I_{p_1} & 0 & 0 & 0 \\ 0 & \sigma_\delta^2 I_{p_2} & 0 & 0 \\ 0 & 0 & \sigma_\xi^2 \Lambda & 0 \\ 0 & 0 & 0 & \sigma_\eta^2 I_m \end{pmatrix},$$

where Λ is the correlation matrix of the additional spatial component, which is assumed to be from an AR(1)*AR(1) process, as recommended by Grondona *et al.* (1996), Gilmour *et al.* (1997) and Cullis *et al.* (1998) (see section 9.1.1).

Definition 9.4

Let ρ_r and ρ_c be the lag 1 within-row and within-column correlation parameters, respectively, for the AR(1)*AR(1) process. $\qquad \blacksquare$

For long narrow plots, $\rho_c > \rho_r$ will be likely.

Definition 9.5
For ease of reference, let

$$\Psi = (\sigma_\gamma^2, \sigma_\delta^2, \sigma_\xi^2, \sigma_\eta^2). \qquad \blacksquare$$

For design purposes, it is necessary to assume that V is known. It is also assumed that V is to be used in the estimation or prediction of $\underline{\tau}_n$ and/or $\underline{\tau}_s$.

In practice, for data from a completed trial, estimation will usually use a fitted variance structure. The design efficiency implications, discussed in chapters 9 to 11, will be approximately correct if the assumed V is close to the fitted V.

9.2.1 Models 1, 2 and 3: Estimation and prediction

9.2.1.1 Model 1

Recall that for model 1, $\underline{\tau}_s$, and $\underline{\tau}_n$ in equation (9.2) are fixed effects. Hence

$$E(\underline{y}) = \underline{1}_m \mu + X_s \underline{\tau}_s + X_n \underline{\tau}_n,$$

and $\quad \mathrm{var}(\underline{y}) = Z_r \, \mathrm{var}(\underline{\gamma}) Z_r' + Z_c \, \mathrm{var}(\underline{\delta}) Z_c' + \mathrm{var}(\underline{\xi}) + \mathrm{var}(\underline{\eta})$

$$= \sigma_\gamma^2 (I_{p_1} \otimes J_{p_2}) + \sigma_\delta^2 (J_{p_1} \otimes I_{p_2}) + \sigma_\xi^2 \Lambda + \sigma_\eta^2 I_m$$

$$= V_1 .$$

Note that the rank of the $m \times (v+1)$ matrix $[\underline{1}_m \mid X_s \mid X_n]$ is v.

Definition 9.6
For model 1, let

$$\mathrm{var}(y_{j_1, j_2}) = \sigma_{(1)}^2.$$

Also, let

$$\mathrm{corr}(y_{j_1, j_2}, y_{j_1 + g_2, j_2 + g_1}) = \rho_{g_1, g_2}^{(1)},$$

where y_{j_1, j_2} is the yield of the plot in row j_1 and column j_2. $\qquad \blacksquare$

Under model 1,

$$\sigma^2_{(1)} = \sigma^2_\gamma + \sigma^2_\delta + \sigma^2_\xi + \sigma^2_\eta,$$

and for $(g_1, g_2) \neq (0,0)$,

$$\rho^{(1)}_{g_1,0} = \left(\sigma^2_\gamma + \sigma^2_\xi \rho_r^{|g_1|} \right) \Big/ \sigma^2_{(1)};$$

$$\rho^{(1)}_{0,g_2} = \left(\sigma^2_\delta + \sigma^2_\xi \rho_c^{|g_2|} \right) \Big/ \sigma^2_{(1)};$$

and $\quad \rho^{(1)}_{g_1,g_2} = \sigma^2_\xi \rho_r^{|g_1|} \rho_c^{|g_2|} \Big/ \sigma^2_{(1)}.$

For illustrative purposes, consider an unreplicated design with $p_1 = 2$, $p_2 = 3$, $t = 2$ and $c = r = 2$. Under model 1 with $\Psi = (\frac{1}{8}, \frac{3}{4}, \frac{3}{4}, \frac{1}{4})$ and $(\rho_r, \rho_c) = (\frac{1}{5}, \frac{2}{3})$,

$$\sigma^2_{(1)} = 15/8 = 1.875;$$

$$\rho^{(1)}_{1,0} = 11/75 \approx 0.147; \quad \rho^{(1)}_{2,0} = 31/375 \approx 0.083; \quad \rho^{(1)}_{0,1} = 16/25 = 0.64;$$

$$\rho^{(1)}_{1,1} = 6/125 = 0.048; \quad \rho^{(1)}_{2,1} = 6/625 \approx 0.010.$$

The gls estimator (see section 2.4) of $\underline{\tau}$ is

$$\hat{\underline{\tau}} = C_1^- X' V_1^* \underline{y}, \tag{9.3}$$

where $C_1 = X' V_1^* X$. It follows from (9.3) that, if $\underline{c}' \underline{\tau}$ is an estimable contrast, $\text{var}(\underline{c}' \hat{\underline{\tau}}) = \underline{c}' C_1^- \underline{c}$. Equivalently, $\hat{\underline{\tau}}$ can be taken as $C_{1a}^{-1} X' V_1^{-1} \underline{y}$, where $C_{1a} = X' V_1^{-1} X$ is of rank v, and $\text{var}(\hat{\underline{\tau}}) = C_{1a}^{-1}$.

9.2.1.2   Model 2

Now consider model 2, where $\underline{\tau}_s$ in equation (9.2) is a vector of fixed effects, and $\underline{\tau}_n$ is a vector of random effects, such that $(\underline{\theta}', \underline{\tau}_n')'$ has zero mean and variance matrix

$$\begin{pmatrix} \text{var}(\underline{\theta}) & 0 \\ 0 & \sigma^2_n G_n \end{pmatrix}.$$

This means that

$$E(\underline{y}) = 1_m \mu + X_s \underline{\tau}_s,$$

and $\mathrm{var}(\underline{y}) = \sigma_n^2 X_n G_n X_n{}' + V_1 = V_2.$

The rank of the $m \times (c+1)$ matrix $[1_m \mid X_s]$ is $c+1$.

Under model 2 with $G_n = I_t$, $\mathrm{cov}(y_{j_1,j_2}, y_{j_1+g_2,j_2+g_1})$ for $(g_1, g_2) \neq (0,0)$ is the same as in model 1, but $\mathrm{var}(y_{j_1,j_2})$ depends on the variety (new or control) allocated to the plot in row j_1 and column j_2. Hence, the dependence process given by V_2 is not stationary. It is easy to show that when the $(j_1, j_2)^{\mathrm{th}}$ plot contains a new variety,

$$\mathrm{var}(y_{j_1,j_2}) = \sigma_n^2 + \sigma_{(1)}^2 = \sigma_{(2,n)}^2,$$

and when the $(j_1, j_2)^{\mathrm{th}}$ plot contains a standard (control) variety,

$$\mathrm{var}(y_{j_1,j_2}) = \sigma_{(1)}^2 = \sigma_{(2,s)}^2.$$

Let $\rho_{g_1,g_2}^{(2,nn)}$, $\rho_{g_1,g_2}^{(2,ss)}$ and $\rho_{g_1,g_2}^{(2,ns)}$ denote $\mathrm{corr}(y_{j_1,j_2}, y_{j_1+g_2,j_2+g_1})$ for $(g_1, g_2) \neq (0,0)$ under model 2 when the $(j_1,j_2)^{\mathrm{th}}$ and $(j_1+g_2, j_2+g_1)^{\mathrm{th}}$ plots

- both contain new varieties
- both contain control varieties
- contain a new and control variety,

respectively. Then, for $G_n = I_t$, $(g_1, g_2) \neq (0,0)$, and $x_1, x_2 \in \{n, s\}$,

$$\rho_{g_1,0}^{(2,x_1 x_2)} = \left(\sigma_\gamma^2 + \sigma_\xi^2 \rho_r^{|g_1|}\right) \Big/ \left(\sigma_{(2,x_1)} \sigma_{(2,x_2)}\right);$$

$$\rho_{0,g_2}^{(2,x_1 x_2)} = \left(\sigma_\delta^2 + \sigma_\xi^2 \rho_c^{|g_2|}\right) \Big/ \left(\sigma_{(2,x_1)} \sigma_{(2,x_2)}\right);$$

and $\rho_{g_1,g_2}^{(2,x_1 x_2)} = \sigma_\xi^2 \rho_r^{|g_1|} \rho_c^{|g_2|} \Big/ \left(\sigma_{(2,x_1)} \sigma_{(2,x_2)}\right).$

Consider an unreplicated design with $p_1 = 2$, $p_2 = 3$, $t = 2$ and $c = r = 2$ under model 2 with $\Psi = (\frac{1}{4}, \frac{1}{4}, \frac{1}{4}, \frac{1}{4})$, $(\rho_r, \rho_c) = (\frac{1}{3}, \frac{2}{3})$ and $\sigma_n^2 = \frac{1}{2}$. Here

$$\sigma_{(2,n)}^2 = 19/8 = 2.375 \quad \text{and} \quad \sigma_{(2,s)}^2 = 15/8 = 1.875,$$

and for the design

$$\begin{array}{|c|c|c|} \hline 1 & \cdot & 1 \\ \hline 2 & 2 & \cdot \\ \hline \end{array}$$

some of the correlations are

$$\text{corr}(y_{1,1}, y_{1,2}) = \rho_{1,0}^{(2,ns)} \approx 0.130;$$

$$\text{corr}(y_{2,1}, y_{2,2}) = \rho_{1,0}^{(2,nm)} = 11/95 \approx 0.116;$$

$$\text{corr}(y_{1,1}, y_{2,1}) = \rho_{0,1}^{(2,ss)} = 16/25 = 0.64;$$

$$\text{corr}(y_{1,2}, y_{2,2}) = \rho_{0,1}^{(2,ns)} \approx 0.569;$$

$$\text{corr}(y_{1,2}, y_{2,3}) = \rho_{1,1}^{(2,nm)} = 18/475 \approx 0.038.$$

Note that the correlations of pairs of plots, which are the same lag apart, can be different.

The BLUE of the estimable contrast $\underline{c}_s'\underline{\tau}_s$ is $\underline{c}_s'\hat{\underline{\tau}}_s$, where

$$\hat{\underline{\tau}}_s = (X_s'V_2^* X_s)^{-1} X_s'V_2^* \underline{y}. \tag{9.4}$$

The best linear unbiased predictor (BLUP) (see section 2.4.5) of $\underline{c}_n'\underline{\tau}_n$ is $\underline{c}_n'\tilde{\underline{\tau}}_n$, where

$$\tilde{\underline{\tau}}_n = \sigma_n^2 G_n X_n'V_2^* (\underline{y} - X_s\hat{\underline{\tau}}_s). \tag{9.5}$$

A derivation of BLUPs is given by Searle *et al.* (1992, section 7.4). This derivation gives

$$(\hat{\mu}, \hat{\underline{\tau}}_s') = (X_{1,s}'V_2^{-1}X_{1,s})^{-1} X_{1,s}'V_2^{-1}\underline{y}, \quad \text{(which is the gls estimator)}$$

where $X_{1,s} = [\underline{1}_m \mid X_s]$, and $\tilde{\underline{\tau}}_n$ as

$$\tilde{\underline{\tau}}_n = \sigma_n^2 G_n X_n'V_2^{-1} \left(\underline{y} - X_{1,s}(\hat{\mu}, \hat{\underline{\tau}}_s')'\right).$$

This derivation is shown in Appendix A3.1 to give the same $\hat{\underline{\tau}}_s$ and $\tilde{\underline{\tau}}_n$ as in (9.4) and (9.5).

Henderson (1975) also considered best linear unbiased prediction and showed that

$$\begin{pmatrix} \hat{\mu} \\ \hat{\underline{\tau}}_s \\ \tilde{\underline{\tau}}_n \end{pmatrix} = C_{(2)}^{-1} \begin{pmatrix} X_{1,s}' \\ X_n' \end{pmatrix} V_1^{-1} \underline{y},$$

where

$$C_{(2)} = \left(\begin{array}{c|c} X_{1,s}'V_1^{-1}X_{1,s} & X_{1,s}'V_1^{-1}X_n \\ \hline X_n'V_1^{-1}X_{1,s} & X_n'V_1^{-1}X_n + \sigma_n^{-2}G_n^{-1} \end{array} \right). \tag{9.6}$$

Equivalently, in terms of V_1^*,

$$\begin{pmatrix} \hat{\underline{\tau}}_s \\ \tilde{\underline{\tau}}_n \end{pmatrix} = C_2^{-1} \begin{pmatrix} X_s' \\ X_n' \end{pmatrix} V_1^* \underline{y}, \tag{9.7}$$

where

$$C_2 = \left(\begin{array}{c|c} X_s'V_1^*X_s & X_s'V_1^*X_n \\ \hline X_n'V_1^*X_s & X_n'V_1^*X_n + \sigma_n^{-2}G_n^{-1} \end{array} \right). \tag{9.8}$$

Definition 9.7
Let C_i^- (for $i=1$) and C_i^{-1} (for $i=2,3$) be partitioned as

$$\left(\begin{array}{c|c} C_i^{(ss)} & C_i^{(sn)} \\ \hline C_i^{(ns)} & C_i^{(nn)} \end{array} \right). \qquad \blacksquare$$

It is shown in Appendix A3.2 that

$$C_2^{(ss)} = \left(X_s'V_2^*X_s \right)^{-1}, \quad C_2^{(sn)} = C_2^{(ns)\prime} = -\sigma_n^2 C_2^{(ss)} X_s'V_2^*X_n G_n$$

and

$$C_2^{(nn)} = \sigma_n^2 \left(G_n - \sigma_n^2 G_n X_n'V_2^*X_n G_n + \sigma_n^2 G_n X_n'V_2^*X_s C_2^{(ss)} X_s'V_2^*X_n G_n \right).$$

In Appendix A3.3 it is shown that

$$\text{var}(\hat{\underline{\tau}}_s) = C_2^{(ss)}, \quad \text{var}(\tilde{\underline{\tau}}_n - \underline{\tau}_n) = \text{mse}(\tilde{\underline{\tau}}_n) = C_2^{(nn)},$$

and $\text{cov}(\hat{\underline{\tau}}_s, \tilde{\underline{\tau}}_n - \underline{\tau}_n) = C_2^{(sn)}$.

9.2.1.3 Model 3

Now consider model 3. Here both $\underline{\tau}_s$ and $\underline{\tau}_n$ in equation (9.2) are vectors of random effects, such that $(\underline{\theta}', \underline{\tau}_s', \underline{\tau}_n')'$ has zero mean and variance matrix

$$
\begin{pmatrix}
\mathrm{var}(\underline{\theta}) & 0 & 0 \\
0 & \sigma_s^2 G_s & 0 \\
0 & 0 & \sigma_n^2 G_n
\end{pmatrix}.
$$

Hence,

$$
E(\underline{y}) = 1_m \mu \quad \text{and} \quad \mathrm{var}(\underline{y}) = \sigma_s^2 X_s G_s X_s' + V_2 = V_3.
$$

It can be shown, similarly to model 2, that the BLUP of $\underline{c}'\underline{\tau}$ is $\underline{c}'\widetilde{\underline{\tau}}$, where

$$
\widetilde{\underline{\tau}} = C_3^{-1} X' V_1^* \underline{y},
$$

$$
C_3 = X' V_1^* X + G^{-1} \text{ (of full rank)},
$$

and $\quad G = \begin{pmatrix} \sigma_s^2 G_s & 0 \\ 0 & \sigma_n^2 G_n \end{pmatrix}.$

The inverse of C_3 can be given as

$$
C_3^{-1} = G - GX' V_3^* XG,
$$

and $\quad \mathrm{var}(\widetilde{\underline{\tau}} - \underline{\tau}) = \mathrm{mse}(\widetilde{\underline{\tau}}) = C_3^{-1}.$

Cullis *et al.* (1989) state that *"for most EGVTs the test lines are either genetically independent or there is insufficient knowledge of the pedigrees."* Also, Cullis *et al.* (1998) assume that the random control variety effects have the same distribution as the random test treatment effects. Therefore $G_n = I_t$ and $G_s = I_c$ are assumed henceforth, unless otherwise stated. Note that $\sigma_s^2 = \sigma_n^2$ is called the *genetic variance*.

Under model 3, the dependence process given by V_3 is not stationary. Let $\rho_{g_1,g_2}^{(3,u)}$ denote $\text{corr}(y_{j_1,j_2}, y_{j_1+g_2,j_2+g_1})$ for model 3, where $u = 1$ if the plots with row and column co-ordinates (j_1, j_2) and $(j_1 + g_2, j_2 + g_1)$ both contain the same control variety, and $u = 0$ otherwise. Then for $(g_1, g_2) \neq (0,0)$,

$$\rho_{g_1,0}^{(3,u)} = \left(u\sigma_n^2 + \sigma_\gamma^2 + \sigma_\xi^2 \rho_r^{|g_1|}\right)/\sigma_{(3)}^2 ;$$

$$\rho_{0,g_2}^{(3,u)} = \left(u\sigma_n^2 + \sigma_\delta^2 + \sigma_\xi^2 \rho_c^{|g_2|}\right)/\sigma_{(3)}^2 ;$$

and $\quad \rho_{g_1,g_2}^{(3,u)} = \left(u\sigma_n^2 + \sigma_\xi^2 \rho_r^{|g_1|}\rho_c^{|g_2|}\right)/\sigma_{(3)}^2 ,$

where

$$\text{var}(y_{j_1,j_2}) = \sigma_n^2 + \sigma_{(1)}^2 = \sigma_{(3)}^2.$$

Consider an unreplicated design with $p_1 = 2$, $p_2 = 3$, $t = 2$ and $c = r = 2$ under model 3 with $\Psi = (\frac{1}{8}, \frac{3}{4}, \frac{3}{4}, \frac{1}{4})$, $(\rho_r, \rho_c) = (\frac{1}{3}, \frac{2}{3})$ and $\sigma_n^2 = \frac{1}{2}$. Here

$$\sigma_{(3)}^2 = 19/8 = 2.375,$$

and for the design

1	•	1
2	2	•

some of the correlations are

$$\text{corr}(y_{1,1}, y_{1,2}) = \rho_{1,0}^{(3,0)} = 11/95 \approx 0.116;$$

$$\text{corr}(y_{2,1}, y_{2,2}) = \rho_{1,0}^{(3,1)} = 31/95 \approx 0.326;$$

$$\text{corr}(y_{1,1}, y_{2,1}) = \text{corr}(y_{1,2}, y_{2,2}) = \rho_{0,1}^{(3,0)} = 48/95 \approx 0.505;$$

$$\text{corr}(y_{1,2}, y_{2,3}) = \rho_{1,1}^{(3,1)} = 118/475 \approx 0.248.$$

9.2.2 Efficiency criteria

The aim of EGVTs is to select good new varieties for further testing. Recall that Lin & Poushinsky (1983) proposed that the estimated yields for the new varieties be adjusted, and then the new varieties corresponding to a pre-assigned proportion of the best adjusted values be selected for further testing.

At NSW Agriculture, current practice is to model the new variety effects as random effects (Cullis *et al.*, 1998), and to fit a spatial model for the dependence using software called ASREML (Gilmour *et al.*, 1995). Then the fitted dependence structure is used to obtain predictors of the new variety effects. These new variety effects are ranked, and approximately the best one third (Cullis *et al.*, 1998) of the new varieties are selected for further evaluation.

There is no commonly agreed simple criterion for comparing designs for unreplicated trials, where the aim is to select the best new varieties for further testing. It is assumed here that only the yield will be used to determine the performance of a new variety. In practice, however, other factors, such as disease resistance and grain quality (for cereals), are also likely to be considered.

The A_{ss}-, A_{nn}-, A_{ns}- and A-values, defined in Definition 9.8 (given below) are the average variance of all pairwise comparisons among control varieties, among new varieties, between control and new varieties, and among all varieties, respectively. Recall from section 9.1.2 that these values correspond to the four ways to assess the efficiency of unreplicated designs that were proposed by Federer & Raghavarao (1975). Also, recall that Federer *et al.* (1975) suggest that A_{ns}-values be used in screening experiments.

Definition 9.8

Given that C_1^-, C_2^{-1} and C_3^{-1} are partitioned as in Definition 9.7, the following values are defined for model i:

$$A_{ss}\text{-value} = 2(c-1)^{-1}\left\{\text{tr}(C_i^{(ss)}) - c^{-1}\underline{1}_c{}'C_i^{(ss)}\underline{1}_c\right\};$$

$$A_{nn}\text{-value} = 2(t-1)^{-1}\left\{\text{tr}(C_i^{(nn)}) - t^{-1}\underline{1}_t{}'C_i^{(nn)}\underline{1}_t\right\};$$

$$A_{ns}\text{-value} = (ct)^{-1}\left\{t\,\text{tr}(C_i^{(ss)}) + c\,\text{tr}(C_i^{(nn)}) - 2\underline{1}_c{}'C_i^{(sn)}\underline{1}_t\right\};$$

$$A\text{-value} = 2(v-1)^{-1}\left\{\text{tr}\left(\begin{array}{c|c} C_i^{(ss)} & C_i^{(sn)} \\ \hline C_i^{(ns)} & C_i^{(nn)} \end{array}\right) - v^{-1}\underline{1}_v{}'\left(\begin{array}{c|c} C_i^{(ss)} & C_i^{(sn)} \\ \hline C_i^{(ns)} & C_i^{(nn)} \end{array}\right)\underline{1}_v\right\}.$$

∎

The expressions for the A_{ss}-, A_{nn}- and A-values given in Definition 9.8 follow from the expression in (2.21) in section 2.5.2, when D^- in (2.21) is replaced by

$$C_i^{(ss)}, \quad C_i^{(nn)} \quad \text{and} \quad \left(\begin{array}{c|c} C_i^{(ss)} & C_i^{(sn)} \\ \hline C_i^{(ns)} & C_i^{(nn)} \end{array}\right),$$

respectively.

Note that another way to assess the efficiency of unreplicated designs, suggested by Dourleijn (1993), is with respect to the average pairwise variance between the new varieties and the average of the control varieties.

The four values in Definition 9.8 are linearly related:

$$v(v-1)\,(A\text{-value}) = 2ct(A_{ns}\text{-value}) + t(t-1)(A_{nn}\text{-value}) + c(c-1)(A_{ss}\text{-value}).$$

This means that for c small and t large, the A- and A_{nn}-values will be highly correlated.

It is shown in chapter 10 that the A-, A_{nn}- and A_{ns}- values correlate well with the probability of selecting high yielding varieties in unreplicated trials.

9.3 Algorithms to obtain efficient EGVTs

As mentioned in chapter 1, attention is restricted in this thesis to the allocation of treatments to plots. For EGVTs, it is sufficient to consider the allocation of control varieties to the plots, with the new varieties being allocated randomly to the remaining plots.

There has been little work on the design of efficient EGVTs for spatial models, such as the model assumed by Gilmour *et al.* (1997). Eccleston & Chan (1998) demonstrated the use of a hybrid simulated annealing algorithm (due to Martin & Eccleston, 1997), and a tabu search (see section 3.3) algorithm to find A_{ns}-efficient designs on a small example of an unreplicated trial, given that the variance structure is fully specified. The Martin & Eccleston (1997) algorithm is used here in chapters 10 and 11. The outline of a general tabu search algorithm in section 3.3, describes three memory functions. However, the tabu search algorithm of Eccleston & Chan (1998) is a simpler implementation with only one memory function, which corresponds to a tabu list of designs deemed to be efficient as the search progresses.

Both the simulated annealing and tabu search algorithms take a random design as the *starting design*. In general, *neighbours* of a design are obtained by randomly interchanging two treatments (a new variety with a control variety, or a control variety with a different control variety). A series of treatment interchanges from the starting design leads to the *final design* at the completion of one *run* of the algorithm. Assuming that the algorithms are allowed to consider a fixed number of designs, they can be set up so that, either

> many designs are considered in one run (or a few runs)

or   few designs are considered in each run, but many runs are carried out. Experimentation with the algorithms suggests that the latter approach, with multiple runs, is more likely to yield better designs.

Building from a very small expository example of an unreplicated design in Martin & Eccleston (1997), Eccleston & Chan (1998) considered unreplicated designs for a 10×5 array with $c = 2$, $r = 5$ and $t = 40$, under model 1 with $\Psi = (0, 0, 1, 0)$ and $(\rho_r, \rho_c) = (\frac{1}{3}, \frac{2}{3})$. Using the simulated annealing and tabu search algorithms, the best design given for this example, by Eccleston & Chan (1998), with respect to the A_{ns}-value (not, as stated, the A-value), is

•	•	•	•	•
•	1	•	•	•
•	•	2	•	2
2	•	•	1	•
•	•	•	•	•
•	•	•	•	•
•	2	•	•	1
1	•	•	2	•
•	•	1	•	•
•	•	•	•	2

Its A_{ns}-value is 0.8497, although a slightly better design, with A_{ns}-value = 0.8495 is given as case 4 in Appendix A3.5. Eccleston & Chan (1998) also considered the following design, which has the check plots systematically arranged in two diagonals, with the number of self-diagonal adjacencies maximised.

1	•	•	•	•
•	1	•	•	•
•	•	1	•	•
•	•	•	1	•
•	•	•	•	1
2	•	•	•	•
•	2	•	•	•
•	•	2	•	•
•	•	•	2	•
•	•	•	•	2

This design has A_{ns}-value = 0.9231. The A_{ns}-efficiency for this design (with respect to the A_{ns}-value for the best design found) is 0.920. The design with the same check plots as in the previous design but with no self diagonal adjacencies (i.e. with the control varieties alternating in the diagonals) was found to have a better A_{ns}-value = 0.8714, which has A_{ns}-efficiency of 0.975.

9.3.1 Speeding up the search algorithms

For each design considered in an algorithmic search (such as by using the simulated annealing and tabu search algorithms described in Eccleston & Chan, 1998), the A-value, under model 1, can be calculated by obtaining a generalised inverse of C_1 (or the inverse of C_{1a}). For model i ($i = 2,3$), the A-value can be determined by calculating the inverse of C_i under model $i = 2,3$. This can be very time consuming since C_i ($i = 1,2,3$), a $v \times v$ matrix, is usually very large for EGVTs. Hence, the search for good designs can be very slow. Methods to speed up this search process are now given.

First consider model 1. The gls estimate of $\underline{\tau}$, given in section 9.2, involves a generalised inverse of C_1 or equivalently the inverse of C_{1a}. For simplicity $\hat{\underline{\tau}} = C_{1a}^{-1} X' V_1^{-1} \underline{y}$ is considered here. The elements of $\underline{y}$ are re-ordered such that

$$P\underline{y} = (\underline{y}_s{}', \underline{y}_n{}')' = \underline{y}_{(1)},$$

where P is a $m \times m$ permutation matrix, and $\underline{y}_s$ and $\underline{y}_n$ are vectors of responses for the plots with control and new varieties, respectively. The treatment design matrix is also re-arranged corresponding to the ordering in $\underline{y}_{(1)}$. This gives

$$PX = X_{(1)} = \begin{pmatrix} X_{ss} & 0 \\ 0 & X_{nn} \end{pmatrix},$$

where X_{ss} and X_{nn} are the control variety and new variety design matrices corresponding to $\underline{y}_s$ and $\underline{y}_n$, respectively. It is assumed that $X_{nn} = I_t$ without loss of generality, since the ordering of the new varieties in the plots does not affect the estimation or variance of contrasts. Also, $var(\underline{y}) = V_1$ is re-arranged as

$$\mathrm{var}(\underline{y}_{(1)}) = PV_1P' = V_{(1)} = \left(\begin{array}{c|c} V_{ss} & V_{sn} \\ \hline V_{ns} & V_{nn} \end{array}\right),$$

and $\quad V_{(1)}^{-1} = \left(\begin{array}{c|c} V^{(ss)} & V^{(sn)} \\ \hline V^{(ns)} & V^{(nn)} \end{array}\right).$

Then

$$C_{1a} = X_{(1)}'V_{(1)}^{-1}X_{(1)} \quad \text{and} \quad \hat{\tau} = C_{1a}^{-1}X_{(1)}'V_{(1)}^{-1}\underline{y}_{(1)}.$$

Let C_{1a}^{-1} be partitioned as in Definition 9.7, i.e.

$$C_{1a}^{-1} = \left(\begin{array}{c|c} C_{1a}^{(ss)} & C_{1a}^{(sn)} \\ \hline C_{1a}^{(ns)} & C_{1a}^{(nn)} \end{array}\right).$$

By applying the formula (A1.23) in Appendix A1.5 for the inverse of a partitioned matrix to

$$C_{1a} = \left(\begin{array}{c|c} X_{ss}'V^{(ss)}X_{ss} & X_{ss}'V^{(sn)}X_{nn} \\ \hline X_{nn}'V^{(ns)}X_{ss} & X_{nn}'V^{(nn)}X_{nn} \end{array}\right) = \left(\begin{array}{c|c} X_{ss}'V^{(ss)}X_{ss} & X_{ss}'V^{(sn)} \\ \hline V^{(ns)}X_{ss} & V^{(nn)} \end{array}\right),$$

it follows that

$$C_{1a}^{(ss)} = M^{-1},$$

$$C_{1a}^{(sn)} = -M^{-1}X_{ss}'V^{(sn)}(V^{(nn)})^{-1},$$

and $\quad C_{1a}^{(nn)} = (V^{(nn)})^{-1} + (V^{(nn)})^{-1}V^{(sn)}X_{ss}M^{-1}X_{ss}'V^{(sn)}(V^{(nn)})^{-1},$

where

$$M = X_{ss}'\left\{V^{(ss)} - V^{(sn)}(V^{(nn)})^{-1}V^{(ns)}\right\}X_{ss}.$$

By applying the formula (A1.23) from Appendix A1.5 to $V_{(1)}^{-1}$ it follows that

$$V_{ss} = \left\{V^{(ss)} - V^{(sn)}(V^{(nn)})^{-1}V^{(ns)}\right\}^{-1}, \tag{9.9}$$

$$V_{sn} = -V_{ss}V^{(sn)}(V^{(nn)})^{-1}, \tag{9.10}$$

$$V_{nn} = (V^{(nn)})^{-1} + (V^{(nn)})^{-1}V^{(ns)}V_{ss}V^{(sn)}(V^{(nn)})^{-1}.$$

By the equation in (9.10):

$$V_{nn} = (V^{(nn)})^{-1} + V_{ns}V_{ss}^{-1}V_{sn}. \tag{9.11}$$

Hence,

$$C_{1a}^{(ss)} = M^{-1} = \left(X_{ss}'V_{ss}^{-1}X_{ss}\right)^{-1} \quad \text{(by (9.9))};$$

$$C_{1a}^{(sn)} = M^{-1}X_{ss}'V_{ss}^{-1}V_{sn} \quad \text{(by (9.10))};$$

$$C_{1a}^{(nn)} = V_{nn} - V_{ns}V_{ss}^{-1}V_{sn} + V_{ns}V_{ss}^{-1}X_{ss}M^{-1}X_{ss}'V_{ss}^{-1}V_{sn}$$

$$\text{(by (9.10) and (9.11))}.$$

This means that for each design considered in an algorithmic search, C_{1a}^{-1} can be obtained by inverting the usually much smaller matrices V_{ss} and M, which are of size $(m-t) \times (m-t)$ and $c \times c$, respectively. This derivation is related to Method (a) in Federer & Raghavarao (1975).

Although the gls estimates of $\underline{\tau}_s$ and $\underline{\tau}_n$ are not needed for the search algorithms, they can be obtained by using V_{ss}^{-1} and M^{-1}:

$$\hat{\underline{\tau}}_s = M^{-1}X_{ss}'V_{ss}^{-1}\underline{y}_s$$

and $\quad \hat{\underline{\tau}}_n = X_{nn}'\left\{\underline{y}_n - V_{ns}V_{ss}^{-1}\left(\underline{y}_s - X_{ss}\hat{\underline{\tau}}_s\right)\right\}.$

For the simulations in chapter 10 under model 1, the gls estimates of $\underline{\tau}_s$ and $\underline{\tau}_n$ were obtained using these expressions.

For model 2, V_2 depends on the allocation of control and new varieties to the plots (i.e. on X_n). This means that a search algorithm, which inverts the matrix V_2 for each design considered, is likely to be slow for m large. A method to speed up the search algorithm, similar to that given in the Appendix of Cullis $et\ al.$ (1998) is now described for $G_n = I_t$.

Let U be the $m \times (m - t)$ check-plot incidence matrix, such that $(U)_{l_1, l_2} = 1$ if plot l_1 is the l_2^{th} check plot, and $(U)_{l_1, l_2} = 0$ otherwise. The matrices UU' and $X_n X_n'$ are related:

$$X_n X_n' = I_m - UU'.$$

Note that

$$U = P \begin{pmatrix} I_{m-t} \\ 0 \end{pmatrix} \quad \text{and} \quad X_n = P \begin{pmatrix} 0 \\ I_t \end{pmatrix},$$

for a $m \times m$ permutation matrix P.

To illustrate this, consider again the design

$$\begin{array}{|c|c|c|} \hline 1 & \bullet & 1 \\ \hline 2 & 2 & \bullet \\ \hline \end{array}$$

which has $p_1 = 2$, $p_2 = 3$, $t = 2$ and $c = r = 2$. It has

$$U = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad \text{and} \quad X_n = \begin{pmatrix} 0 & 0 \\ 1 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 1 \end{pmatrix},$$

so that UU' and $X_n X_n'$ are diagonal matrices with diagonals $(1,0,1,1,1,0)$ and $(0,1,0,0,0,1)$, respectively.

Also, let

$$V_I = V_1 + \sigma_n^2 I_m.$$

Then V_2 can be written as

$$V_2 = V_I + \sigma_n^2 (X_n X_n' - I_m) = V_I - \sigma_n^2 UU'.$$

Applying formula (A1.24) from Appendix A1.5 to V_2 gives

$$V_2^{-1} = V_I^{-1} + V_I^{-1} U S_1^{-1} U' V_I^{-1},$$

where $S_1 = \sigma_n^{-2} I_{m-t} - U' V_I^{-1} U$.

Given that the $m \times m$ matrix V_I, which is invariant to the allocation of varieties to the plots, is inverted once at the start of the algorithm, substantial time savings are likely when m is large, since for each design considered, V_2^{-1} can be obtained by inverting S_1 a $(m-t) \times (m-t)$ matrix.

For model 3, V_3^{-1} with $G_s = I_c$ and $G_n = I_t$, can be expressed (similarly to model 2) as

$$V_3^{-1} = V_2^{-1} - V_2^{-1} X_s S_2^{-1} X_s ' V_2^{-1},$$

where V_2^{-1} is as for model 2, and $S_2 = \sigma_s^{-2} I_c - X_s ' V_2^{-1} X_s$. Therefore, V_3^{-1} can be obtained by inverting S_1 and the $c \times c$ matrix S_2 for each design considered by the search algorithm, given that V_I^{-1} is derived at the start of the algorithm.

10 Simple criteria to compare EGVT designs

10.1 Introduction

In this chapter some simple criteria are considered for their appropriateness to compare different designs (i.e. different allocations of control varieties to the plots) for an EGVT, when the aim is to select the highest yielding new varieties for further testing.

Definition 10.1
- Let $\pi_{q_1,z}$ denote the probability that the z new varieties with the largest estimated (or predicted) new variety effects include the q_1 ($q_1 \leq z < t$) best new varieties.
- Let $\omega_{q_2,z}$ denote the probability that the z new varieties with the largest estimated (or predicted) new variety effects include at least one of the q_2 ($q_2 \leq z < t$) best new varieties. ■

Andrews & Curnow (1996) compared the efficacy of selecting a fixed number of new varieties in a replicated agricultural variety selection programme, where the aim was to maximise the expected mean yield of the selected varieties, to the efficacy of selecting sufficient varieties to achieve some minimum or expected probability that a specified number of best varieties are among those selected. They carried out simulations in which estimates of $\pi_{q_1,z}$ and $\omega_{q_2,z}$ were obtained. As well as comparing test varieties amongst themselves, they also considered the situation where control varieties were compared with test varieties.

Unfortunately, estimates of $\pi_{q_1,z}$ and $\omega_{q_2,z}$ can only usually be obtained from simulations. Instead, it would be useful to consider measurements associated with $\pi_{q_1,z}$ and $\omega_{q_2,z}$ that are readily available.

When $\underline{\tau}_n$ is assumed to be a vector of random effects, as in models 2 and 3, a simple criterion is to maximise the average squared correlation between $\tau_{n,l}$ and $\widetilde{\tau}_{n,l}$ over $l = 1,2,...,t$, where $\tau_{n,l}$ is the effect of the lth new variety and $\widetilde{\tau}_{n,l}$ is its predictor. If this average squared correlation is high (i.e. near 1) then it is likely that this measurement would be a well associated with $\pi_{q_1,z}$ and/or $\omega_{q_2,z}$.

Two papers which consider the correlation between the true and predicted variety effects are Yeo & David (1984) and Cullis *et al.* (1992). Yeo & David (1984) considered the general problem of choosing the best q objects out of t objects, "*when instead of measurements y_i ($i = 1,...,t$) of primary interest, only associated measurements x_i are readily available.*" They gave a table of $\pi_{q,z}$, under the assumption that the t pairs (x_i, y_i) are a random sample from a bivariate normal distribution. These values of $\pi_{q,z}$ depend on the correlation between the two variables, which is assumed to be equal for all pairs of variables. As an example of an application, they considered a variety trial, where variety effects were modelled as uncorrelated normal variates with zero mean, and $\pi_{q,z}$ depends on the correlation between the true and estimated variety effects, which is assumed to be equal for all varieties. Note that for EGVTs under models 2 and 3, the correlation between the lth true and predicted new variety effects (see equation (10.2) below) is not necessarily the same for all l.

Cullis *et al.* (1992) carried out a simulation study to compare five methods of analysis (including the spatial analysis of Cullis *et al.*, 1989) of EGVTs, using a measurement which they called the *relative response to selection* (RSS). The RSS is a function of the correlation coefficient of the true (simulated) and estimated (or predicted) new variety effects. Methods of analysis with a high RSS were favoured over methods with a low RSS.

For model i ($i = 2,3$), the squared correlation between the lth true and predicted new variety effects is

$$\text{corr}^2(\tau_{n,l}, \tilde{\tau}_{n,l}) = \frac{\text{cov}^2(\tau_{n,l}, \tilde{\tau}_{n,l})}{\{\text{var}(\tau_{n,l})\,\text{var}(\tilde{\tau}_{n,l})\}}$$

$$= \frac{\text{var}(\tilde{\tau}_{n,l})}{\text{var}(\tau_{n,l})}, \tag{10.1}$$

since $\text{cov}(\tau_{n,l}, \tilde{\tau}_{n,l}) = \text{var}(\tilde{\tau}_{n,l})$ (by (A3.13) and (A3.14) in Appendix A3.3). Assuming, as in section 9.2.1, that $G_n = I_t$, gives

$$\text{corr}^2(\tau_{n,l}, \tilde{\tau}_{n,l}) = 1 - \sigma_n^{-2}\left(C_i^{(nn)}\right)_{ll}. \tag{10.2}$$

Now consider maximising the average squared correlation, i.e. maximising

$$t^{-1}\sum_{l=1}^{t}\text{corr}^2(\tau_{n,l}, \tilde{\tau}_{n,l}) = 1 - \sigma_n^{-2}\text{tr}\left(C_i^{(nn)}\right).$$

This is equivalent to minimising $\text{tr}\left(C_i^{(nn)}\right)$. Recall that the A_{nn}-value is a function of $\text{tr}\left(C_i^{(nn)}\right)$:

$$A_{nn}\text{-value} = 2(t-1)^{-1}\left\{\text{tr}(C_i^{(nn)}) - t^{-1}\mathbf{1}_t{'}C_i^{(nn)}\mathbf{1}_t\right\}.$$

Unreplicated designs considered in the simulation studies described in section 10.3, suggest that when t is large, $\text{tr}\left(C_i^{(nn)}\right)$ is approximately equal to $\frac{1}{2}(t-1)$ times the A_{nn}-value. Therefore, for t large, the criterion of maximising the average squared correlation between $\tau_{n,l}$ and $\tilde{\tau}_{n,l}$ seems to be approximately the same as minimising the A_{nn}-value. Also, recall that for c small and t large, the A- and A_{nn}-values will be highly correlated.

For model 1, $\underline{\tau}_n$ is fixed, so $\text{corr}(\tau_{n,l}, \tilde{\tau}_{n,l})$ cannot be used. However, it may still be useful to consider $\text{tr}\left(C_1^{(nn)}\right)$ as a potential associated measurement of $\pi_{q_1,z}$ and/or $\omega_{q_2,z}$.

As well as considering $\text{tr}\left(C_i^{(nn)}\right)$ and the A- and A_{nn}-values as potential associated measurements, it may also be useful to consider the A_{ns}- and A_{ss}-values since they are suggested by Federer & Raghavarao (1975) (see section 9.1.2); although the A_{ss}-value is not expected to be useful. Simulation studies to investigate if any of these 5 measurements are well associated with $\pi_{q_1,z}$ and/or $\omega_{q_2,z}$, are described in this chapter. The methodology of the simulation studies is given in section 10.2, and the results are summarised in section 10.3. A discussion of the conclusions from the simulation studies is given in section 10.4.

10.2 Simulation methodology

Simulated yields from the model in (9.2) can be used to estimate $\pi_{q_1,z}$ and $\omega_{q_2,z}$. These estimates can then be compared to the potential associated measurements. The simulations that were carried out here used MATLAB version 4.2c.1 to generate the yields.

The elements of the vector of random errors $\underline{\eta}$, which has $E(\underline{\eta}) = \underline{0}_m$ and $\text{var}(\underline{\eta}) = \sigma_\eta^2 I_m$, were generated as independent $N(0, \sigma_\eta^2)$ values using the MATLAB function $\texttt{randn}$, which gives pseudo-independent $N(0,1)$ values.

The additional spatial components (or trend effects) are assumed to be from an AR(1)*AR1(1) process, and are generated by the procedure described in Appendix A3.4. In the simulation study in Cullis *et al.* (1989), the trend within each row was assumed to be from an ARIMA(0,1,0) process, and the elements of the vector of first-differenced trend effects were generated as independent normal, zero mean, values. In Cullis *et al.* (1992), twenty sets of *uniformity data* were considered. Uniformity data are data from trials where a single variety is grown on all plots (i.e. essentially a design with just 1

treatment). Cullis *et al.* (1992) assumed model 2 with $\sigma_\gamma^2 = \sigma_\delta^2 = 0$, and from each set of uniformity data, the value of the trend effect for each plot in the simulation was obtained. The value of σ_η^2 (the variance of the random errors) was also obtained from the uniformity data, and then used to generate the simulated data.

Now consider the generation of the control and new variety effects. Andrews & Curnow (1996) simulated yields from trials with $c = 1$ control variety, and took the control effect to be zero and the variety effects to be independent $N(0,1)$ values. Cullis *et al.* (1989, 1992) generated the new variety effects as independent $N(0, \sigma_n^2)$ values. Cullis *et al.* (1989) noted that plant breeders in the NSW Department of Agriculture suggest that *"genetic variance should be larger than the error variance, although in some trials the genetic variance may be as small as ⅓ of the error variance."* To take account of this, the genetic variance (σ_n^2) values of 0.2, 1 and 5 were considered in Cullis *et al.* (1989), with error variance, σ_η^2, taken as 1. Note that Cullis *et al.* (1989) took the variance of the differenced trend effect to be 0.01, 0.1 and 1, and Cullis *et al.* (1992) took $\sigma_n^2 / \sigma_\eta^2 = 0.5, 1, 5$. Both papers assumed $c = 1$, as in Andrews & Curnow (1996). However, the control variety effect was generated differently: as 80% of the average of the new variety effects.

When $\underline{\tau}_s$ and/or $\underline{\tau}_n$ are fixed effects, they could have particular values assigned to them. However, for the simulation studies in this chapter, in order to represent typical observed effects, the elements of $\underline{\tau}_s$ and/or $\underline{\tau}_n$ have been generated from an independent $N(0, \sigma_n^2)$ distribution. Without loss of generality, it is assumed that $\sigma_\xi^2 + \sigma_\eta^2 = 1$. To reflect what is likely in practice,

as recommended by Dr. B. Cullis of NSW Agriculture (personal correspondence, 1998), $\sigma_n^2/(\sigma_\zeta^2 + \sigma_\eta^2) = \sigma_n^2$ is taken to be between 0.1 and 1. Also, in some of the simulations in section 10.3.3, σ_n^2 is taken as 5.

For each simulated trial, the vectors $\underline{\tau}_n$, $\underline{\tau}_s$, $\underline{\eta}$ and $\underline{\zeta}$ were generated independently of each other as described above, giving a simulated vector of yields $\underline{y}$ ($\mu = 0$ assumed) from a normal distribution with mean and variance depending on which of the models, 1, 2 or 3, is assumed, and also, for models 2 and 3, on the design (i.e. an allocation of control varieties) used.

For a given design, the potential associated measurements can be calculated. Then by simulating a large number, N, of trials, estimates of $\pi_{q_1,z}$ and $\omega_{q_2,z}$, denoted by $\hat{\pi}_{q_1,z}$ and $\hat{\omega}_{q_2,z}$, respectively, can be obtained for this design. From the simulated yields for a particular trial, $\hat{\underline{\tau}}_n$ (or $\tilde{\underline{\tau}}_n$) can be calculated under the assumption that var($\underline{y}$) is known. In practice, for data from a completed trial, estimation will usually use a fitted variance structure. However, the possible differences arising from this are not considered in this thesis. The z greatest estimated (or predicted) new variety effects are then assumed to be selected. Over N trials, $\hat{\pi}_{q_1,z}$ and $\hat{\omega}_{q_2,z}$ are calculated as the proportion of the N simulated trials in which the z selected new varieties include

i)   the q_1 best varieties

ii) at least one of the q_2 best varieties,

respectively.

By obtaining $\hat{\pi}_{q_1,z}$ and $\hat{\omega}_{q_2,z}$ over a set of designs which cover a wide range of the potential associated measurements, $\hat{\pi}_{q_1,z}$ and $\hat{\omega}_{q_2,z}$ can then be compared with the potential associated measurements to see if any of these measurements are well associated with $\pi_{q_1,z}$ and $\omega_{q_2,z}$. For the simulation studies in section 10.3 (except in section 10.3.1), in order to have designs with a wide range of values for the potential associated measurements, the set of designs considered comprise the three subsets of designs, $\mathcal{B}$, $\mathcal{G}$ and $\mathcal{R}$, as described in Definition 10.2.

Definition 10.2
- Let $\mathcal{R}$ be a set of designs for which control varieties are allocated randomly.
- Let $\mathcal{B}$ be a set of designs selected to have high values of the potential associated measurements.
- Let $\mathcal{G}$ be a set of designs selected to have low values of the potential associated measurements.
∎

Designs in the subsets $\mathcal{B}$ and $\mathcal{G}$ are obtained using the simulated annealing algorithm of Martin & Eccleston (1997). For the purpose of finding a design with a high (or low) value of a potential associated measurement, one run of the algorithm is executed (see section 9.3), and since designs with a good spread of both high and low values of the potential associated measurements are required, the algorithm is set up so that fewer designs are considered in one run than would be considered if the design with the best/optimal measurement was required.

10.3 Simulation results

The results of several simulation studies are presented in this section. Most of the simulation studies described here assume model 1. As an initial preliminary study, a very small array, for which all the different designs can be easily enumerated, is considered in section 10.3.1. Further preliminary studies, for a larger array, are outlined in section 10.3.2. In sections 10.3.3 and 10.3.4, two larger studies are considered over several different variance structures and genetic variance settings.

10.3.1 Preliminary study – on a 4×4 array with $c = 2$

A preliminary simulation study, under model 1, on a 4×4 array with $c = r = 2$ (and $t = 12$) is considered in this section. Although EGVTs are unlikely to be this small, for a small example like this, the simulation can be conducted over all the possible *different* designs. Two designs are deemed to be different if they have different C_1 matrices. The variance components are set at

$\sigma_\gamma^2 = \sigma_\delta^2 = \sigma_\eta^2 = 0$ and $\sigma_\zeta^2 = 1$ (i.e. $\Psi = \Psi_1 = (0, 0, 1, 0)$, called the *purely spatial model*). The parameters of Λ are set at $(\rho_r, \rho_c) = (\frac{1}{2}, \frac{1}{2})$, which may be reasonable in practice when plots are square or nearly square. This example was also considered by Martin & Eccleston (1997) to illustrate their algorithm.

A complete enumeration of the designs gives 736 different designs. It is clear that the number of ways of allocating the two replications of the two control varieties is

$$\frac{1}{2}\binom{16}{2}\binom{14}{2} = 5460.$$

This is reduced to 736 different designs, since reversals, horizontal and vertical reflections, NW-SE and NE-SW diagonal reflections of a design give designs with the same C_1 matrix.

The control and new variety effects are simulated with genetic variance $\sigma_n^2 = 1$. The number of simulated trials for each design is $N = 10,000$. From these 10,000 trials, $\hat{\pi}_{1,3} = \hat{\omega}_{1,3}$ is obtained. Here, $z = 3$ is taken as 25% of t, and $q_1 = q_2 = 1$ is $8\frac{1}{3}$% of t. Over the 736 designs, $\hat{\pi}_{1,3}$ lies between 0.943 and 0.959, with median value 0.952. For other q_1 and z, a wider range of $\hat{\pi}_{q_1,z}$ may result (for $q_1 = 2$ and $z = 4$, say). For a lower genetic variance than taken here, it is likely that a lower median of $\hat{\pi}_{1,3}$ would result, since new variety effects and their estimates would be less spread out, hence making accurate selection less likely. Also, for a higher genetic variance, it is expected that accurate selection of high yielding varieties would be more likely (see Table 10.4 in section 10.3.3, and Table 10.8 in section 10.3.4).

Plots of $\hat{\pi}_{1,3}$ against the A-, A_{nn}-, A_{ns}-, A_{ss}- and $tr(C_1^{(nn)})$- values are given in Figure 10.1a to Figure 10.1e. The Spearman rank correlation coefficient (a measure of a monotonic relationship) between each of the potential associated measurements and $\hat{\pi}_{1,3}$, is given in parentheses for each of Figure 10.1a to Figure 10.1e. From Figure 10.1, for the example being considered here, the A-, A_{nn}- and $tr(C_1^{(nn)})$- values are likely to be reasonably well associated with $\pi_{1,3}$, with $\hat{\pi}_{1,3}$ high for low A-, A_{nn}- and $tr(C_1^{(nn)})$- values, and low $\hat{\pi}_{1,3}$ for high measurements. However, there is no clear relationship between $\hat{\pi}_{1,3}$ and the A_{ns}- and A_{ss}- values, especially between $\hat{\pi}_{1,3}$ and the A_{ss}- values. The Spearman rank correlation coefficients in Figure 10.1 suggest that the A_{nn}- value is the best associated measurement (from the five measurements considered) of $\pi_{1,3}$ for this example.

Figure 10.1

Plots of $\hat{\pi}_{1,3}$ against the A-, A_{nn}-, A_{ns}-, A_{ss}-, $\text{tr}\left(C_1^{(nn)}\right)$- values, for the simulation study in section 10.3.1 with Spearman rank correlation coefficients in parentheses.

a) $\hat{\pi}_{1,3}$ against A-value (-0.40)

b) $\hat{\pi}_{1,3}$ against A_{nn}-value (-0.48)

c) $\hat{\pi}_{1,3}$ against A_{ns}-value (-0.19)

d) $\hat{\pi}_{1,3}$ against A_{ss}-value (0.02)

e) $\hat{\pi}_{1,3}$ against $\text{tr}\left(C_1^{(nn)}\right)$-value (-0.34)
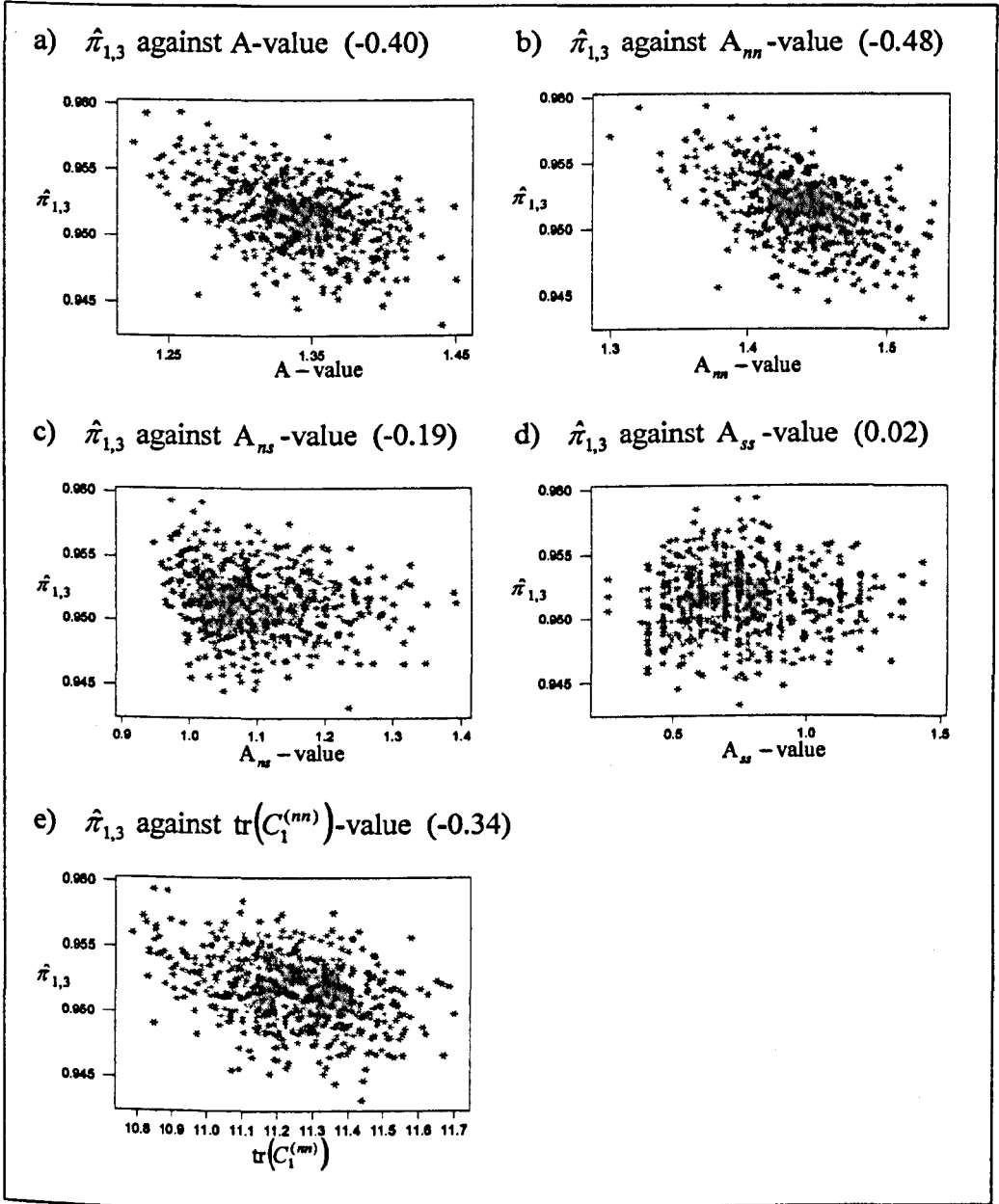
10.3.2 Preliminary studies – on a 10×10 array with $c = 2$

Simulation studies under models 1 and 2 were conducted on a more realistically sized 10×10 array, with $c = 2$, $r = 10$, and Ψ, (ρ_r, ρ_e) and σ_n^2 as in the 4×4 example described above. For the simulation study under model 1, 500 designs were considered, comprising 16 designs with high A-, A_{nn}-, A_{ns}- and A_{ss}- values (4 designs with respect to each of these 4 measurements), 16 designs with low A-, A_{nn}-, A_{ns}- and A_{ss}- values, and 468 randomly selected designs. The simulation study under model 2 had 200 randomly selected designs, as well as 24 designs with high A-, A_{nn}-, A_{ns}- and A_{ss}- values (6 designs with respect to each of these 4 measurements), and 24 designs with low A-, A_{nn}-, A_{ns}- and A_{ss}- values.

For both simulation studies $N = 5,000$ trials were simulated for each design, from which $\hat{\pi}_{2,10}$ and $\hat{\omega}_{2,10}$ were estimated. The minimum, median and maximum values of $\hat{\pi}_{2,10}$ and $\hat{\omega}_{2,10}$, which are very similar for both studies, are given in Table 10.1. The $\hat{\omega}_{2,10}$ are very close to 1. This may mean that any relationship between $\hat{\omega}_{2,10}$ and potential associated measurements may be difficult to discern.

Table 10.1
Minimum, median and maximum of $\hat{\pi}_{2,10}$ and $\hat{\omega}_{2,10}$ over 500 designs for the model 1 study, and over 248 designs for the model 2 study in section 10.3.2. (to 3 decimal places, except when value is exact)

	$\hat{\pi}_{2,10}$			$\hat{\omega}_{2,10}$		
	min.	median	max.	min.	median	max.
Model 1	0.981	0.988	0.993	0.997	0.999	1
Model 2	0.984	0.991	0.995	0.998	0.999	1

For both studies, the Spearman rank correlation coefficients (given in Table 10.2) between $\hat{\pi}_{2,10}$ and the A-, A_{nn}-, A_{ns}- and $\text{tr}\left(C_i^{(nn)}\right)$- values ($i = 1,2$) are very similar (close to -0.35), even though both studies have a different number of designs. For each study, the correlation coefficients between $\hat{\pi}_{2,10}$ and the A-, A_{nn}-, A_{ns}- and $\text{tr}\left(C_i^{(nn)}\right)$- values are very similar since the A-, A_{nn}-, and $\text{tr}\left(C_i^{(nn)}\right)$- values are highly inter-correlated, with Spearman rank correlation coefficients greater than 0.998 and 0.999, for the model 1 and model 2 studies, respectively. The correlation coefficients between the A-/A_{nn}-/$\text{tr}\left(C_i^{(nn)}\right)$- values and the A_{ns}-values are also high (greater than 0.95 and 0.94, for the model 1 and model 2 studies, respectively). The Spearman rank correlation coefficient between $\hat{\pi}_{2,10}$ and the A_{ss}-value is near zero for both studies.

Table 10.2
Spearman rank correlation coefficients between $\hat{\pi}_{2,10}$ and the A-, A_{nn}-, $\text{tr}\left(C_i^{(nn)}\right)$-, A_{ns}- and A_{ss}- values ($i = 1,2$) for the simulation study in section 10.3.2 (to 2 decimal places).

	A-	A_{nn}-	$\text{tr}\left(C_i^{(nn)}\right)$-	A_{ns}-	A_{ss}-
Model 1	-0.35	-0.35	-0.35	-0.35	0.07
Model 2	-0.35	-0.35	-0.35	-0.34	0.00

Now consider $\hat{\omega}_{2,10}$ for the two studies. Table 10.3 gives the Spearman rank correlation coefficients between $\hat{\omega}_{2,10}$ and the A-, A_{nn}-, $\text{tr}\left(C_i^{(nn)}\right)$ and A_{ns}- values. The association seems to be weaker than for $\hat{\pi}_{2,10}$, which may be due to the $\hat{\omega}_{2,10}$ being close to 1. Also, note that the correlation coefficients (except for the A_{ss}-value) are slightly higher for model 2 than for model 1. As for $\hat{\pi}_{2,10}$, the correlation coefficient between $\hat{\omega}_{2,10}$ and the A_{ss}-value is near zero for both studies (see Table 10.3).

Table 10.3
Spearman rank correlation coefficients between $\hat{\omega}_{2,10}$ and the A-, A_{nn}-, $\mathrm{tr}\!\left(C_i^{(nn)}\right)$-, A_{ns}- and A_{ss}- values ($i = 1,2$) for the simulation study in section 10.3.2 (to 2 decimal places).

	A-	A_{nn}-	$\mathrm{tr}\!\left(C_i^{(nn)}\right)$-	A_{ns}-	A_{ss}-
Model 1	-0.22	-0.22	-0.22	-0.23	0.01
Model 2	-0.18	-0.18	-0.18	-0.20	0.00

The studies described in this section provide more evidence to suggest that the A_{ss}-value is not well associated with $\pi_{q_1,z}$ or $\omega_{q_2,z}$. Also, there seems to be little difference over models 1 and 2, in the association between the potential associated measurements and $\pi_{q_1,z}$ or $\omega_{q_2,z}$.

Under model 3, a simulation study, with the same settings as in the studies for models 1 and 2 described above, was also carried out. This study gave Spearman rank correlation coefficients that were very close to the correlation coefficients for model 2.

10.3.3 Simulation study – on a 20×8 array with $c = 2$

The simulation study described in this section uses a 20×8 array, with $c = 2$, $r = 10$ ($t = 140$), under model 1. Approximately 14% of the plots are check plots, which satisfies the recommendation of Kempton (1984) (see section 9.1.2). One hundred and fifty designs were considered. To ensure a wide

range of values, these designs comprised 15 designs with high A-, A_{nn}- and A_{ns}- values (5 designs with respect to each of these 3 measurements), 15 designs with low A-, A_{nn}- and A_{ns}- values, and 120 randomly selected designs. Designs with high (low) A_{nn}-values are likely to have high (low) $\text{tr}\left(C_1^{(nn)}\right)$- values, since the A_{nn}- and $\text{tr}\left(C_1^{(nn)}\right)$- values are likely to be highly correlated. The A_{ss}-criterion is not considered here, since the preliminary studies (in sections 10.3.1 and 10.3.2) suggest that it is of little use as an associated criterion to maximising $\pi_{q_1,z}$ or $\omega_{q_2,z}$.

The variance components were set at $\Psi_1 = (0, 0, 1, 0)$ and $\Psi_2 = (\frac{1}{4}, \frac{5}{8}, \frac{5}{8}, \frac{3}{8}) = (\frac{1}{4}, \frac{3}{4}, \frac{3}{4}, \frac{1}{4})$, where $\sigma_\xi^2 + \sigma_\eta^2 = 1$, as recommended by Dr. B. Cullis (personal correspondence, 1998) (see section 10.2). Recall that Ψ_1 is the purely spatial model. The settings in Ψ_2 have $\sigma_\delta^2 > \sigma_\gamma^2$ to reflect the situation with long narrow plots. The correlation parameters, (ρ_r, ρ_c), were set at $(\frac{1}{2}, \frac{1}{2})$, $(\frac{1}{2}, \frac{1}{3})$ and $(\frac{1}{10}, \frac{9}{10})$, which may be reasonable for square or nearly square plots, long thin plots and very long thin plots, respectively. The genetic variance, σ_n^2, is taken as $\frac{1}{5}$, 1 and 5. Simulations were conducted over all 18 combinations of Ψ, (ρ_r, ρ_c) and σ_n^2, with $N = 5,000$ trials being simulated for each of the 150 designs. Note that the 30 non-random designs were selected separately, as described in section 10.2, for each of the 6 variance structures (i.e. for the 6 combinations of Ψ and (ρ_r, ρ_c)).

For each trial, $z = 35 = \frac{1}{4}t$ of the new varieties were assumed to be selected, and estimates of $\pi_{7,35}$, $\pi_{1,35}$ and $\omega_{7,35}$ were derived from the simulations. Cullis *et al.* (1998) say that about $\frac{1}{3}$ of the new varieties go on for further testing, in which case $z = 47$ may be a more appropriate setting for z. The possible differences arising from this are not considered in this section. However, the study in section 10.3.4 takes z to be about $\frac{1}{3}$ of t. For the 18 combinations of Ψ, (ρ_r, ρ_c) and σ_n^2, the minimum, median and maximum values of $\hat{\pi}_{7,35}$ over the 150 designs are given in Table 10.4. As expected, $\hat{\pi}_{7,35}$ decreases as σ_n^2 decreases, with $\hat{\pi}_{7,35}$ very low for $\sigma_n^2 = \frac{1}{3}$. Also, the median of $\hat{\pi}_{7,35}$ is lower for Ψ_2 than for Ψ_1.

Table 10.4
Minimum, median and maximum of $\hat{\pi}_{7,35}$ over 150 designs for the simulation study in section 10.3.3 (to 3 decimal places for $\sigma_n^2 = \frac{1}{3}$, 5; to 2 decimal places, otherwise).

σ_n^2	(ρ_r, ρ_c)	Ψ_1			Ψ_2		
		min.	median	max.	min.	median	max.
5	$(\frac{1}{2}, \frac{1}{2})$	0.942	0.962	0.976	0.779	0.887	0.914
	$(\frac{1}{3}, \frac{2}{3})$	0.939	0.958	0.971	0.776	0.886	0.917
	$(\frac{1}{10}, \frac{9}{10})$	0.947	0.988	1.000	0.795	0.942	0.972
1	$(\frac{1}{2}, \frac{1}{2})$	0.31	0.38	0.43	0.13	0.22	0.25
	$(\frac{1}{3}, \frac{2}{3})$	0.31	0.37	0.40	0.13	0.22	0.25
	$(\frac{1}{10}, \frac{9}{10})$	0.34	0.65	0.81	0.14	0.34	0.43
$\frac{1}{3}$	$(\frac{1}{2}, \frac{1}{2})$	0.013	0.024	0.031	0.005	0.010	0.015
	$(\frac{1}{3}, \frac{2}{3})$	0.015	0.023	0.032	0.004	0.011	0.015
	$(\frac{1}{10}, \frac{9}{10})$	0.017	0.089	0.156	0.005	0.020	0.032

Table 10.5

Minimum, median and maximum of $\hat{\pi}_{1,35}$ over 150 designs for the simulation study in section 10.3.3 (to 3 decimal places for $\sigma_n^2 = 1, 5$; to 2 decimal places for $\sigma_n^2 = \frac{1}{3}$, except when value is exact).

σ_n^2	(ρ_r, ρ_c)	Ψ_1			Ψ_2		
		min.	median	max.	min.	median	Max.
5	$(\frac{1}{2}, \frac{1}{2})$	0.999	1	1	0.996	0.999	1
	$(\frac{1}{3}, \frac{2}{3})$	0.999	1.000	1	0.992	0.999	1
	$(\frac{1}{10}, \frac{9}{10})$	0.999	1	1	0.994	1.000	1
1	$(\frac{1}{2}, \frac{1}{2})$	0.939	0.958	0.968	0.863	0.911	0.928
	$(\frac{1}{3}, \frac{2}{3})$	0.937	0.955	0.966	0.855	0.909	0.927
	$(\frac{1}{10}, \frac{9}{10})$	0.941	0.985	0.998	0.853	0.944	0.965
$\frac{1}{3}$	$(\frac{1}{2}, \frac{1}{2})$	0.67	0.70	0.72	0.56	0.62	0.65
	$(\frac{1}{3}, \frac{2}{3})$	0.66	0.69	0.71	0.56	0.62	0.66
	$(\frac{1}{10}, \frac{9}{10})$	0.67	0.88	0.82	0.57	0.68	0.73

The minimum, median and maximum values of $\hat{\pi}_{1,35}$ are given in Table 10.5. For $\sigma_n^2 = 5$, the $\hat{\pi}_{1,35}$-values are either very close to 1 or equal to 1, and hence it would be difficult to compare $\hat{\pi}_{1,35}$ with the potential associated measurements. The values of $\hat{\omega}_{7,35}$ are also, in many cases, equal to 1, over all the σ_n^2 settings considered. Hence, $\hat{\omega}_{7,35}$ (for all of the σ_n^2 settings considered) and $\hat{\pi}_{1,35}$ (for $\sigma_n^2 = 5$) are not considered further. In retrospect, a lower value of q_2 (for $\omega_{q_2,35}$) would have been better.

As in the 10×10 example, which was discussed in section 10.3.2, the A-, A_{nn}- and $\mathrm{tr}\left(C_1^{(nn)}\right)$- values are highly inter-correlated, with Spearman rank correlation coefficients greater than 0.999. The correlation coefficients between the A-/A_{nn}-/$\mathrm{tr}\left(C_1^{(nn)}\right)$- values and the A_{ns}-values are also high (greater than 0.96). Hence, only the A_{nn}- and A_{ns}- values are considered in the rest of this section.

Figure 10.2 shows $\hat{\pi}_{7,35}$ plotted against the A_{nn}- and A_{ns}- values for Ψ_2, $(\rho_r, \rho_c) = (\frac{1}{3}, \frac{2}{3})$ and $\sigma_n^2 = 1$. There seems to be a strong linear relationship between the A_{nn}-value and $\hat{\pi}_{7,35}$, and apparently a non-linear relationship between the A_{ns}-value and $\hat{\pi}_{7,35}$. For the other combinations of parameter settings, the plots are similar.

Figure 10.2
Plots of $\hat{\pi}_{7,35}$ against the A_{nn}- and A_{ns}- values for Ψ_2, $(\rho_r, \rho_c) = (\frac{1}{3}, \frac{2}{3})$ and $\sigma_n^2 = 1$, for the simulation study in section 10.3.3.

a) $\hat{\pi}_{7,35}$ against A_{nn}-value   b) $\hat{\pi}_{7,35}$ against A_{ns}-value
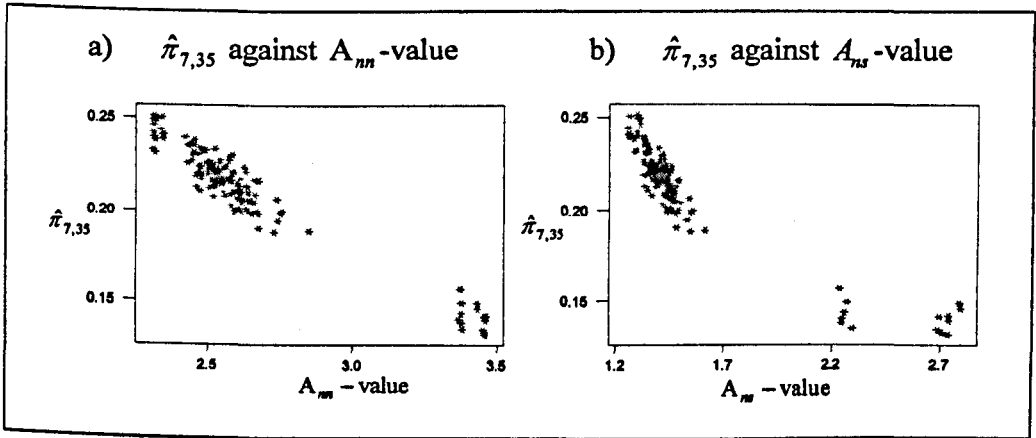
Spearman rank correlation coefficients between the A_{nn}- and A_{ns}- values and $\hat{\pi}_{7,35}$, given in Table 10.6, show that, as either the A_{nn}-value or the A_{ns}- value decreases the value of $\hat{\pi}_{7,35}$ tends to increase. As expected, the correlation is stronger when $\sigma_n^2 = 1.5$ than when $\sigma_n^2 = \frac{1}{3}$. Also, the correlation is better for Ψ_2 than for Ψ_1, except when $\sigma_n^2 = \frac{1}{3}$ and $(\rho_r, \rho_c) = (\frac{1}{10}, \frac{9}{10})$. The correlation is also stronger for $(\rho_r, \rho_c) = (\frac{1}{10}, \frac{9}{10})$ than for $(\rho_r, \rho_c) = (\frac{1}{2}, \frac{1}{2})$, $(\frac{1}{3}, \frac{2}{3})$. There seems to be little difference in the correlations for the A_{nn}- and A_{ns}- values, although the correlation coefficients are very slightly better for the A_{nn}-value than for the A_{ns}-value in most cases. Table 10.7 gives the Spearman rank correlation coefficients for $\hat{\pi}_{1,35}$ for $\sigma_n^2 = \frac{1}{3}, 1$. As for $\hat{\pi}_{7,35}$,

both the A_{nn}- and A_{ns}- values correlate well with $\hat{\pi}_{1,35}$. Plots of $\hat{\pi}_{1,35}$ against the A_{nn}- and A_{ns}- values are very similar to the plots for $\hat{\pi}_{7,35}$. For example, compare Figure 10.2 with Figure 10.3.

Table 10.6
Spearman rank correlation coefficients between the A_{nn}- and A_{ns}- values and $\hat{\pi}_{7,35}$ for the simulation study in section 10.3.3 (to 2 decimal places).

σ_n^2	(ρ_r, ρ_c)	Ψ_1		Ψ_2	
		A_{nn}-	A_{ns}-	A_{nn}-	A_{ns}-
5	$(\frac{1}{2}, \frac{1}{2})$	-0.66	-0.65	-0.89	-0.88
	$(\frac{1}{3}, \frac{3}{3})$	-0.67	-0.66	-0.91	-0.90
	$(\frac{1}{10}, \frac{9}{10})$	-0.90	-0.89	-0.97	-0.97
1	$(\frac{1}{2}, \frac{1}{2})$	-0.70	-0.69	-0.88	-0.87
	$(\frac{1}{3}, \frac{3}{3})$	-0.74	-0.71	-0.87	-0.86
	$(\frac{1}{10}, \frac{9}{10})$	-0.98	-0.98	-0.96	-0.96
$\frac{1}{5}$	$(\frac{1}{2}, \frac{1}{2})$	-0.32	-0.33	-0.52	-0.50
	$(\frac{1}{3}, \frac{3}{3})$	-0.42	-0.40	-0.45	-0.42
	$(\frac{1}{10}, \frac{9}{10})$	-0.94	-0.94	-0.75	-0.75

Figure 10.3
Plots of $\hat{\pi}_{1,35}$ against the A_{nn}- and A_{ns}- values for Ψ_2, $(\rho_r, \rho_c) = (\frac{1}{3}, \frac{3}{3})$ and $\sigma_n^2 = 1$, for the simulation study in section 10.3.3.

a) $\hat{\pi}_{1,35}$ against A_{nn}-value   b) $\hat{\pi}_{1,35}$ against A_{ns}-value
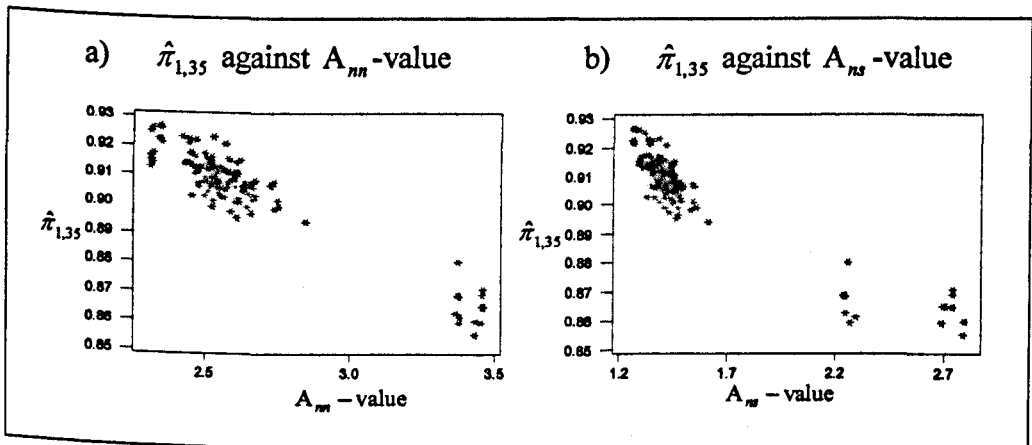
Table 10.7
Spearman rank correlation coefficients between the A_{nn}- and A_{ns}- values and $\hat{\pi}_{1,35}$, for $\sigma_n^2 = \frac{1}{3}, 1$, for the simulation study in section 10.3.3. (to 2 decimal places)

σ_n^2	(ρ_r, ρ_c)	Ψ_1		Ψ_2	
		A_{nn}-	A_{ns}-	A_{nn}-	A_{ns}-
1	$(\frac{1}{2}, \frac{1}{2})$	-0.66	-0.67	-0.71	-0.71
	$(\frac{1}{3}, \frac{2}{3})$	-0.55	-0.52	-0.77	-0.77
	$(\frac{1}{10}, \frac{9}{10})$	-0.91	-0.90	-0.92	-0.91
$\frac{1}{3}$	$(\frac{1}{2}, \frac{1}{2})$	-0.48	-0.48	-0.67	-0.66
	$(\frac{1}{3}, \frac{2}{3})$	-0.48	-0.48	-0.76	-0.73
	$(\frac{1}{10}, \frac{9}{10})$	-0.93	-0.94	-0.86	-0.84

The simulations in this section provide evidence to suggest that when c is small and t is large, the A-, A_{nn}-, A_{ns}- and $\text{tr}\left(C_1^{(nn)}\right)$- values are all well associated with $\pi_{q_1,z}$. The strength of this association seems to be dependent on the genetic variance and on the variance structure.

10.3.4   Simulation study – on a 20×8 array with $c = 5$

The simulation study considered in this section has the same sized array as the study in section 10.3.3 (i.e. 20×8). Here, however, there are $c = 5$ control varieties and $t = 134$ new varieties. Four of these control varieties are replicated 6 times and the fifth control variety is replicated twice (i.e. $r = (6,6,6,6,2)'$). The fifth control variety may be taken to represent a standard variety with respect to quality rather than yield. This would reflect current practice at NSW Agriculture, where a standard variety to assess quality, with fewer replications than the standard varieties to assess yield, is included. Note that $16\frac{1}{4}\%$ of the plots are check plots. These settings of p_1, p_2, r and c are also considered in chapter 11, where the robustness of some systematic designs is investigated.

As well as $\Psi_2 = (\frac{1}{4}, \frac{2}{8}, \frac{2}{8}, \frac{2}{8})$, which was considered in section 10.3.3,

$\Psi_3 = (\frac{5}{10}, \frac{2}{10}, \frac{6}{10}, \frac{4}{10}) = (\frac{1}{2}, \frac{1}{2}, \frac{3}{5}, \frac{2}{5})$ was also assumed here. The variance

component settings given by Ψ_3 have $\sigma_\gamma^2 = \sigma_\delta^2$, and were recommended by

Dr. B. Cullis of NSW Agriculture (personal correspondence, 1998). Recall

that he also recommended that $\sigma_n^2 = \frac{1}{10}, \frac{1}{2}, 1$ be assumed. The correlation

parameters were set at $(\rho_r, \rho_c) = (\frac{1}{2}, \frac{1}{2}), (\frac{1}{3}, \frac{2}{3})$. This gives 12 combinations of

Ψ, (ρ_r, ρ_c) and σ_n^2.

For each of the 4 combinations of Ψ and (ρ_r, ρ_c), 150 designs were selected

as in section 10.3.3. For each of these designs, $N = 5,000$ trials were

simulated, and estimates of $\pi_{7,45}$, $\pi_{1,45}$ and $\omega_{7,45}$ were obtained. Here z is

taken as approximately $\frac{1}{3}$ of t. Table 10.8 gives the minimum, median and

maximum values of $\hat{\pi}_{7,45}$ over the 150 designs. It can be seen that all the

estimates of $\pi_{7,45}$, over the 12 combinations of Ψ, (ρ_r, ρ_c) and σ_n^2, are less

than $\frac{1}{2}$. If the simulation study (including the range of σ_n^2) reflects what is

likely in practice, then such low estimates of $\pi_{7,45}$ suggest that only a few of

the best new varieties are likely to go on for further testing. If this is the case,

the success of the entire programme would arguably be undermined at the

EGVT stage (see the quote from Cullis *et al.* (1998), given in section 9.1). For

the purposes of this investigation, however, the actual values of $\hat{\pi}_{q_1,z}$ or $\hat{\omega}_{q_2,z}$

are not of particular importance, except, that is, when they are very near to

zero or one, in which case, any relationship with the potential associated

measurements is unlikely to be discernible. The values of $\hat{\omega}_{7,45}$ are very close

to 1 (for all the σ_n^2 settings), and from Table 10.8, it is clear that the $\hat{\pi}_{7,45}$-

values are close to 0 when $\sigma_n^2 = \frac{1}{10}$. Hence, $\hat{\pi}_{7,45}$ (for $\sigma_n^2 = \frac{1}{10}$) and $\hat{\omega}_{7,45}$ (for

all the σ_n^2 settings) are not considered further. In retrospect, a lower setting of

q_2 would have been better for $\omega_{q_2,45}$, and a higher value of q_1 would have

been better for $\pi_{q_2, 45}$ when $\sigma_n^2 = \frac{1}{10}$. The minimum, median and maximum values of $\hat{\pi}_{1, 45}$ are given in Table 10.9. As would be expected, the values of $\hat{\pi}_{1, 45}$ are much higher than the values of $\hat{\pi}_{7, 45}$.

Table 10.8
Minimum, median and maximum of $\hat{\pi}_{7, 45}$ over 150 designs for the simulation study in section 10.3.4 (to 3 decimal places for $\sigma_n^2 = \frac{1}{10}$; to 2 decimal places, otherwise).

σ_n^2	(ρ_r, ρ_c)	Ψ_2			Ψ_3		
		min.	median	max.	min.	median	max.
1	$(\frac{1}{2}, \frac{1}{2})$	0.31	0.42	0.46	0.29	0.34	0.37
	$(\frac{1}{3}, \frac{2}{3})$	0.30	0.42	0.47	0.27	0.33	0.37
$\frac{1}{2}$	$(\frac{1}{2}, \frac{1}{2})$	0.12	0.17	0.20	0.10	0.13	0.15
	$(\frac{1}{3}, \frac{2}{3})$	0.11	0.17	0.21	0.10	0.12	0.14
$\frac{1}{10}$	$(\frac{1}{2}, \frac{1}{2})$	0.007	0.014	0.021	0.006	0.011	0.016
	$(\frac{1}{3}, \frac{2}{3})$	0.007	0.014	0.020	0.006	0.010	0.017

Table 10.9
Minimum, median and maximum of $\hat{\pi}_{1, 45}$ over 150 designs for the simulation study in section 10.3.4 (to 2 decimal places).

σ_n^2	(ρ_r, ρ_c)	Ψ_2			Ψ_3		
		min.	median	max.	min.	median	max.
1	$(\frac{1}{2}, \frac{1}{2})$	0.92	0.95	0.97	0.91	0.93	0.95
	$(\frac{1}{3}, \frac{2}{3})$	0.92	0.95	0.97	0.91	0.93	0.95
$\frac{1}{2}$	$(\frac{1}{2}, \frac{1}{2})$	0.82	0.87	0.89	0.81	0.84	0.86
	$(\frac{1}{3}, \frac{2}{3})$	0.82	0.87	0.90	0.81	0.84	0.86
$\frac{1}{10}$	$(\frac{1}{2}, \frac{1}{2})$	0.57	0.62	0.64	0.57	0.60	0.62
	$(\frac{1}{3}, \frac{2}{3})$	0.58	0.62	0.64	0.57	0.59	0.62

As in section 10.3.3, the A-, A_{nn}- and $\text{tr}\left(C_1^{(nn)}\right)$- values are highly inter-correlated, with Spearman rank correlation coefficient greater than 0.998. The correlation coefficients between the A-/A_{nn}-/$\text{tr}\left(C_1^{(nn)}\right)$- values and A_{ns} - values are also high (greater than 0.842) but not as high as in section 10.3.3.

Therefore, only the A_{nn}- and A_{ns}- values are considered in the rest of this section.

Table 10.10 gives the Spearman rank correlation coefficients between the A_{nn}- and A_{ns}- values and $\hat{\pi}_{7,45}$ for $\sigma_n^2 = \frac{1}{2}$, 1, which suggest that both the A_{nn}- and A_{ns}- values are well associated with $\pi_{7,45}$. Plots of $\hat{\pi}_{7,45}$ against the A_{nn}- and A_{ns}- values are similar to those for the simulation study in section 10.3.3. Plots for Ψ_2, $(\rho_r, \rho_c) = (\frac{1}{3}, \frac{2}{3})$ and $\sigma_n^2 = 1$ (the same settings as the plots in section 10.3.3) are given as Figure 10.4.

Recall from the simulation study in section 10.3.3, that the correlation coefficients between the A_{nn}- and $\hat{\pi}_{7,35}$-values were very slightly better than the correlation coefficients between the A_{ns}- and $\hat{\pi}_{7,35}$-values, in most cases. Here, for $\hat{\pi}_{7,45}$, the difference in the correlation coefficients between the A_{nn}- and A_{ns}- values is slightly greater than in section 10.3.3, with better correlation coefficients for the A_{nn}-values than for the A_{ns}-values, in 7 of the 8 combinations considered. Also, the correlation is better, in most cases, for Ψ_2 than for Ψ_3, and for $(\rho_r, \rho_c) = (\frac{1}{3}, \frac{2}{3})$ than for $(\rho_r, \rho_c) = (\frac{1}{2}, \frac{1}{2})$. As expected, the correlation is also better for $\sigma_n^2 = 1$ than for $\sigma_n^2 = \frac{1}{2}$. Similar conclusions are drawn from the Spearman rank correlation coefficients for $\hat{\pi}_{1,45}$, given in Table 10.11.

Table 10.10

Spearman rank correlation coefficients between the A_{nn}- and A_{ns}- values and $\hat{\pi}_{7,45}$, for $\sigma_n^2 = \frac{1}{2}, 1$, for the simulation study in section 10.3.4 (to 2 decimal places).

σ_n^2	(ρ_r, ρ_c)	Ψ_2		Ψ_3	
		A_{nn}-	A_{ns}-	A_{nn}-	A_{ns}-
1	$(\frac{1}{2}, \frac{1}{2})$	-0.80	-0.74	-0.65	-0.57
	$(\frac{1}{3}, \frac{2}{3})$	-0.85	-0.79	-0.71	-0.63
$\frac{1}{2}$	$(\frac{1}{2}, \frac{1}{2})$	-0.71	-0.68	-0.58	-0.54
	$(\frac{1}{3}, \frac{2}{3})$	-0.77	-0.73	-0.51	-0.53

Figure 10.4

Plots of $\hat{\pi}_{7,45}$ against the A_{nn}- and A_{ns}- values for Ψ_2, $(\rho_r, \rho_c) = (\frac{1}{3}, \frac{2}{3})$ and $\sigma_n^2 = 1$, for the simulation study in section 10.3.4.

a) $\hat{\pi}_{7,45}$ against A_{nn}-value   b) $\hat{\pi}_{7,45}$ against A_{ns}-value
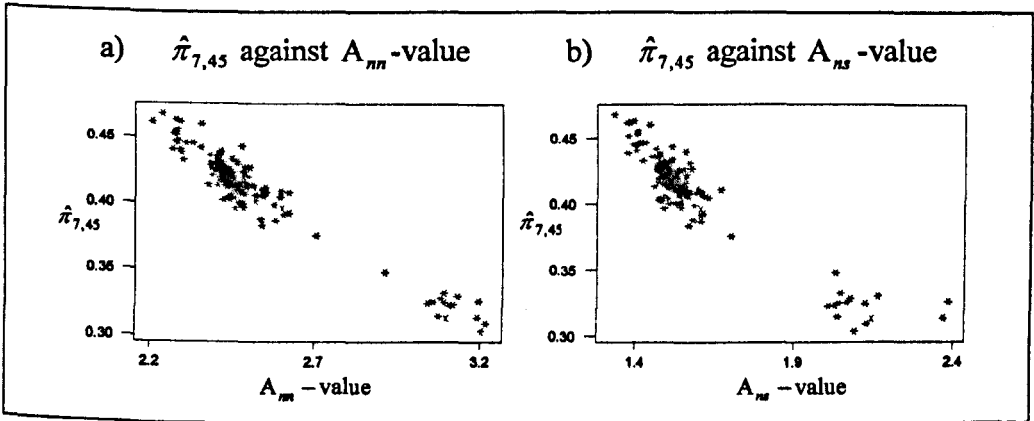
Table 10.11

Spearman rank correlation coefficients between the A_{nn}- and A_{ns}- values and $\hat{\pi}_{1,45}$, for the simulation study in section 10.3.4 (to 2 decimal places).

σ_n^2	(ρ_r, ρ_c)	Ψ_2		Ψ_3	
		A_{nn}-	A_{ns}-	A_{nn}-	A_{ns}-
1	$(\frac{1}{2}, \frac{1}{2})$	-0.62	-0.62	-0.58	-0.48
	$(\frac{1}{3}, \frac{2}{3})$	-0.75	-0.71	-0.52	-0.46
$\frac{1}{2}$	$(\frac{1}{2}, \frac{1}{2})$	-0.65	-0.63	-0.52	-0.51
	$(\frac{1}{3}, \frac{2}{3})$	-0.71	-0.70	-0.42	-0.48
$\frac{1}{10}$	$(\frac{1}{2}, \frac{1}{2})$	-0.53	-0.48	-0.37	-0.31
	$(\frac{1}{3}, \frac{2}{3})$	-0.51	-0.50	-0.28	-0.27

10.4 Discussion

Most of the simulation studies described in section 10.3 assumed model 1. The exceptions are the preliminary studies under models 2 and 3 (see section 10.3.2), which suggest that, for given Ψ, (ρ_r, ρ_c) and σ_n^2, the strength of the association between $\pi_{q_1, z}$ and the potential associated measurements, is likely to be similar over all the models, 1, 2 and 3. However, it would not be sensible to draw conclusions for models 2 and 3 from the studies under model 1, without conducting further simulation studies for models 2 and 3. Hence, the discussion in the rest of this section is with respect to model 1 only.

When c is small and t large, as is usually the case for EGVTs, the simulations suggest that of the 5 potential associated measurements investigated, all but the A_{ss}-value seem to be well associated with $\pi_{q_1, z}$. That is, the A-, A_{nn}-, A_{ns}- and $\text{tr}\left(C_1^{(nn)}\right)$- values are likely to be useful in comparing designs with respect to the efficacy of the selection of high yielding new varieties.

For the settings of Ψ and (ρ_r, ρ_c) considered in section 10.3 under model 1, Table 10.12 gives $\rho_{0,1}^{(1)} / \rho_{1,0}^{(1)}$.

Table 10.12
Values of $\rho_{0,1}^{(1)} / \rho_{1,0}^{(1)}$ under model 1 (to 1 decimal place, except when exact).

(ρ_r, ρ_c)	Ψ_1	Ψ_2	Ψ_3
$(\frac{1}{2}, \frac{1}{2})$	1	2.3	1
$(\frac{1}{3}, \frac{2}{3})$	3	4.4	1.4
$(\frac{1}{10}, \frac{9}{10})$	9	7.1	1.9

The strength of the association between the A-, A_{nn}-, A_{ns}- and $\text{tr}\left(C_1^{(nn)}\right)$- values and $\pi_{q_1, z}$ seems to depend, not only on the genetic variance, as might be expected, but also on the correlation structure, with a stronger association when the lag 1 column correlation is greater than the lag 1 row correlation (i.e.

when $\rho_{0,1}^{(1)} / \rho_{1,0}^{(1)} > 1$). As seen in section 10.3, the association was stronger for Ψ_2 than for Ψ_1 or Ψ_3, and also for $(\rho_r, \rho_c) = (\frac{1}{5}, \frac{3}{5})$, $(\frac{1}{10}, \frac{9}{10})$ than for $(\rho_r, \rho_c) = (\frac{1}{2}, \frac{1}{2})$.

There is some evidence to suggest that the A-, A_{nn}- and $\mathrm{tr}\left(C_1^{(nn)}\right)$- criteria are slightly better associated criteria to maximising $\pi_{q_1,z}$ than the A_{ns}-criterion. Some further investigations to compare the reliability of the A_{nn}- and A_{ns}- criteria are described in chapter 11.

As well as considering how well the A-, A_{nn}-, A_{ns}- and $\mathrm{tr}\left(C_1^{(nn)}\right)$- values are associated with $\pi_{q_1,z}$ for designs over a wide range of these values, it would be interesting to see how the Spearman rank correlation coefficients change if designs in the set $\mathcal{B}$ (designs selected to have high A-, A_{nn}-, A_{ns}- and $\mathrm{tr}\left(C_1^{(nn)}\right)$- values) are omitted. From the plots of $\hat{\pi}_{q_1,z}$ against the A_{nn}- and A_{ns}- values (see Figure 10.4, for example) the Spearman rank correlation coefficients between $\hat{\pi}_{q_1,z}$ and the A_{nn}- and A_{ns}- values are likely to be slightly worse (higher) when designs in $\mathcal{B}$ are omitted. This is the case, for example, for the study in section 10.3.4 with Ψ_2, $(\rho_r, \rho_c) = (\frac{1}{5}, \frac{3}{5})$ and $\sigma_n^2 = 1$. For this example, the correlation coefficients between $\hat{\pi}_{7,45}$ and the A_{nn}- and A_{ns}- values, when all designs are considered, are -0.85 and -0.79, respectively, and the correlation coefficients are -0.79 and -0.72, respectively, when designs in $\mathcal{B}$ are omitted.

In addition to finding measurements which are well associated with $\pi_{q_1,z}$, an examination of the spread of these measurements would be useful. For example, consider the A_{nn}- and A_{ns}- values in Figure 10.4 (i.e. for Ψ_2 and $(\rho_r, \rho_c) = (\frac{1}{5}, \frac{3}{5})$). The minimum and maximum A_{nn}- and A_{ns}- values over

the 3 subsets of designs G, R and B (defined in Definition 10.2) are given in Table 10.13. Recall that the sets G and B each contain 15 designs, and R contains 120 designs. The range of the A_{nn}- and A_{ns}- values over all the designs is large. The relative efficiency of the A_{nn}-worst design (A_{nn}-value $= 3.22$) to the A_{nn}-best design (A_{nn}-value $= 2.20$) is 0.68 (to 2 decimal places), and the relative efficiency of the A_{ns}-worst design (A_{ns}-value $= 2.38$) to the A_{ns}-best design (A_{ns}-value $= 1.33$) is 0.56 (to 2 decimal places). This shows that designs with high A_{nn}- (A_{ns}-) values are substantially worse than designs with low A_{nn}- (A_{ns}-) values, suggesting that designs with high A_{nn}- (A_{ns}-) values should be avoided.

Table 10.13
Minimum and maximum A_{nn}- and A_{ns}- values over the 3 subsets of designs G, R and B, for Ψ_2 and $(\rho_r, \rho_c) = (\frac{1}{3}, \frac{1}{3})$, for the simulation study in section 10.3.4 (to 2 decimal places).

	G		R		B	
	min.	max.	min.	max.	min.	max.
A_{nn}-value	2.20	2.33	2.35	2.70	2.91	3.22
A_{ns}-value	1.33	1.43	1.44	1.70	2.01	2.38

A comparison between the A_{nn}-/A_{ns}- values of designs in R and B, shows that designs in B can be much worse than designs selected randomly, with the relative efficiency of the A_{nn}-worst design in B (A_{nn}-value $= 3.22$) to the A_{nn}-best design in R (A_{nn}-value $= 2.35$) approximately equal to 0.73, and the relative efficiency of the A_{ns}-worst design in B (A_{ns}-value $= 2.38$) to the A_{ns}-best design in R (A_{ns}-value $= 1.44$) approximately equal to 0.61. This suggests that very inefficient designs are unlikely to be selected randomly.

By using the best design obtained from a few runs of the simulated annealing algorithm (see section 10.2), there can be a moderate gain in efficiency over using a randomly selected design. This is illustrated by the relative efficiency of the worst design in $\mathcal{R}$ to the best design in $\mathcal{G}$ of 0.81 and 0.78 (to 2 decimal places) with respect to the A_{nn} - and A_{ns} - values, respectively. More extensive algorithmic searches are likely to give a much greater gain in efficiency compared to a randomly selected design.

The relative efficiencies given above and the conclusions drawn from them are for one particular example only. However, the spread of the A_{nn} - and A_{ns} - values in Figure 10.2 and Figure 10.3, suggests that similar conclusions can be drawn for the other examples.

As well as investigating the properties of efficient designs, it is useful to know about inefficient designs, so that they can be avoided. The inefficient designs used in the simulation studies in section 10.3 generally had check plots clustered together. For the 20×8 example with $c = 5$ control varieties, which was considered in section 10.3.4, an example of a A_{nn}-inefficient design, and an example of a A_{ns} - inefficient design, used in the simulation for Ψ_3 and $(\rho_r, \rho_c) = (\frac{1}{2}, \frac{1}{2})$ are given in Figure 10.5. The A_{nn}-inefficient design has all the check plots clustered together in the right half of the array, and the A_{ns} - inefficient design has the check plots in a few columns, with many column self-adjacencies of the control varieties. The efficiencies of these designs, with respect to the best design found from an extensive search (see case 3 in Appendix A3.7) are given in parentheses in Figure 10.5. Worse designs than these are almost certainly possible, since these designs were obtained from only a few runs of the simulated annealing algorithm.

Figure 10.5

A_{nn}- and A_{ns}-inefficient designs for Ψ_3 and $(\rho_r, \rho_c) = (\tfrac{1}{2}, \tfrac{1}{2})$. Efficiencies (to 2 decimal places) given in parentheses.

A_{nn}-inefficient design (0.84)	A_{ns}-inefficient design (0.69)
<pre>• • • • 1 5 2 • • • • • • 1 3 1 • 4 2 3 4 • • • • 3 2 • 4 • • • • • 1 4 4 • • • • • • • • • • • • • • • 3 • • • • • • • 4 • • • • • • 2 5 • • • • • • • • • • • • 3 • 2 1 • • • • • 2 3 1 •</pre>	<pre>• • • • • • • • • • • • • • • 3 • • 1 • • • • • • • • • • • • 4 • 4 • • • • • • • 4 • 3 • 2 • • • • • 3 • 2 1 • • • • 3 • 2 1 • • • • • • 2 • • • • • 3 • • • • • • • • • • • • • • • 3 • • 1 • • • • 4 • 2 1 • • • • 4 • • 1 • • • • • • 2 • • • • • 4 • • • • • • 5 • • • • • • • 5 •</pre>

11 Efficiency of some systematic EGVT designs

11.1 Introduction

Systematic designs are often used for EGVTs. A systematic design for an EGVT has the check plots systematically distributed in the array. This chapter examines the efficiency and robustness of some systematic designs for EGVTs over different models and variance structures. Some examples of systematic designs were given in section 9.1.2. These examples included designs with the check plots in diagonals (see section 9.1.2), as is the current practice at NSW Agriculture. Also, the example of an EGVT from the International Maize and Wheat Improvement Center (given in section 9.1.2) had check plots in diagonals. For long narrow plots, with the short side of the plots within rows, as in Figure 9.1, wheat trials at the Plant Breeding Institute, Cambridge, UK, have had the check plots allocated to a few rows (Kempton, 1984, and Besag & Kempton, 1986).

By considering approximations to the A_{nn}- and A_{ns}-values under model 1, Martin *et al.* (2000) derive some theoretical results on efficient unreplicated designs. The 10×5 example from Eccleston & Chan (1998), which has $c = 2$, $r = 5$ and $t = 40$, is used as an illustrative example by Martin *et al.* (2000). This example was also considered in Chan *et al.* (1998), and some systematic designs for this example are investigated in section 11.2.

Example 11.1.

This example has a 10×5 array with $c = 2$ and $r = 5$. ∎

For the investigations in this chapter, as well as Example 11.1, a second example (Example 11.2) is examined in section 11.3.

Example 11.2

This example has a 20×8 array with $c = 5$ and $\underline{r} = (6,6,6,6,2)'$. ∎

Recall that Example 11.2 was also considered in section 10.3.4. A variety of systematic arrangements of the check plots is investigated for these two examples, including designs with check plots in diagonals and in a few rows.

As in much of chapter 10, the A_{nn}- and A_{ns}- criteria are used. The efficiency of a systematic design, with respect to the A_{nn}- or A_{ns}-value, is found by a comparison with an optimal (i.e. the design with the lowest possible A_{nn}- or A_{ns}-value) or near-optimal design. An extensive search of the design space was carried out using the annealing algorithm of Martin & Eccleston (1997), and the best design obtained from this search was used to calculate the efficiency of the systematic design. The efficiency and robustness of some systematic designs for Example 11.1 are examined in section 11.2 under models 1, 2 and 3. Section 11.3 looks at Example 11.2 under models 1 and 3. A discussion of the conclusions for this chapter is given in section 11.4.

11.2 Some systematic designs for Example 11.1

In this section, various systematic designs are considered for Example 11.1. Although the number of plots in this example is less than there would usually be in an EGVT, results from this small example are likely to be relevant to larger examples. Also, optimal designs are easier to find for small examples than for larger examples.

The systematic designs considered for Example 11.1 are given in Figure 11.1. Designs D_1 and D_2 have the check plots in diagonals (*diagonal* designs), with like and unlike diagonal control variety adjacencies, respectively. The diagonal designs D_1 and D_2 are typical of current practice at NSW Agriculture (Dr. B. Cullis, personal correspondence, 1999).

Figure 11.1
Systematic designs, D_1 to D_{13}, for Example 11.1
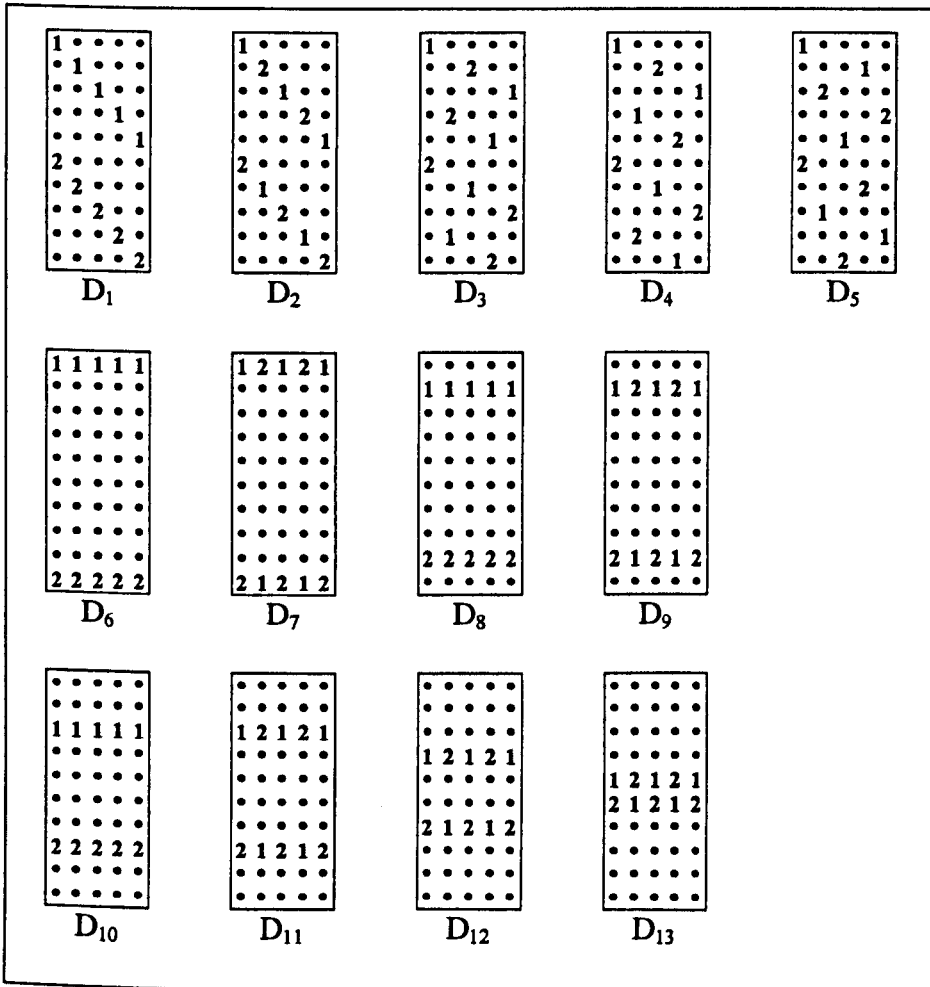
Designs D_3 to D_5 are called *knight's move* designs, since any pair of check plots are at least a knight's move apart (i.e. lag $(1, 2)$ or lag $(2, 1)$ apart). If $\rho_{1,0}^{(1)}$ and $\rho_{0,1}^{(1)}$ are roughly equal and not too large (and all other correlation values are small), Martin *et al.* (2000) show that both the A_{nn}- and A_{ns}-efficient designs have the check plots reasonably apart. That is, as few lag $(1, 0)$, $(0, 1)$, $(2, 0)$, $(0, 2)$, $(1, 1)$ and $(1, -1)$ (see Figure 3.1 in section 3.1.1.4) check plot adjacencies as possible. Also, for $\rho_{0,1}^{(1)}$ not too large and all other correlations small, Martin *et al.* (2000) show that the A_{ns}-efficient designs have as few row and column adjacencies of like control varieties, as many

control-new variety adjacencies in rows and columns, as few lag (2, 0) and (0, 2) like control adjacencies and as many lag (2, 0) and (0, 2) control-new variety adjacencies as possible. Hence, knight's move designs are likely to be efficient for some correlation structures.

When $t = (p_1 - q)p_2$ (i.e. $\sum r_i = qp_2$) for a positive integer q, let a *row* design be a design with all the check plots in q rows. For Example 11.1, $t = (p_1 - 2)p_2$ and D_6 to D_{13} are row designs which include pairs of designs (D_{2i+4}, D_{2i+5}), for $i = 1,2,3$, such that both designs in a pair have the check plots in rows i and $11 - i$, where rows are labelled 1 to 10 from top to bottom. Designs D_{2i+4} and D_{2i+5}, have the number of like and unlike row control variety adjacencies maximised, respectively. Designs D_{12} and D_{13} have the check plots in rows 4 and 7, and rows 5 and 6, respectively, with no like control variety adjacencies. For model 1, Martin *et al.* (2000) show that when $\rho_{0,1}^{(1)}$ is not too large and all other correlations are small (i.e. when the lag 1 within-column correlation is dominant), the A_{nn}-efficient designs have as many row and column adjacencies of new varieties (especially column adjacencies) and as many control-new variety column adjacencies as possible. Hence, some row designs are likely to be A_{nn}-efficient in some circumstances.

Most of the systematic designs in Figure 11.1 have been chosen for consideration since theoretical results from Martin *et al.* (2000) suggest that they are likely to be efficient for certain dependence structures under model 1; such as when $\rho_{0,1}^{(1)}$ is not too large and all other correlations are small, which is likely to be the case for long narrow plots (see section 9.1.1). When $t = p_1(p_2 - q)$, let a *column* design be a design with all the check plots in q columns. Some column designs will be A_{nn}-efficient when $\rho_{1,0}^{(1)}$ is large and all other correlations are small (Martin *et al.*, 2000). However, column designs are not considered here since attention is restricted to square (or near-square) plots and long narrow plots, as in Figure 9.1.

Many other systematic arrangements of the check plots are clearly possible, including other diagonal designs, knight's move designs and row designs. However, examining the efficiency and robustness of a large number of systematic designs would be complicated and unwieldy. Instead, an examination of a few representative systematic designs (D_1 to D_{13}) is carried out. This should provide some preliminary results, and may suggest other systematic designs worth investigating later.

The following settings of $\Psi = (\sigma_\gamma^2, \sigma_\delta^2, \sigma_\zeta^2, \sigma_\eta^2)$ are considered here:

$\Psi_1 = (0, 0, 1, 0)$, $\Psi_2 = (\frac{1}{4}, \frac{1}{4}, \frac{1}{4}, \frac{1}{4})$, $\Psi_3 = (\frac{1}{10}, \frac{1}{10}, \frac{6}{10}, \frac{1}{10})$ and $\Psi_4 = (1, 1, 0, 1)$. As in chapter 10, $\sigma_\zeta^2 + \sigma_\eta^2 = 1$ is assumed without loss of generality. The settings Ψ_1, Ψ_2, Ψ_3 and Ψ_4 are also assumed in Chan et al. (1998), and Ψ_1, Ψ_2 and Ψ_3 were considered in chapter 10. Let Ψ_1, Ψ_2 and Ψ_3 be called the *spatial models*, since $\sigma_\zeta^2 \neq 0$, and let Ψ_4 be the *non-spatial model*, since the variance of the additional spatial component is zero. Note that Ψ_4 has $\sigma_\gamma^2 = \sigma_\delta^2 = \sigma_\eta^2 = 1$. To reflect what is likely in practice, the ratio $\sigma_n^2/(\sigma_\zeta^2 + \sigma_\eta^2)$ is taken as $\frac{1}{10}$, $\frac{1}{2}$ and 1, as in section 10.3.4. The correlation parameters (ρ_r, ρ_c) of the AR(1)*AR(1) process are taken as $(\frac{1}{2}, \frac{1}{2})$, $(\frac{1}{2}, \frac{2}{3})$ and $(\frac{1}{10}, \frac{9}{10})$, as in section 10.3.3.

11.2.1 Example 11.1 under model 1

Model 1 (see section 9.2.1.1) is assumed in this section. There are 10 combinations of the settings of Ψ and (ρ_r, ρ_c), called cases 1 to 10 in Table 11.1. The ratios of the lag 1 column to row correlations, $\rho_{0,1}^{(1)}/\rho_{1,0}^{(1)}$, are also given in Table 11.1.

Table 11.1

Case numbers and the ratio $\rho_{0,1}^{(1)}/\rho_{1,0}^{(1)}$ for the 10 combinations of the settings of Ψ and (ρ_r, ρ_c) for Example 11.1 under model 1. The ratios $\rho_{0,1}^{(1)}/\rho_{1,0}^{(1)}$ are given in parentheses (to 1 decimal place, except when exact). † indicates that the combination is also considered for Example 11.2 under model 1

(ρ_r, ρ_c)	Ψ_1	Ψ_2	Ψ_3	Ψ_4
$(\frac{1}{2}, \frac{1}{2})$	1 (1) †	2 (2.3) †	3 (1) †	
$(\frac{1}{2}, \frac{2}{3})$	4 (3) †	5 (4.4) †	6 (1.4) †	10 (1) †
$(\frac{1}{10}, \frac{9}{10})$	7 (9)	8 (7.1)	9 (1.9)	

The best designs found for each case, from an extensive search with respect to the A_{nn}- and A_{ns}- values, are given in Appendix A3.5. The example being considered here has a small number of plots, which made it feasible to have a very large number of runs (100) of the algorithm of Martin & Eccleston (1997), so that the 20 resulting designs (10 cases and the 2 criteria) are very likely to be the optimal designs.

Nineteen of the 20 best designs found for the 10 cases have binary columns (i.e. no variety occurs more than once in any column). The exception is for case 1 under the A_{nn}-criterion. Also, when $\rho_{0,1}^{(1)} > \rho_{1,0}^{(1)}$ (case 2 and cases 4 to 9) the best designs found do not have check plots in the top or bottom rows. For the spatial models (cases 1 to 9), check plots in the same column are at least lag 3 apart (often lag 5 apart). When $\rho_{1,0}^{(1)} = \rho_{0,1}^{(1)}$, except for the non-spatial model (i.e. for cases 1 and 3), the best designs found have many pairs of the check plots a knight's move apart. As expected from Martin *et al.* (2000), when $\rho_{0,1}^{(1)} > \rho_{1,0}^{(1)}$ (case 2 and cases 4 to 9), row designs (often D_{10} and D_{11}) are the best designs found with respect to the A_{nn}-value. Under the A_{ns}-criterion, the best designs found have many of the check plots a knight's move apart. For the non-spatial model (case 10), the A_{nn}- and A_{ns}-best

designs found have several lag 1 row and column adjacencies of unlike control varieties (Martin *et al.*, 2000).

Table 11.2 and Table 11.3, respectively, give the values of $\{1 - (A_{nn}\text{-efficiency})\} \times 10,000$ and $\{1 - (A_{ns}\text{-efficiency})\} \times 10,000$ for the systematic designs D_1 to D_{13}. This means that for a given case, the best of these designs has the lowest entry in the corresponding column of Table 11.2 or Table 11.3. For example, the entry 988, for case 1 and design D_1 in Table 11.2 corresponds to an A_{nn}-efficiency of 0.9012. Also, the entry 0 in Table 11.2 and Table 11.3 corresponds to an efficiency of 1.0000.

Table 11.2
$\{1 - (A_{nn}\text{-efficiency})\} \times 10,000$ for D_1 to D_{13} under model 1.
(lowest value in bold)

(ρ_r, ρ_c)		$(\frac{1}{2}, \frac{1}{2})$			$(\frac{1}{3}, \frac{2}{3})$			$(\frac{1}{10}, \frac{9}{10})$			
Ψ		Ψ_1	Ψ_2	Ψ_3	Ψ_1	Ψ_2	Ψ_3	Ψ_1	Ψ_2	Ψ_3	Ψ_4
Case No.		1	2	3	4	5	6	7	8	9	10
$\rho_{0,1}^{(1)}/\rho_{1,0}^{(1)}$		1	2.3	1	3	4.4	1.4	9	7.1	1.9	1
D_1	diagonal	988	634	248	487	688	290	1279	1079	680	**54**
D_2	designs	449	361	39	241	530	134	1025	935	550	**54**
D_3	knight's	138	335	**1**	260	562	127	1137	953	546	**54**
D_4	move	**56**	332	34	206	557	146	1124	958	556	**54**
D_5	designs	60	342	49	191	554	152	1070	952	558	**54**
D_6		1463	477	525	1004	717	350	2184	532	233	249
D_7		1314	415	508	914	698	353	2057	543	250	249
D_8		1234	184	387	340	184	80	478	**40**	24	249
D_9	row	965	72	358	177	150	85	234	57	45	249
D_{10}	designs	1218	108	351	160	**32**	**0**	249	15	**0**	249
D_{11}		958	**0**	324	**0**	**0**	5	**0**	34	19	249
D_{12}		1105	166	389	250	257	110	1472	447	160	249
D_{13}		1581	764	660	1157	1059	500	3460	1149	439	249
Best & near-best designs from D_1 to D_{13}		D_4 & D_5	D_{11}	D_2 to D_5	D_{11}	D_{10} & D_{11}	D_{10} & D_{11}	D_{11}	D_8 to D_{11}	D_8 to D_{11}	D_1 to D_5

Table 11.3

$\{1 - (A_{ns}\text{-efficiency})\} \times 10{,}000$ for D_1 to D_{13} under model 1.
(lowest value in bold)

(ρ_r, ρ_c)		$(\frac{1}{2}, \frac{1}{2})$			$(\frac{1}{5}, \frac{3}{5})$			$(\frac{1}{10}, \frac{9}{10})$			
Ψ		Ψ_1	Ψ_2	Ψ_3	Ψ_1	Ψ_2	Ψ_3	Ψ_1	Ψ_2	Ψ_3	Ψ_4
Case No.		1	2	3	4	5	6	7	8	9	10
$\rho_{0,1}^{(1)} / \rho_{1,0}^{(1)}$		1	2.3	1	3	4.4	1.4	9	7.1	1.9	1
D_1	diagonal	1533	769	462	797	484	282	1455	490	337	**14**
D_2	designs	382	135	25	252	**157**	31	988	272	178	**14**
D_3	knight's	197	150	15	345	226	49	1177	316	187	**14**
D_4	move	**24**	97	12	232	185	42	1132	309	190	**14**
D_5	designs	27	107	25	204	175	43	1057	294	187	**14**
D_6		3540	2476	3296	2062	1813	2779	3130	1696	2842	3087
D_7		2411	1434	2120	1487	1151	1738	2705	995	1702	1931
D_8		3058	2073	3118	1210	1251	2552	1358	1171	2674	3087
D_9	row	1666	881	1868	467	488	1445	721	404	1486	1931
D_{10}	designs	2865	1912	3047	840	1027	2461	623	1004	2614	3087
D_{11}		1431	691	1780	**76**	244	1333	**0**	239	1414	1931
D_{12}		1646	877	1852	322	467	1410	1122	522	1487	1931
D_{13}		2749	1781	2269	1507	1337	1782	3093	1142	1685	1931

Over the 10 cases considered, the A_{nn}-efficiencies of the systematic designs, D_1 to D_{13}, range from 0.6540 (the entry 3460 for D_{13} in Table 11.2) to 1. For the spatial models, the A_{nn}-worst design is D_{13} in 8 of 9 cases. This is perhaps not surprising given the A_{nn}-inefficient design presented in Figure 10.5 in section 10.4. If D_{13} is excluded, the A_{nn}-efficiencies range from 0.7816 (the entry 2184 in Table 11.2) to 1.

For the spatial models, Table 11.4 lists the best design from D_1 to D_{13} under model 1. The minimum A_{nn}- and A_{ns}- efficiencies of the best of these designs, over the 10 cases, are 0.9944 and 0.9761, respectively.

Table 11.4
Best systematic designs from D_1 to D_{13} under model 1.
Case numbers in parentheses. Spatial models only.

(ρ_r, ρ_c)	Ψ_1		Ψ_2		Ψ_3	
	A_{ns}-	A_{nn}-	A_{ns}-	A_{nn}-	A_{ns}-	A_{nn}-
$(\frac{1}{2}, \frac{1}{2})$	D_4	D_4 (1)	D_4	D_{11} (2)	D_4	D_3 (3)
$(\frac{1}{3}, \frac{2}{3})$	D_{11}	D_{11} (4)	D_2	D_{11} (5)	D_2	D_{10} (6)
$(\frac{1}{10}, \frac{9}{10})$	D_{11}	D_{11} (7)	D_{11}	D_{10} (8)	D_2	D_{10} (9)

As expected from Martin *et al.* (2000), when $\rho_{0,1}^{(1)} / \rho_{1,0}^{(1)} > 1$, the A_{nn}-best design from D_1 to D_{13} is a row design (either D_{10} or D_{11}). For cases 1 and 3, where $\rho_{0,1}^{(1)} / \rho_{1,0}^{(1)} = 1$ (spatial models), a knight's move design (D_3 or D_4) is the A_{nn}-best design from D_1 to D_{13}.

In this paragraph, comparisons are among all 13 designs D_1 to D_{13}. The A_{ns}-efficiencies for these designs range from 0.6460 (the entry 3540 in Table 11.3) to 1. The A_{ns}-worst design is the row design D_6. For the spatial models, the A_{ns}-best designs are D_2 or D_4 when $\rho_{0,1}^{(1)} / \rho_{1,0}^{(1)} \leq 2.3$ (cases 1, 2, 3, 6 and 9). Design D_{11} is the A_{ns}-best design for many of the other cases (cases 4, 7 and 8). Note that for case 5, where $\rho_{0,1}^{(1)} / \rho_{1,0}^{(1)} \approx 4.4$, the A_{ns}-best design is D_2.

Over the 10 cases, the designs D_2 to D_5, have reasonably high efficiencies with respect to both the A_{nn}- and A_{ns}- values. The A_{nn}- efficiencies for D_2 to D_5 range from 0.8863 to 0.9999, with median 0.9667, and the A_{ns}-efficiencies range from 0.8823 to 0.9988, with median 0.9824. The row designs, D_6 to D_{12}, have reasonably high A_{nn}- efficiency, but can have low A_{ns}-efficiencies over the 10 cases. The A_{nn}- efficiencies for D_6 to D_{12} range from 0.7816 to 1.0000, with median 0.9751, and the A_{ns}-efficiencies range from 0.6460 to 1.0000, with median 0.8344.

11.2.1.1 Estimated selection probabilities

Recall from the simulation studies in section 10.3 that both the A_{nn}- and A_{ns}-values correlate well with selection probabilities, with some evidence to suggest that the correlation is a little better for the A_{nn}-values. The estimated selection probabilities for the systematic designs, D_1 to D_{13}, are examined here to see if they provide more evidence to favour the A_{nn}-criterion.

Estimates of $\pi_{2,10}$ ($\hat{\pi}_{2,10}$) were obtained as described in section 10.2, from $N = 10,000$ trials of simulated yields for designs D_1 to D_{13}, over the 10 cases. The $\hat{\pi}_{2,10}$-values are given in Table 11.5. The estimated standard error of the $\hat{\pi}_{2,10}$-values is approximately 0.005 for most cases, which gives an approximate 95% confidence interval of $\hat{\pi}_{2,10} \pm 0.01$ for each $\pi_{2,10}$-value. For each case, the highest $\hat{\pi}_{2,10}$-values (these are values which are greater than the highest value (to 3 decimal places) minus 0.005) are given in bold in Table 11.5. Note that D_{13} has the lowest (or near to the lowest) $\hat{\pi}_{2,10}$-value for most cases.

Table 11.5

Estimated $\pi_{2,10}$ ($\times 1{,}000$) for D_1 to D_{13} under model 1.
(highest values in bold)

(ρ_r, ρ_c)	$(\tfrac{1}{2}, \tfrac{1}{2})$			$(\tfrac{1}{3}, \tfrac{2}{3})$			$(\tfrac{1}{10}, \tfrac{9}{10})$			
Ψ	Ψ_1	Ψ_2	Ψ_3	Ψ_1	Ψ_2	Ψ_3	Ψ_1	Ψ_2	Ψ_3	Ψ_4
Case No.	1	2	3	4	5	6	7	8	9	10
$\rho_{0,1}^{(1)} / \rho_{1,0}^{(1)}$	1	2.3	1	3	4.4	1.4	9	7.1	1.9	1
D_1 diagonal	561	452	**419**	563	469	404	834	575	445	**338**
D_2 designs	577	461	411	**577**	477	401	837	562	440	**338**
D_3 knight's	574	462	413	**577**	467	400	833	582	453	334
D_4 move	**584**	461	400	569	468	399	829	578	447	328
D_5 designs	571	466	417	574	472	403	830	584	452	324
D_6	538	465	406	533	476	405	802	590	459	330
D_7	543	461	402	547	462	405	798	580	457	326
D_8	557	463	400	558	465	404	838	602	439	320
D_9 row	556	466	406	574	467	409	845	585	440	326
D_{10} designs	554	476	401	564	471	410	847	602	459	319
D_{11}	554	479	405	**577**	476	409	849	599	458	331
D_{12}	565	463	397	571	467	400	825	567	446	316
D_{13}	540	449	382	544	457	400	760	558	446	324

Consider the pair of row designs (D_{2i+4}, D_{2i+5}) for $i = 1,2,3$, where each pair has the same check plots (i.e. the pairs (D_6, D_7), (D_8, D_9), (D_{10}, D_{11})). Let D_{2i+4} be called a *row like-control* design since like control variety adjacencies in rows are maximised, and let D_{2i+5}, which has no like control variety adjacencies, be called a *row unlike-control* design. Design D_{2i+4} has a much lower A_{ns}-efficiency than design D_{2i+5}, but both designs have similar A_{nn}-efficiencies. However, note that for cases 1 to 5 and case 7, the differences in the A_{nn}-efficiencies for D_{2i+4} and D_{2i+5} ($i = 1,2,3$) have the same sign as the differences in the A_{ns}-efficiencies for these designs.

Let $\pi_{2,10}(D_i)$ be the selection probability for design D_i. Over the designs (D_{2i+4}, D_{2i+5}) $(i = 1,2,3)$, if the A_{nn}-value correlates well with $\pi_{2,10}$ then $\pi_{2,10}(D_{2i+4}) \approx \pi_{2,10}(D_{2i+5})$ would be expected, and if the A_{ns}-value correlates well with $\pi_{2,10}$ then $\pi_{2,10}(D_{2i+4}) < \pi_{2,10}(D_{2i+5})$ would be expected. For cases 1 to 9 and the 3 pairs of designs (D_{2i+4}, D_{2i+5}), the 27 differences $\hat{\pi}_{2,10}(D_{2i+4}) - \hat{\pi}_{2,10}(D_{2i+5})$ are given in Table 11.6. These differences are very small, ranging from −0.016 to 0.017, with median 0.001; and are negative in only 14 of the 27 combinations. This suggests that the A_{ns}-value is not, for these designs, well associated with the selection probabilities.

Table 11.6

Differences $\hat{\pi}_{2,10}(D_{2i+4}) - \hat{\pi}_{2,10}(D_{2i+5})$ $(i = 1,2,3)$ under model 1.

(ρ_r, ρ_c)	$(\frac{1}{2}, \frac{1}{2})$			$(\frac{1}{3}, \frac{2}{3})$			$(\frac{1}{10}, \frac{9}{10})$		
Ψ	Ψ_1	Ψ_2	Ψ_3	Ψ_1	Ψ_2	Ψ_3	Ψ_1	Ψ_2	Ψ_3
Case No.	1	2	3	4	5	6	7	8	9
$\rho_{0,1}^{(1)} / \rho_{1,0}^{(1)}$	1	2.3	1	3	4.4	1.4	9	7.1	1.9
(D_6, D_7)	-0.004	0.004	0.004	-0.014	0.014	0.000	0.004	0.010	0.002
(D_8, D_9)	0.001	-0.003	-0.006	-0.016	-0.002	-0.005	-0.008	0.017	-0.001
(D_{10}, D_{11})	0.000	-0.003	-0.004	-0.014	-0.005	0.001	-0.003	0.003	0.001

A comparison of $\hat{\pi}_{2,10}$ for the 6 cases when the best designs from D_1 to D_{13} under the A_{ns}- and A_{nn}-criteria are different (cases 2, 3, 5, 6, 8 and 9) (see Table 11.4), shows that for all cases except case 5, $\hat{\pi}_{2,10}$ is greater for the A_{nn}-best design; although the difference is small for cases 6 and 8. Note also that the designs with the highest $\hat{\pi}_{2,10}$-values (marked in bold in Table 11.5) include the A_{nn}-best design from D_1 to D_{13} in 8 out of 9 cases, thus providing more evidence to support the use of the A_{nn}-criterion rather than the A_{ns}-criterion in this section.

Now consider case 10 (Ψ_4) over designs D_1 to D_{13}. There is not a large difference in the A_{nn}-efficiencies (either 0.9946 or 0.9751), but the A_{ns}-efficiencies vary a great deal; they are either 0.9986 (for D_1 to D_5), 0.8069 (for row unlike control designs) or 0.6913 (for row like control designs). The $\hat{\pi}_{2,10}$-values are fairly similar (ranging from 0.316 to 0.338) suggesting that there is no evidence that the selection probabilities for the row like control designs, D_6, D_8 and D_{10}, are different to the selection probabilities for the other row designs.

In section 11.2.1.2, A_{nn}-efficiency is considered, unless otherwise stated.

11.2.1.2 *An examination of the A_{nn}-efficiencies for D_1 to D_{13} under model 1*

Now consider the A_{nn}-efficiencies from Table 11.2 in more detail, beginning with the spatial models. Of the 2 diagonal designs, D_2 is better than D_1 over all 9 cases (under both criteria); the difference in the efficiencies between these two designs ranges from 0.013 to 0.054. The 3 knight's move designs, D_3 to D_5, have similar efficiencies; the difference in the efficiencies between the best and worst knight's move designs ranges from 0.0006 to 0.0083. For the row designs, as stated above, there is little difference in the efficiencies between designs with row like-control and row unlike-control designs. As might be expected (see section 10.4), since check plots are close together, design D_{13} has efficiency lower than the best from the other row designs. Clearly D_{10} and D_{11} are the best from the row designs, D_6 to D_{13}, although in some cases (Ψ_3, for example) the efficiency is similar for D_8 and D_9. For the non-spatial model (Ψ_4), D_1 to D_5 are equally the best from D_1 to D_{13}, under both criteria. Also, row designs, D_6 to D_{13}, have a relative A_{nn}-efficiency of 0.98 compared to D_1 to D_5.

For the cases considered here, Table 11.2 (foot) lists the A_{mn}-best and near-best designs from D_1 to D_{13}. A design is deemed to be *best/near-best* if it has efficiency greater than or equal to 99.5% of the efficiency of the best design from D_1 to D_{13}. This suggests that either diagonal or knight's move designs be used when $\rho_{0,1}^{(1)} / \rho_{1,0}^{(1)}$ is near 1, and row designs be used for $\rho_{0,1}^{(1)} / \rho_{1,0}^{(1)}$ greater than about 2.

As well as identifying good systematic designs from D_1 to D_{13} for specific situations, it is useful to consider the robustness of the designs. Assume that there is no prior information on the variance components, other than that $\sigma_\xi^2 > 0$, and that $\rho_r, \rho_c > 0$ and the ratio ρ_c / ρ_r depends mainly on the plot size ratio. Then for square plots and long thin plots $\rho_c \approx \rho_r$ and $\rho_c > \rho_r$, respectively, are likely. Over the 10 cases considered, all designs from D_1 to D_{12} are reasonably robust with efficiency greater than 0.78.

The robustness of designs D_1 to D_{13} is considered for six categories of prior information about the plot size ratio. These six categories, called categories (a) to (f) are listed in Table 11.7. Since it is assumed that ρ_c / ρ_r depends mainly on the plot size ratio, an approximate range for ρ_c / ρ_r, corresponding to each of the categories is also given in Table 11.7. Note that over the 6 categories, these ranges for ρ_c / ρ_r are not exclusive.

Table 11.7

Categories for prior information on plot size ratio, approximate ranges for ρ_c/ρ_r, and setting(s) of (ρ_r, ρ_c) (and corresponding cases) used to determine if a design is robust.

Category	Prior information on plot size ratio	Approximate range for ρ_c/ρ_r	(ρ_r, ρ_c) setting(s)	Cases for model 1	Cases for models 2 and 3
(a)	Square or near-square plots	$\frac{1}{2} \le \rho_c/\rho_r \le 2$	$(\frac{1}{2}, \frac{1}{2})$	1 to 3	1 to 3, 11 to 13, 21 to 23
(b)	Long thin plots	$2 \le \rho_c/\rho_r \le 5$	$(\frac{1}{3}, \frac{2}{3})$	4 to 6	4 to 6, 14 to 16, 24 to 26
(c)	Very long thin plots	$\rho_c/\rho_r \ge 5$	$(\frac{1}{10}, \frac{9}{10})$	7 to 9	7 to 9, 17 to 19, 27 to 29
(d)	Not very long thin plots	$\frac{1}{2} \le \rho_c/\rho_r \le 5$	$(\frac{1}{2}, \frac{1}{2})$, $(\frac{1}{3}, \frac{2}{3})$	1 to 6	1 to 6, 11 to 16, 21 to 26
(e)	Not square plots	$\rho_c/\rho_r \ge 2$	$(\frac{1}{3}, \frac{2}{3})$, $(\frac{1}{10}, \frac{9}{10})$	4 to 9	4 to 9, 14 to 19, 24 to 29
(f)	Little prior information on plot shape	$\rho_c/\rho_r \ge \frac{1}{2}$	$(\frac{1}{2}, \frac{1}{2})$, $(\frac{1}{3}, \frac{2}{3})$, $(\frac{1}{10}, \frac{9}{10})$	1 to 9	1 to 9, 11 to 19, 21 to 29.

For each category, a design D_i ($i = 1,\ldots,13$) is deemed to be *robust* if the minimum and median A_{nn}-efficiencies (over the cases for which ρ_c/ρ_r are included in the corresponding range for ρ_c/ρ_r) are greater than m_1 and m_2, respectively, where m_1 and m_2 are near 1. The designs (from D_1 to D_{13}) deemed to be robust (with respect to A_{nn}-efficiency) for 3 settings of m_1, m_2 are given in Table 11.8. For example, for category (d), the cases included in the range $\frac{1}{2} \le \rho_c/\rho_r \le 5$ are cases 1 to 6. Over these cases, D_2 has minimum and median A_{nn}-efficiencies of 0.9470 and 0.9699, respectively. Hence, for category (d), D_2 is deemed to be robust for $m_1 = 0.85$ and $m_2 = 0.95$. However, D_2 is not deemed to be robust for category (d) when $m_1 = 0.9$ and $m_2 = 0.98$ (see Table 11.8). Note that for each category, the range for ρ_c/ρ_r

given in Table 11.7 is approximate, since the cases considered do not have ρ_c/ρ_r at the upper and lower values of the range. For example, for category (d), $(\frac{1}{2} \le \rho_c/\rho_r \le 5)$, ρ_c/ρ_r is equal to either 1 (cases 1 to 3) or 3 (cases 4 to 6) for the cases considered. Also, for some categories ((a), (b) and (c)), the cases considered have only one setting of ρ_c/ρ_r.

For the spatial models, the most robust ($m_1 = 0.9$ and $m_2 = 0.99$) designs, for square or near-square plots (category (a)), are D_4 and D_5, otherwise (categories (b) to (f)) D_{10} or D_{11} are the most robust.

Table 11.8
Robustness of D_1 to D_{13} (for $\sigma_\xi^2 > 0$) under model 1.

Category	Prior information on plot size ratio	$m_1 = 0.85$ $m_2 = 0.95$	$m_1 = 0.9$ $m_2 = 0.98$	$m_1 = 0.9$ $m_2 = 0.99$
(a)	Square or near-square plots	D_2 to D_5, D_8 to D_{12}	D_3 to D_5	D_4 to D_5
(b)	Long thin plots	D_1 to D_5, D_8 to D_{12}	D_5, D_8 to D_{11}	D_{10} to D_{11}
(c)	Very long thin plots	D_8 to D_{12}	D_8 to D_{11}	D_8 to D_{11}
(d)	Not very long thin plots	D_2 to D_5, D_8 to D_{12}	D_3 to D_5, D_9 to D_{11}	D_{11}
(e)	Not square plots	D_8 to D_{12}	D_8 to D_{11}	D_{10} to D_{11}
(f)	Little prior information on plot shape	D_2 to D_5, D_8 to D_{12}	D_9 to D_{11}	D_{11}

11.2.2 Example 11.1 under model 2

For model 2 (see section 9.2.1.2), there are 30 combinations of the settings for Ψ, (ρ_r, ρ_c) and σ_n^2. These 30 combinations are called cases 1 to 30 in Table 11.9.

Table 11.9

Case numbers for the 30 combinations of the settings of Ψ, (ρ_r, ρ_c) and σ_n^2 for models 2 and 3. † indicates that the combination is also considered for Example 11.2 under model 3.

σ_n^2	(ρ_r, ρ_c)	Ψ_1	Ψ_2	Ψ_3	Ψ_4
$\frac{1}{10}$	$(\frac{1}{2}, \frac{1}{2})$	1 †	2	3 †	
	$(\frac{1}{3}, \frac{2}{3})$	4 †	5	6 †	10 †
	$(\frac{1}{10}, \frac{9}{10})$	7	8	9	
$\frac{1}{2}$	$(\frac{1}{2}, \frac{1}{2})$	11	12	13	
	$(\frac{1}{3}, \frac{2}{3})$	14	15	16	20
	$(\frac{1}{10}, \frac{9}{10})$	17	18	19	
1	$(\frac{1}{2}, \frac{1}{2})$	21 †	22	23 †	
	$(\frac{1}{3}, \frac{2}{3})$	24 †	25	26 †	30 †
	$(\frac{1}{10}, \frac{9}{10})$	27	28	29	

The A_{nn}- and A_{ns}- best designs found for the 30 cases are listed in Appendix A3.6. For all except 3 of the 30 cases, the A_{nn}-best designs found are one of the systematic designs given in Figure 11.1, usually D_6. Also, note that the A_{nn}-best design found for case 13 is a column design. Most of the A_{ns}-best designs found have many pairs of check plots a knight's move apart. However, for Ψ_1 with $\sigma_n^2 = \frac{1}{10}$ (cases 1, 4 and 7), the A_{ns}-best designs found have many like control variety diagonal adjacencies, with like control varieties clustered together away from the top and bottom edge plots. For the non-spatial model (Ψ_4), any design with one check plot in each row and with 2 different control varieties in each column (such as D_1 to D_5) seems to be A_{ns}-optimal for $\sigma_n^2 = \frac{1}{10}, \frac{1}{2}, 1$, and A_{nn}-optimal for $\sigma_n^2 = 1$. Any design with the check plots in 2 rows and with 2 different control varieties in each column (such as D_6 to D_{13}) seems to be A_{nn}-optimal for $\sigma_n^2 = \frac{1}{10}, \frac{1}{2}$.

The A_{nn}- and A_{ns}- efficiencies of D_1 to D_{13} are given in Table 11.10 and Table 11.11, respectively. All these designs have reasonably high A_{nn}-efficiencies (greater than 0.82), but the A_{ns}-efficiencies are, in some cases, very low (less than 0.3). Similarly to model 1, D_1 to D_5 have high efficiencies over all the cases and under both criteria. The minimum, median and maximum A_{nn}-efficiencies (A_{ns}-efficiencies) for D_1 to D_5 over all 30 cases are 0.9490 (0.8529), 0.9942 (0.9761) and 1.0000 (1.0000), respectively. The row designs, D_6 to D_{13}, can have very high A_{nn}-efficiencies (median A_{nn}-efficiency of 0.9947 over all 30 cases) and very low A_{ns}-efficiencies (median A_{ns}-efficiency of 0.6527).

Table 11.10
$\{1 - (A_{nn}\text{-efficiency})\} \times 10,000$ for D_1 to D_{13} under model 2.
(lowest value in bold)
Table 11.10a $\sigma_n^2 = \frac{1}{10}$

(ρ_r, ρ_c)		$(\frac{1}{2}, \frac{1}{2})$			$(\frac{1}{3}, \frac{3}{5})$			$(\frac{1}{10}, \frac{9}{10})$			
Ψ		Ψ_1	Ψ_2	Ψ_3	Ψ_1	Ψ_2	Ψ_3	Ψ_1	Ψ_2	Ψ_3	Ψ_4
Case No.		1	2	3	4	5	6	7	8	9	10
D_1	diagonal	114	48	30	114	55	35	361	84	46	6
D_2	designs	73	36	24	94	48	32	334	80	45	6
D_3	knight's	74	39	26	91	49	33	336	82	46	6
D_4	move	79	37	25	94	49	33	331	82	46	6
D_5	designs	79	37	24	94	49	33	334	82	46	6
D_6		**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
D_7		10	2	1	6	3	2	11	9	5	**0**
D_8		69	32	16	105	44	24	351	62	29	**0**
D_9	row	87	35	18	115	50	28	368	73	34	**0**
D_{10}	designs	70	35	19	106	49	28	412	84	41	**0**
D_{11}		88	38	21	115	54	32	424	91	45	**0**
D_{12}		85	38	21	113	53	31	427	95	48	**0**
D_{13}		88	39	22	114	54	32	540	99	50	**0**
Best & near-best designs from D_1 to D_{13}		D_6 & D_7	ALL	ALL	D_6 & D_7	D_2 to D_{10}	ALL	D_6 & D_7	D_6 & D_7	ALL	ALL

Table 11.10b $\quad \sigma_n^2 = \frac{1}{2}$

(ρ_r, ρ_c)		$(\frac{1}{2}, \frac{1}{2})$			$(\frac{1}{5}, \frac{3}{5})$			$(\frac{1}{10}, \frac{9}{10})$			
Ψ		Ψ_1	Ψ_2	Ψ_3	Ψ_1	Ψ_2	Ψ_3	Ψ_1	Ψ_2	Ψ_3	Ψ_4
Case No.		11	12	13	14	15	16	17	18	19	20
D_1	diagonal	171	98	53	187	136	75	313	211	91	4
D_2	designs	40	49	30	125	105	59	249	189	83	4
D_3	knight's	69	63	38	136	114	66	283	195	86	4
D_4	move	51	55	34	126	111	64	262	196	86	4
D_5	designs	51	55	33	127	113	65	261	197	87	4
D_6		57	0	4	0	0	0	19	0	0	0
D_7		67	2	7	7	10	8	18	26	16	0
D_8		123	60	35	139	84	45	6	97	53	0
D_9	row	144	63	39	153	99	58	0	130	71	0
D_{10}	designs	131	75	45	160	110	63	254	176	94	0
D_{11}		150	77	49	171	125	74	254	200	107	0
D_{12}		143	84	53	168	131	79	525	249	132	0
D_{13}		230	122	74	275	174	104	1159	325	164	0
Best & near-best designs from D_1 to D_{13}		D_2 to D_7	D_2, D_6, D_7	D_1 to D_{12}	D_6 & D_7	D_6 & D_7	D_6 to D_8	D_6 to D_9	D_6 & D_7	D_6 & D_7	ALL

Table 11.10c $\sigma_n^2 = 1$

(ρ_r, ρ_c)		$(\frac{1}{2}, \frac{1}{2})$			$(\frac{1}{3}, \frac{2}{3})$			$(\frac{1}{10}, \frac{9}{10})$			
Ψ		Ψ_1	Ψ_2	Ψ_3	Ψ_1	Ψ_2	Ψ_3	Ψ_1	Ψ_2	Ψ_3	Ψ_4
Case No.		21	22	23	24	25	26	27	28	29	30
D_1	diagonal	221	95	39	139	151	56	510	270	72	0
D_2	designs	24	13	0	44	99	27	420	228	53	0
D_3	knight's	62	36	12	71	116	37	472	237	56	0
D_4	move	28	25	8	48	112	36	448	239	58	0
D_5	designs	28	26	8	48	113	37	440	239	58	0
D_6		187	2	30	1	0	0	462	0	0	24
D_7		185	0	33	0	11	11	434	33	21	24
D_8		213	45	48	50	53	24	51	48	33	24
D_9	row	208	41	52	49	71	42	0	89	58	24
D_{10}	designs	216	63	60	81	92	48	259	146	82	24
D_{11}		212	60	64	80	108	64	228	179	101	24
D_{12}		214	78	74	94	133	78	794	286	149	24
D_{13}		375	171	124	324	246	142	1785	455	220	24
Best & near-best designs from D_1 to D_{13}		D_2 to D_5	D_2 to D_9	D_1 to D_8	D_2, D_4 to D_9	D_6 & D_7	D_2 to D_{10}	D_8 & D_9	D_6 to D_8	D_6 to D_8	ALL

Table 11.11

$\{1-(A_{ns}\text{-efficiency})\}\times 10{,}000$ for D_1 to D_{13} under model 2

(lowest value in bold)

Table 11.11a $\quad \sigma_n^2 = \frac{1}{10}$

(ρ_r,ρ_c)		$(\frac{1}{2},\frac{1}{2})$			$(\frac{1}{3},\frac{2}{3})$			$(\frac{1}{10},\frac{9}{10})$			
Ψ		Ψ_1	Ψ_2	Ψ_3	Ψ_1	Ψ_2	Ψ_3	Ψ_1	Ψ_2	Ψ_3	Ψ_4
Case No.		1	2	3	4	5	6	7	8	9	10
D_1	diagonal	**379**	186	**235**	297	185	168	294	180	92	**0**
D_2	designs	1471	601	525	863	705	700	376	554	509	**0**
D_3	knight's	1193	508	522	751	622	676	322	563	539	**0**
D_4	move	1310	494	408	838	554	551	384	490	462	**0**
D_5	designs	1301	465	363	819	505	497	362	458	437	**0**
D_6		6606	6314	7556	3994	5131	7188	2639	5193	7430	7659
D_7		5137	4754	6258	2930	3737	5863	2189	3832	6162	6428
D_8		5711	5837	7433	2301	4595	7080	621	4842	7368	7659
D_9	row	3823	4007	6006	1029	2941	5630	241	3305	6032	6428
D_{10}	designs	5706	5797	7405	2286	4513	7044	553	4702	7333	7659
D_{11}		3812	3934	5948	1007	2823	5565	155	3145	5981	6428
D_{12}		3808	3953	5973	1003	2861	5592	**144**	3170	5985	6428
D_{13}		5461	4980	6348	2704	3624	5823	1260	3424	6041	6428

Table 11.11b $\quad \sigma_n^2 = \frac{1}{2}$

(ρ_r,ρ_c)		$(\frac{1}{2},\frac{1}{2})$			$(\frac{1}{3},\frac{2}{3})$			$(\frac{1}{10},\frac{9}{10})$			
Ψ		Ψ_1	Ψ_2	Ψ_3	Ψ_1	Ψ_2	Ψ_3	Ψ_1	Ψ_2	Ψ_3	Ψ_4
Case No.		11	12	13	14	15	16	17	18	19	20
D_1	diagonal	**314**	240	227	225	**170**	**130**	363	101	51	**0**
D_2	designs	372	226	264	259	302	349	241	231	256	**0**
D_3	knight's	327	237	305	**212**	296	368	269	256	284	**0**
D_4	move	369	185	206	252	247	285	253	217	241	**0**
D_5	designs	364	**168**	**179**	249	227	258	248	206	230	**0**
D_6		4507	4522	6067	2294	3362	5600	1885	3320	5807	6426
D_7		2980	2995	4529	1499	2198	4120	1538	2211	4339	4961
D_8		3594	4049	5913	1187	2921	5474	471	3029	5733	6426
D_9	row	1927	2401	4272	423	1668	3904	189	1860	4215	4961
D_{10}	designs	3567	3999	5876	1128	2840	5431	313	2915	5692	6426
D_{11}		1884	2328	4210	351	1570	3839	**36**	1743	4162	4961
D_{12}		1872	2349	4237	337	1593	3861	211	1757	4164	4961
D_{13}		3327	3229	4637	1421	2147	4088	1264	1956	4223	4961

Table 11.11c $\quad \sigma_n^2 = 1$

(ρ_r, ρ_c)		$(\tfrac{1}{2}, \tfrac{1}{2})$			$(\tfrac{1}{5}, \tfrac{3}{5})$			$(\tfrac{1}{10}, \tfrac{9}{10})$			
Ψ		Ψ_1	Ψ_2	Ψ_3	Ψ_1	Ψ_2	Ψ_3	Ψ_1	Ψ_2	Ψ_3	Ψ_4
Case No.		21	22	23	24	25	26	27	28	29	30
D_1	diagonal	483	277	226	305	173	121	539	83	49	0
D_2	designs	207	105	171	172	171	228	340	124	179	0
D_3	knight's	226	146	222	170	192	262	412	155	205	0
D_4	move	204	81	131	166	145	193	375	126	175	0
D_5	designs	200	69	110	164	133	174	363	118	167	0
D_6		3872	3773	5280	1911	2687	4782	1999	2667	5016	5668
D_7		2453	2360	3739	1220	1673	3342	1648	1698	3572	4165
D_8		3056	3341	5120	1005	2304	4655	594	2393	4938	5668
D_9	row	1548	1850	3496	346	1244	3147	255	1389	3456	4165
D_{10}	designs	3004	3283	5081	912	2227	4612	310	2296	4900	5668
D_{11}		1475	1775	3436	243	1156	3087	0	1292	3408	4165
D_{12}		1477	1806	3464	244	1183	3108	406	1334	3415	4165
D_{13}		2797	2606	3855	1215	1682	3329	1647	1559	3483	4165

11.2.2.1 Estimated selection probabilities

As for model 1, there is little difference in the A_{nn}-efficiencies between row like-control and row unlike-control designs, however, row like-control designs have much lower A_{ns}-efficiency. Hence, the differences in estimated selection probabilities, $\hat{\pi}_{2,10}$, for pairs of row designs were compared as in section 11.2.1.1. These 81 differences (27 cases and 3 pairs of designs) are very small for the spatial models (Ψ_1, Ψ_2 and Ψ_3). Their minimum, median and maximum are −0.0167, −0.0007 and 0.0159, respectively, and only 45 of them are less than zero. This indicates that the A_{ns}-value may not, for these designs, be well associated with the selection probabilities.

Note that for many cases the differences in the A_{nn}-efficiencies for D_{2i+4} and D_{2i+5} ($i = 1,2,3$) have opposite signs to the differences in the A_{ns}-efficiencies for these designs (cf. model 1).

Now consider the non-spatial model (Ψ_4). Here, designs D_6 to D_{13} have very low A_{ns}-efficiency (less than 0.58) but these designs have A_{nn}-efficiency equal to or very near to the A_{nn}-efficiency of the best design found. The diagonal and knight's move designs (D_1 to D_5) have A_{ns}-efficiency equal to that of the A_{ns}-best designs found. The row like-control designs have equal A_{ns}-efficiencies, as do the row unlike-control designs; the latter group being more A_{ns}-efficient than the former. If, over D_1 to D_{13}, the A_{ns}-values correlate well with the selection probabilities, $\pi_{2,10}$, then $\pi_{2,10}$ for D_1 to D_5 should be greater than $\pi_{2,10}$ for both these groups of row designs. Also, if, over D_1 to D_{13}, the A_{nn}-values correlate well with $\pi_{2,10}$ then all designs should have very similar $\pi_{2,10}$.

For Ψ_4 and a given setting of σ_n^2, let $\hat{\pi}_I$ be the average of the estimated selection probabilities for D_1 to D_5. Also, let $\hat{\pi}_{II}$ be the average of the estimated selection probabilities for D_6, D_8 and D_{10} (row like control designs), and let $\hat{\pi}_{III}$ be the average of the estimated selection probabilities for D_7, D_9, D_{11}, D_{12} and D_{13} (row unlike control designs). The differences, $\hat{\pi}_I - \hat{\pi}_{II}$ ($\hat{\pi}_I - \hat{\pi}_{III}$), are 0.005 (0.006), 0.000 (0.006) and 0.012 (0.012), for $\sigma_n^2 = \frac{1}{10}, \frac{1}{2}$ and 1, respectively. The estimated standard errors of these differences are approximately 0.003 for $\sigma_n^2 = \frac{1}{10}$, and 0.005 for $\sigma_n^2 = \frac{1}{2}$, 1. This suggests that the A_{ns}-criterion may be better for Ψ_4, but the evidence is not strong enough to not use the A_{nn}-criterion.

In section 11.2.2.2, only the A_{nn}-efficiency is considered.

11.2.2.2   An examination of the A_{nn}-efficiencies for D_1 to D_{13} under model 2

Now consider the A_{nn}-efficiencies of designs D_1 to D_{13} in more detail. For the spatial models, D_1 to D_{11} are highly efficient (A_{nn}-efficiency greater than 0.949). As for model 1, D_2 is slightly better than D_1 for all 27 cases. There is little difference between the knight's move designs, D_3 to D_5; the difference in the A_{nn}-efficiency between the best and worst knight's move designs is less than 0.0034. The best and near-best designs with respect to the A_{nn}-values are given in Table 11.10. Designs D_6 and D_7 are best or near-best for all cases expect for cases 21 and 27, which both have Ψ_1 and $\sigma_n^2 = 1$. Note that for some cases, such as Ψ_3 when $\sigma_n^2 = \frac{1}{10}$, and Ψ_4 for all 3 settings of σ_n^2, all of D_1 to D_{13} are deemed to be near-best.

In 24 of the 30 cases, the best and near-best designs from D_1 to D_{13} include those with the highest estimated $\pi_{2,10}$. For all 30 cases the best and near-best designs have at least the third highest estimated $\pi_{2,10}$. This supports the use of the A_{nn}-criterion in this section.

The robustness of the designs D_1 to D_{13} is considered as in section 11.2.1.2. For the settings $(m_1, m_2) = (0.85, 0.95)$ and $(0.9, 0.98)$ used in Table 11.8, all or nearly all the designs from D_1 to D_{13} are deemed to be robust. Higher values of (m_1, m_2) are used to obtain the robust designs listed in Table 11.12. For the spatial models, designs D_6 and D_7 are the most robust, $(m_1, m_2) = (0.95, 0.9975)$, over the categories considered.

Table 11.12

Robustness of D_1 to D_{13} (for $\sigma_\xi^2 > 0$) under model 2.

Category	Prior information on plot size ratio	$m_1 = 0.9$ $m_2 = 0.99$	$m_1 = 0.95$ $m_2 = 0.995$	$m_1 = 0.95$ $m_2 = 0.9975$
(a)	Square or near-square plots	D_1 to D_{12}	D_2 to D_8	
(b)	Long thin plots	D_2 to D_{12}	D_6 & D_7	
(c)	Very long thin plots	D_6 to D_9	D_6 & D_7	
(d)	Not very long thin plots	D_1 to D_{12}	D_2, D_4 to D_8	D_6 & D_7
(e)	Not square plots	D_2 to D_{10}	D_6 & D_7	
(f)	Little prior information on plot shape	D_1 to D_{12}	D_6 to D_8	

11.2.3 Example 11.1 under model 3

The results for model 3 (see section 9.2.1.3) are very similar to those obtained for model 2 since the best designs found are the same for 49 out of 60 combinations (30 cases and 2 criteria). For the spatial models, D_6 or one of the other systematic designs from D_1 to D_{13} is the A_{nn}-best design found for 56 of these 60 combinations.

For the non-spatial model, any design with all the check plots in one column seems to be A_{nn}-optimal for $\sigma_n^2 = \frac{1}{10}$. For $\sigma_n^2 = \frac{1}{2}$, 1, any design with one check plot in each row and with two different control varieties in each column seems to be A_{nn}-optimal.

The efficiencies of D_1 to D_{13} are similar to those for model 2. As in section 11.2.2, all these designs are A_{nn}-efficient (A_{nn}-efficiency greater than 0.82). The A_{ns}-efficiencies are lower, but not as low as for model 2 (A_{ns}-efficiency greater than 0.65). A comparison of the estimated selection probabilities, $\hat{\pi}_{2,10}$, as in section 11.2.2.1, gives similar results.

Henceforth in this section, A_{nn}-efficiencies will be considered. Note that for the spatial models, the A_{nn}-best design from D_1 to D_{13} had a slightly higher $\hat{\pi}_{2,10}$-value than the A_{ns}-best design in 24 out of 27 cases (the difference in the $\hat{\pi}_{2,10}$-values ranging from 0.003 to 0.037), providing more evidence to support the use of the A_{nn}-values here.

As noted in section 11.2.2.2, designs D_1 to D_{11} have high A_{nn}-efficiencies (greater than 0.955), D_2 is slightly better than D_1, and the knight's move designs (D_3 to D_5) have very similar efficiencies. The best and near-best designs are listed in Table 11.13. Designs D_6 and D_7 are best or near-best for most of the cases expect for cases 21 and 27 (as in section 11.2.2.2). The best and near-best designs from D_1 to D_{13} include the design with the highest estimated $\pi_{2,10}$ in 25 of the 30 cases, and at least the third highest estimated $\pi_{2,10}$ in 29 cases.

Table 11.13
Best and near-best designs from D_1 to D_{13} under model 3.
(with respect to the A_{nn}-efficiency) (case numbers in parentheses)

σ_n^2	$(\frac{1}{2}, \frac{1}{2})$			$(\frac{1}{3}, \frac{2}{3})$			$(\frac{1}{10}, \frac{9}{10})$			
	Ψ_1	Ψ_2	Ψ_3	Ψ_1	Ψ_2	Ψ_3	Ψ_1	Ψ_2	Ψ_3	Ψ_4
$\frac{1}{10}$	D_6 & D_7 (1)	ALL (2)	ALL (3)	D_6 & D_7 (4)	D_1 to D_{10} (5)	ALL (6)	D_6 & D_7 (7)	D_6 & D_7 (8)	ALL (9)	ALL (10)
$\frac{1}{2}$	D_2 to D_7 (11)	D_2, D_6, D_7 (12)	D_1 to D_{12} (13)	D_6 & D_7 (14)	D_6 & D_7 (15)	D_6 to D_8 (16)	D_6 to D_9 (17)	D_6 & D_7 (18)	D_6 & D_7 (19)	ALL (20)
1	D_2 to D_5 (21)	D_2 to D_9 (22)	D_1 to D_7 (23)	D_6 to D_8 (24)	D_6 & D_7 (25)	D_1 to D_{10} (26)	D_8 & D_9 (27)	D_6 to D_8 (28)	D_2 to D_8 (29)	ALL (30)

Using the same settings of (m_1, m_2) as in Table 11.12, the robust designs, listed in Table 11.14, are very similar to those for model 2, with D_6 and D_7 being the most robust.

Table 11.14
Robustness of D_1 to D_{13} (for $\sigma_{\xi}^2 > 0$) under model 3.

Category	Prior information on plot size ratio	$m_1 = 0.9$ $m_2 = 0.99$	$m_1 = 0.95$ $m_2 = 0.995$	$m_1 = 0.95$ $m_2 = 0.9975$
(a)	Square or near-square plots	D_1 to D_{12}	D_2 to D_7	
(b)	Long thin plots	D_2 to D_{11}	D_6 & D_7	
(c)	Very long thin plots	D_6 to D_9	D_6 & D_7	
(d)	Not very long thin plots	D_1 to D_{12}	D_2, D_4 to D_8	D_6 & D_7
(e)	Not square plots	D_2 to D_{10}	D_6 to D_8	
(f)	Little prior information on plot shape	D_1 to D_{11}	D_6 to D_8	

11.3 Systematic designs for Example 11.2

Example 11.2 is investigated in this section. This example has a 20×8 array with $c = 5$ unequally replicated control varieties, such that $\underline{r} = (6,6,6,6,2)'$. It has a larger array of plots and more control varieties than Example 11.1. The systematic designs considered here are displayed in Figure 11.2.

As for Example 11.1, some diagonal designs are considered here. The efficiency of diagonal designs is of particular interest, since designs of this type are used at NSW Agriculture. Designs D_{14} to D_{18} are diagonal designs. Of these diagonal designs, D_{14} and D_{15} have no like control variety diagonal adjacencies, whereas for D_{16} and D_{17} the number of like control variety diagonal adjacencies, for each of control varieties 1 to 4, is eight. For D_{18} each of these control varieties is in a separate diagonal so that the number of like control variety diagonal adjacencies is ten.

Figure 11.2 Some systematic designs for Example 11.2
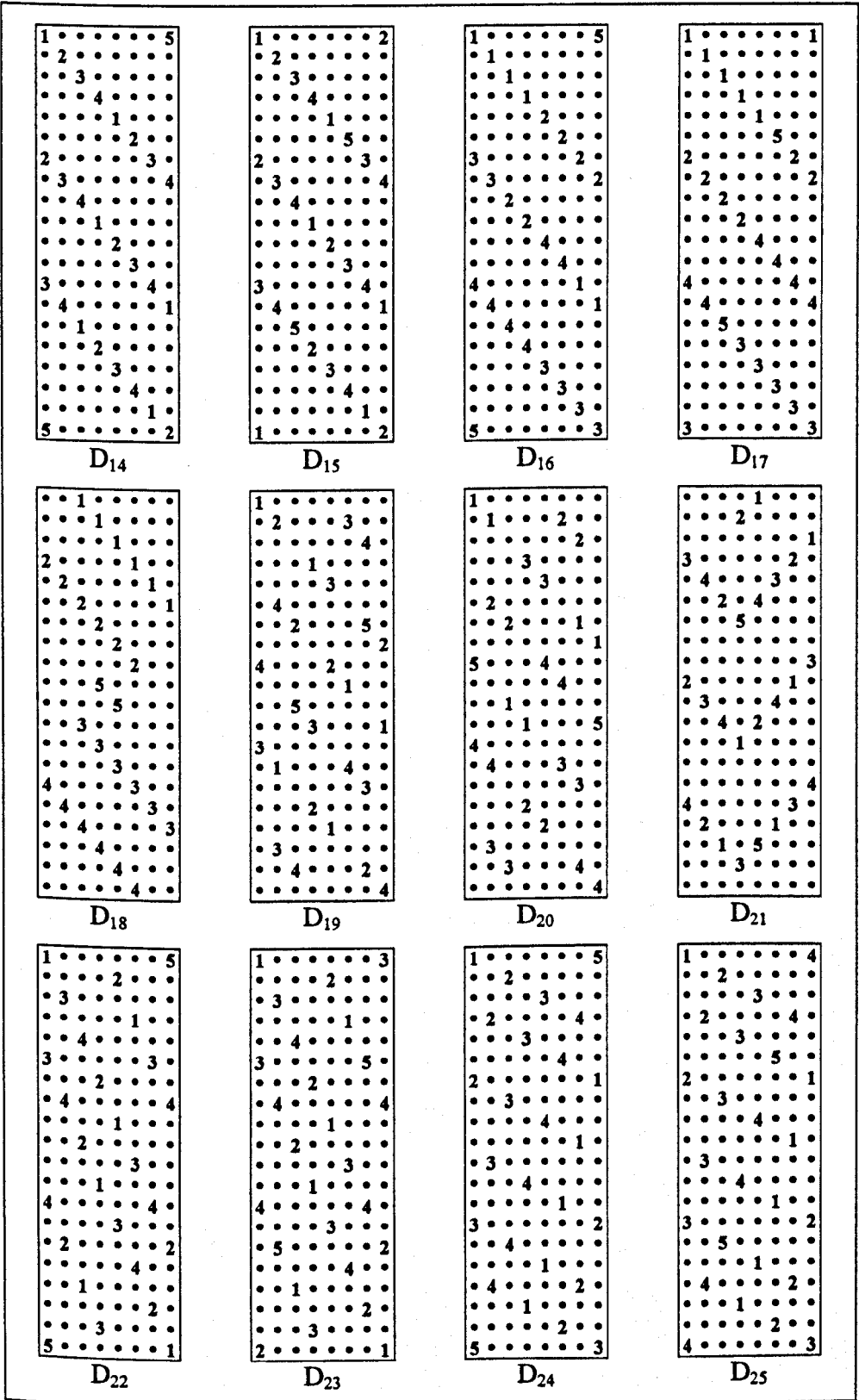
For Example 11.2 it is not possible to have row designs, such as D_1 to D_{13}, which have all the check plots in a few rows with no new varieties in these rows; although designs with 24 of the check plots in 3 rows (with no new varieties in these rows), and 2 check plots placed elsewhere, are possible. However, these designs have not been investigated here since some row designs were considered in some detail for Example 11.1. Some other types of systematic arrangements of the check plots (such as 'diagonal pair' and 'V-shape' designs) are examined here instead. Designs D_{19} and D_{20} have the control varieties in diagonal pairs, with unlike and like pairs, respectively. For D_{21} the check plots are in 'V-shapes', with no like control variety diagonal adjacencies.

Knight's move designs are also examined here, since for Example 11.1 the knight's move designs, D_3 to D_5, had high efficiencies under both criteria and over many of the cases considered. Designs D_{22} to D_{25} are knight's move designs, with the check plots at least lag (1,2) apart for D_{22} and D_{23}, and at least lag (2,1) apart for D_{24} and D_{25}.

Clearly, many more systematic designs are possible than those in Figure 11.2, but in order to avoid a large and complicated investigation only designs D_{14} to D_{25} are considered here.

It is not clear how the positions of the 2 check plots containing control variety 5 should be chosen, since it is only replicated twice (the other 4 control varieties are each replicated 6 times). As a preliminary investigation, to see if the positions of the check plots containing control variety 5 have an appreciable effect on the efficiency, these check plots are placed either on opposite corner plots of the array, or in the inner part of the array. Designs D_{14}, D_{16}, D_{22} and D_{24} have control variety 5 on opposite corner plots. For the other designs, control variety 5 is allocated to plots in the inner part of the

array. A comparison of the efficiencies for these two types of positions for control variety 5, may indicate better positions for this control variety.

Note that columns are binary for all designs except D_{15}, which has non-binary edge columns.

Finding optimal or near-optimal designs will take longer here than for Example 11.1 since the number of plots in the array and the number of check plots is over 3 and $2\frac{1}{2}$ times greater, respectively, than for Example 11.1. Hence, fewer runs are carried out in the algorithm of Martin & Eccleston (1997) than for Example 11.1. This means that the best designs found here are less likely, than in Example 11.1, to be optimal designs.

Since the results were similar for models 2 and 3 in section 11.2, only models 1 and 3 are considered here. For model 1, the 4 settings of Ψ assumed in section 11.2 are considered, and for model 3, Ψ was taken as Ψ_1, Ψ_3 and Ψ_4 with $\sigma_n^2 = \frac{1}{10}$ and 1. For both models, $(\rho_r, \rho_c) = (\frac{1}{2}, \frac{1}{2})$ and $(\frac{1}{3}, \frac{2}{3})$ are assumed. Recall that $\Psi_1 = (0, 0, 1, 0)$, $\Psi_2 = (\frac{1}{4}, \frac{1}{4}, \frac{1}{4}, \frac{1}{4})$, $\Psi_3 = (\frac{2}{10}, \frac{2}{10}, \frac{6}{10}, \frac{2}{10})$ and $\Psi_4 = (1, 1, 0, 1)$.

11.3.1 Example 11.2 under model 1

For model 1 (see section 9.2.1.1), the best designs found under the two criteria for the 7 combinations of settings of (ρ_r, ρ_c) and Ψ, are given in Appendix A3.7. These designs have similar properties to the best designs found for Example 11.1. For ease of reference, the case numbers marked by † in Table 11.1 (in section 11.2.1) are used here. Recall that for each case, $\rho_{0,1}^{(1)} / \rho_{1,0}^{(1)}$ is also given in Table 11.1.

Many of the best designs found have binary columns, except for Ψ_1 (cases 1 and 4) under both criteria, and for Ψ_4 (case 10) under the A_{nn}-criterion. The A_{nn}-best designs found for cases 2, 4 and 5, have the check plots clustered in a few rows. For these 3 cases the lag 1 within-column correlation is dominant (Martin *et al.*, 2000) with $\rho_{0,1}^{(1)}/\rho_{1,0}^{(1)}$ greater than 2. For case 5, where $\rho_{0,1}^{(1)}/\rho_{1,0}^{(1)} \approx 4.4$, only 5 of the 20 rows contain check plots in the best design found. For the cases with low $\rho_{0,1}^{(1)}/\rho_{1,0}^{(1)}$, the check plots in the best designs found tend to be at least a knight's move apart as in Example 11.1.

All the A_{ns}-best designs found for the spatial models contain the arrangement

$$\begin{bmatrix} c_1 & 5 \\ 5 & c_2 \end{bmatrix},$$

where $c_1 \neq c_2$ are two of the control varieties 1, 2, 3 or 4. Also, note that the A_{nn}-best design found for case 3 has many diagonal pair adjacencies of unlike control varieties, as in D_{19}. For the non-spatial model (Ψ_4), the column lag between check plots ranges from 1 to 15, suggesting that this is not an important factor determining efficiency (as in Example 11.1). Note also that the best designs found for Ψ_4 have some diagonal pair adjacencies of both like and unlike control varieties.

In this paragraph, comparisons are among all 12 designs D_{14} to D_{25}. Table 11.15 and Table 11.16, respectively, give the values of $\{1 - (A_{nn}\text{-efficiency})\} \times 10,000$ and $\{1 - (A_{ns}\text{-efficiency})\} \times 10,000$ for these designs. The A_{nn}- and A_{ns}-efficiencies are highly correlated (correlation coefficient greater than 0.93 for the 7 cases), with the A_{nn}-best and A_{ns}-best designs being the same design in 3 out of 7 cases. A comparison of the estimated selection probabilities, $\hat{\pi}_{7,45}$, for the 4 cases when the A_{nn}-best and A_{ns}-best designs are different, suggests that there is insufficient evidence of a

difference in $\pi_{7,45}$ between the A_{nn}-best and A_{ns}-best designs. Hence, it is assumed that both A_{nn}- and A_{ns}- values are good associated measurements of the selection probabilities, and for simplicity, the A_{nn}-efficiency is mostly considered henceforth in this section. However, if row like-control and row unlike-control designs had been considered for Example 11.2, as in Example 11.1, then an examination of the estimated $\pi_{7,45}$ for these row designs may have suggested that, for some row designs, A_{ns}- values are not well associated with $\pi_{7,45}$.

Table 11.15
$\{1 - (A_{nn}\text{-efficiency})\} \times 10,000$ for D_{14} to D_{25} under model 1.
(lowest value in bold)

(ρ_r, ρ_c)		$(\frac{1}{2}, \frac{1}{2})$			$(\frac{1}{3}, \frac{2}{3})$			
Ψ		Ψ_1	Ψ_2	Ψ_3	Ψ_1	Ψ_2	Ψ_3	Ψ_4
$\rho_{0,1}^{(1)} / \rho_{1,0}^{(1)}$		1	2.3	1	3	4.4	1.4	1
Case No.		1	2	3	4	5	6	10
D_{14}	diagonal designs	528	191	94	246	235	80	146
D_{15}		514	294	191	264	346	172	295
D_{16}		872	402	235	389	347	179	142
D_{17}		920	509	453	411	429	353	394
D_{18}		982	643	386	464	591	338	336
D_{19}	diagonal pairs	259	204	119	208	322	119	165
D_{20}		447	307	182	303	391	171	222
D_{21}	V-shapes	447	148	181	**132**	**172**	119	323
D_{22}	knight's move designs	**168**	**133**	108	216	239	104	239
D_{23}		193	210	148	242	319	151	261
D_{24}		301	186	77	256	255	**76**	**138**
D_{25}		302	230	135	274	309	127	221
Best & near-best designs from D_{14} to D_{25}		D_{22} & D_{23}	D_{21} & D_{22}	D_{14}, D_{19}, D_{22}, D_{24}	D_{21}	D_{21}	D_{14}, D_{19}, D_{21}, D_{22} D_{24}	D_{14}, D_{16}, D_{19}, D_{24}

Table 11.16

$\{1 - (A_{ns}\text{-efficiency})\} \times 10{,}000$ for D_{14} to D_{25} under model 1.
(lowest value in bold)

(ρ_r, ρ_c)		$(\tfrac{1}{2}, \tfrac{1}{2})$			$(\tfrac{1}{2}, \tfrac{3}{4})$			
	Ψ	Ψ_1	Ψ_2	Ψ_3	Ψ_1	Ψ_2	Ψ_3	Ψ_4
	$\rho_{0,1}^{(1)}/\rho_{1,0}^{(1)}$	1	2.3	1	3	4.4	1.4	1
	Case No.	1	2	3	4	5	6	10
D_{14}		884	470	**318**	593	399	**280**	188
D_{15}	diagonal designs	726	646	574	540	593	526	625
D_{16}		1509	877	592	878	597	426	178
D_{17}		1464	1054	1079	841	756	874	932
D_{18}		1804	1242	966	985	848	738	683
D_{19}	diagonal pairs	**545**	479	391	476	455	352	330
D_{20}		1033	774	600	703	633	505	493
D_{21}	V-shapes	634	**378**	421	**407**	**324**	372	488
D_{22}	knight's move designs	625	475	491	584	450	452	503
D_{23}		563	577	532	552	550	493	517
D_{24}		813	535	336	665	458	288	**137**
D_{25}		711	590	492	619	531	439	457

All the systematic designs, D_{14} to D_{25}, are reasonably A_{nn}-efficient, with A_{nn}-efficiencies in the range 0.9018 to 0.9924. The A_{ns}-efficiencies are in the range 0.8196 to 0.9863.

For each pair of designs (D_i, D_{i+1}) for $i = 14, 16, 22, 24$, the layout of the check plots is almost the same, except that D_i has control variety 5 is two opposite corner plots and D_{i+1} has control variety 5 in the inner part of the array. Over almost all the cases considered for these pairs of designs, D_i is more A_{nn}- and A_{ns}- efficient, suggesting that, generally, having control variety 5 in the corner plots is likely to give a more A_{nn}- and A_{ns}- efficient design than having control variety 5 in the inner part of the array.

For each of the pairs of designs (D_{14}, D_{16}), (D_{15}, D_{17}) and (D_{19}, D_{20}), the difference in the designs is that the first design in each pair has unlike control variety diagonal adjacencies, and the second has like control variety diagonal adjacencies. A comparison of these designs, with respect to both A_{nn}- and A_{ns}- efficiencies, suggests that, for the spatial models, like control diagonal adjacencies should be avoided. Note also that D_{18}, which has the most like control diagonal adjacencies from designs D_{14} to D_{25}, is the A_{nn}- and A_{ns}- worst from these designs in many cases.

For the spatial models, designs D_{21} (V-shapes) or D_{22} (knight's move) are the A_{nn}-best or near-best from D_{14} to D_{25} for all the cases considered here (see Table 11.15). Since the number of cases considered here is less than for Example 11.1, robustness is considered in terms of minimum A_{nn}-efficiency only. The robust designs from D_{14} to D_{25} are listed in Table 11.17 for categories (a), (b) and (d) only. For square or near-square plots (category (a)) D_{22} and D_{23} are deemed to be the most robust, and for long thin plots (category (b)) D_{14}, D_{21} and D_{22} are the most robust. D_{22} is included in the most robust designs for all 3 categories.

Table 11.17
Robustness of D_{14} to D_{25} (for $\sigma_\xi^2 > 0$) under model 1 with respect to A_{nn}-efficiency.

Category	Prior information on plot size ratio	$m_1 = 0.95$	$m_1 = 0.975$
(a)	Square or near-square plots	D_{19} to D_{25}	D_{22} & D_{23}
(b)	Long thin plots	D_{14} to D_{17}, D_{19} to D_{25}	D_{14}, D_{21} & D_{22}
(d)	Not very long thin plots	D_{19} to D_{25}	D_{22}

11.3.2 Example 11.2 under model 3

Model 3 (see section 9.2.1.3) is assumed in this section. There are 10 combinations (cases) of the settings of Ψ, (ρ_r, ρ_c) and σ_n^2 assumed for Example 11.2 under model 3. The corresponding case numbers (1, 3, 4, 6, 10, 21, 23, 24, 26 and 30) are marked by † in Table 11.9 (in section 11.2.2).

Properties of the 20 best designs found with respect to the A_{nn}- and A_{ns}-criteria (given in Appendix A3.8), are now discussed. Consider firstly the spatial models. For $\sigma_n^2 = \frac{1}{10}$ (cases 1 to 6), the A_{nn}-best designs found have the check plots on the edges of the array. For Ψ_3, $(\rho_r, \rho_c) = (\frac{1}{2}, \frac{1}{2})$ and $\sigma_n^2 = \frac{1}{10}$ (case 3), the best designs found have all the check plots in the edge columns with like control varieties clustered together. For $(\rho_r, \rho_c) = (\frac{1}{3}, \frac{2}{3})$ and $\sigma_n^2 = \frac{1}{10}$ (cases 4 and 6), the A_{nn}-best designs found have like control varieties clustered in the edge rows. When $\sigma_n^2 = 1$ (cases 21, 23, 24 and 26), the A_{nn}-best designs found have most of the check plots in the outer two or three rows and columns, with many of the check plots a knight's move apart for $(\rho_r, \rho_c) = (\frac{1}{2}, \frac{1}{2})$ (cases 21 and 23), and many unlike control variety diagonal pairs for $(\rho_r, \rho_c) = (\frac{1}{3}, \frac{2}{3})$ (cases 24 and 26).

In contrast to the A_{nn}-best designs found, the A_{ns}-best designs found avoid having check plots on the edges, suggesting that A_{ns}-efficient designs are likely to be A_{nn}-inefficient. For Ψ_3 under both settings of σ_n^2 (cases 3, 6, 23 and 26), the A_{ns}-best designs found are binary in rows and columns. Also, for $\sigma_n^2 = 1$ (cases 21, 23, 24 and 26), the A_{ns}-best designs found contain, as for model 1, the arrangement

$$\begin{vmatrix} c_1 & 5 \\ 5 & c_2 \end{vmatrix}.$$

Now consider the non-spatial model (Ψ_4). When $\sigma_n^2 = \frac{1}{10}$ (case 10), the A_{nn}-best design found has the check plots clustered in 5 rows with many like control variety row adjacent pairs. For $\sigma_n^2 = 1$ (case 30), the A_{nn}-best design found is binary in rows and columns and has many check plots a knight's move apart. Under the A_{ns}-criterion for cases 10 and 30, both rows and columns are binary, and the size of the column lag between check plots seems to be unimportant.

In this paragraph, comparisons are among designs D_{14} to D_{25}. The efficiencies of these designs (see Table 11.18 and Table 11.19) show that, as expected, the A_{ns}-best design (often D_{18}) is in many cases the A_{nn}-worst design, especially for $\sigma_n^2 = \frac{1}{10}$. However, note that all the designs are very highly A_{nn}-efficient, with A_{nn}-efficiency in the range 0.9856 to 1. Also, the relative A_{nn}-efficiencies are extremely high (greater than 0.99 for 9 of the 10 cases). For the non-spatial model (Ψ_4), D_{24} is the best design from D_{14} to D_{25} under both criteria.

As for model 1, the estimated selection probabilities for designs D_{14} to D_{25} do not provide any evidence to favour one of the two criteria. This means that either the A_{nn}- or A_{ns}- values could be used as an associated measurement of the selection probabilities. However, since the A_{nn}-efficiencies are all very similar, a detailed examination of the designs with respect to the A_{nn}-criterion, as in section 11.3.1, may not be useful here. Instead, A_{ns}-efficiencies are considered. Over D_{14} to D_{25}, the A_{ns}- efficiencies range from 0.9338 to 1.

A comparison of pairs of designs as in section 11.3.1 (but with respect to the A_{ns}-criterion here), suggests that it is better to have control variety 5 in the inner part of the array, rather than in opposite corners. Unlike control variety diagonal adjacencies are preferred in most cases when $\sigma_n^2 = 1$. For $\sigma_n^2 = \frac{1}{10}$, however, like control variety diagonal adjacencies are preferred in most cases. Also, for the cases considered here, having the check plots lag (2, 1) apart is better than having them lag (1, 2) apart.

Table 11.18
$\{1 - (A_{nn}\text{-efficiency})\} \times 10{,}000$ for D_{14} to D_{25} under model 3.
(lowest value in bold)

σ_n^2		$\frac{1}{10}$					1				
(ρ_r,ρ_c)		$(\frac{1}{2},\frac{1}{2})$		$(\frac{1}{3},\frac{2}{3})$			$(\frac{1}{2},\frac{1}{2})$		$(\frac{1}{3},\frac{2}{3})$		
Ψ		Ψ_1	Ψ_3	Ψ_1	Ψ_3	Ψ_4	Ψ_1	Ψ_3	Ψ_1	Ψ_3	Ψ_4
Case No.		1	3	4	6	10	21	23	24	26	30
D_{14}		37	40	13	12	0	15	15	**4**	**5**	1
D_{15}	diagonal designs	39	41	13	12	0	23	23	10	11	5
D_{16}	diagonal designs	49	46	14	12	0	97	55	21	15	1
D_{17}		50	46	15	13	1	106	63	36	30	17
D_{18}		66	55	19	15	0	144	84	43	28	6
D_{19}	diagonal pairs	46	47	16	14	0	25	25	13	11	2
D_{20}	diagonal pairs	55	51	17	14	0	83	54	24	18	3
D_{21}	V-shapes	49	50	16	15	0	31	29	17	16	5
D_{22}	knight's move designs	37	40	14	12	1	11	15	15	14	10
D_{23}	knight's move designs	38	40	14	12	1	20	23	15	13	7
D_{24}	knight's move designs	36	39	13	12	**0**	21	22	9	7	**0**
D_{25}		37	40	14	12	0	27	28	13	10	2

Table 11.19

$\{1 - (A_{ns}\text{-efficiency})\} \times 10,000$ for D_{14} to D_{25} under model 3.

(lowest value in bold)

σ_n^2		$\frac{1}{10}$					1				
(ρ_r, ρ_c)		$(\frac{1}{2},\frac{1}{2})$		$(\frac{1}{3},\frac{3}{5})$			$(\frac{1}{2},\frac{1}{2})$		$(\frac{1}{3},\frac{3}{5})$		
Ψ		Ψ_1	Ψ_3	Ψ_1	Ψ_3	Ψ_4	Ψ_1	Ψ_3	Ψ_1	Ψ_3	Ψ_4
Case No.		1	3	4	6	10	21	23	24	26	30
D_{14}		510	301	132	121	1	568	412	228	239	10
D_{15}	diagonal designs	433	245	127	116	12	427	285	193	214	47
D_{16}		275	182	101	70	1	662	461	266	215	11
D_{17}		189	122	116	97	77	521	335	285	261	186
D_{18}		**52**	**40**	47	**24**	2	523	329	198	**142**	36
D_{19}	diagonal pairs	388	210	102	98	1	394	260	159	180	16
D_{20}		258	127	102	79	1	546	310	245	198	23
D_{21}	V-shapes	378	195	93	89	2	**386**	**250**	**138**	174	23
D_{22}	knight's move designs	499	300	176	186	52	556	406	324	355	123
D_{23}		426	243	144	147	26	416	276	230	253	74
D_{24}		482	290	132	127	**0**	549	401	246	252	**6**
D_{25}		413	236	118	115	**0**	405	271	185	205	18
Best & near best designs from D_{14} to D_{25}		D_{18}	D_{18}	D_{18} & D_{21}	D_{16} & D_{18}	D_{14} to D_{16}; D_{18} to D_{21}; D_{23} to D_{25}	D_{15}, D_{19}, D_{21}, D_{23} & D_{25}		D_{19}, D_{21}, D_{25}	D_{18}, D_{19}, & D_{21}	D_{14} to D_{16}; D_{18} to D_{21}; D_{24} & D_{25}

Table 11.20

Robustness of D_{14} to D_{25} (for $\sigma_\xi^2 > 0$) under model 3 with respect to A_{ns}-efficiency

Category	Prior information on plot size ratio	$m_1 = m_2 = 0.95$	$m_1 = m_2 = 0.96$
(a)	Square or near-square plots	$D_{15}, D_{19}, D_{21}, D_{23}$ to D_{25}	D_{19} & D_{21}
(b)	Long thin plots	All	All
(d)	Not very long thin plots	$D_{15}, D_{19}, D_{21}, D_{23}$ to D_{25}	D_{19} & D_{21}

For model 1, D_{21} (V-shapes design) was the A_{nn}-best or near-best design from D_{14} to D_{25} for many cases. For model 3, D_{18} and D_{21} are A_{ns}-best or near best for $\sigma_n^2 = \frac{1}{10}$ and $\sigma_n^2 = 1$, respectively. Robust designs are given in Table 11.20, with respect to A_{ns}-efficiencies. The diagonal pair design D_{19} and the knight's move design D_{21} are the most robust over the categories considered.

11.4 Discussion

A discussion of the conclusions drawn from the investigations in this chapter is given here. The results for model 1 were as expected from the theoretical results derived by Martin *et al.* (2000), with the best designs found, and the efficiencies of the systematic designs that were considered, dependent on the variance components Ψ and the correlation parameters (ρ_r, ρ_c). However, for models 2 and 3, as well as the settings of Ψ and (ρ_r, ρ_c), the properties of the best designs found are also dependent on the genetic variance σ_n^2. The results for models 2 and 3 are very similar, but, unlike for model 1, it is difficult to ascertain properties of efficient designs for given Ψ, (ρ_r, ρ_c) and σ_n^2.

The results in chapter 10 suggested that the A_{nn}-values may be slightly better associated measurements of selection probabilities than the A_{ns}-values. Further evidence to support the use of A_{nn}-values is given in section 11.2 by comparing some row designs which have high A_{nn}-values and low A_{ns}-values. However, for most of the systematic designs considered here, excepting the row designs, there seems to be little difference between the A_{nn}- and A_{ns}-values as associated measurements of selection probabilities.

When the range of the efficiencies of the systematic designs considered is very small, as for the A_{nn}-efficiencies in Example 11.2 under model 3, comparisons of these systematic designs may not be useful, unless A_{nn}-values are highly correlated with selection probabilities, and the range of the selection probabilities is not small.

Although designs which have all the check plots on the edges of the array, such as D_6 and D_7, are A_{nn}-efficient for some combinations of Ψ, (ρ_r, ρ_c) and σ_n^2, practitioners are likely to be reluctant to use such designs. Instead, knight's move designs, which have the check plots spread evenly over the array may be preferable, since they generally have both high A_{nn}- and A_{ns}-efficiencies.

In practice, the parameters of the variance structure would usually be estimated from the yield (data). To estimate these parameters well, and if necessary, to assess the (variance) model adequacy, it would usually be preferable to have some check plots close together and some check plots more spread out. To take account of this, a systematic arrangement which has the check plots spread out over the array (such as a knight's move design), with some additional randomly allocated check plots, may be appropriate.

12 Summary and Conclusions

The main conclusions drawn from the results obtained are summarised here (more detailed conclusions were provided at the end of each of chapters 6, 7, 8, 10 and 11). Sections 12.1 and 12.2, consider the work on NRC and EGVT designs, respectively. Suggestions for further work are also presented.

12.1 NRC designs

Recent work on optimal and efficient NRC designs was reviewed in chapter 5. A few corrections to some of the papers considered were also given. Further results for optimal NRC designs were derived in chapters 6 to 8. These optimal NRC designs exist for certain b (number of blocks), and are universally optimal (see section 2.5.4) over all designs in $\mathcal{D}$ (where $\mathcal{D}$ is the set of all connected designs with b blocks of the required size and the required number of treatments t) under gls. Under ols, the optimal designs are universally optimal over designs in $\mathcal{D}$ which have C and var($\underline{q}$) (see section 2.4) completely symmetric, and are weakly universally optimal over designs in $\mathcal{D}$ which have C completely symmetric. These designs can be constructed using SBAs. Fairly simple dependence structures were considered and most of the optimality results obtained are for small-sized blocks.

For blocks of size 2×2 (chapter 6), under a stationary reflection symmetric process, optimal binary and non-binary designs were obtained for all four models I to IV (see chapter 4), under both ols and gls, and for $t \geq 2$. It was shown that binary designs can have very low efficiency for some correlation values.

For blocks of size 3×2 (chapter 7), under a separable process, optimality results were much more difficult to derive than for blocks of size 2×2, and hence, attention was restricted to model IV, gls and $t \geq 6$. Much more work

for blocks of size 3×2 is clearly possible, including finding optimal designs when any of models I to III, ols, or $2 \le t \le 5$ are assumed.

Results obtained for the AR(1)*AR(1) process (chapter 8) under gls and $t \ge k$, provide extensions to Uddin & Morgan (1997a). For blocks of size $p_1 \times p_2$ ($p_1, p_2 \ge 2$) the optimality region for binary designs was specified under model IV, for positive and/or negative correlation values. The results of Uddin & Morgan (1997a) for blocks of size $p_1 \times 2$ ($p_1 \ge 2$) under model IV, were extended to when only one of the two correlation values is negative. Some results under model III for blocks of size $p_1 \times 2$ ($p_1 \ge 2$) were also derived. In addition to this, non-binary designs for blocks of size 3×3 under model IV were determined, for when at least one of the correlation values is positive.

It is likely that the work on the AR(1)*AR(1) process could fairly easily be extended further by:
- specifying optimality regions of binary designs for general sized blocks ($p_1 \times p_2$, $p_1, p_2 \ge 2$) under models I, II and III and gls;
- considering the optimality of binary and non-binary blocks of size 3×3 under models I, II and III, and for $2 \le t \le 8$ under model IV;
- considering ols estimation;

The optimality results obtained for non-binary blocks of size $p_1 \times 2$ and 3×3 under model IV and the AR(1)*AR(1) process do not include the situation when both correlation values are negative. It would be interesting to find the optimal designs for this situation. Also, it would be useful to find optimal designs for other dependence structures, such as for conditional autoregressive processes (see section 2.3.3.3).

The number of blocks required for the optimal NRC designs in chapters 6 to 8 is often large and restrictive. However, the results obtained for gls will give

upper bounds on the efficiency of designs which have a smaller number of blocks. Also, these results could be used to suggest the form of optimal or near optimal designs for a smaller number of blocks, by, for example, having the C-matrix close to complete symmetry (cf. Uddin & Morgan, 1997b).

In practice, the dependence structure and its parameters are not known exactly. Therefore, as well as finding optimal designs, an investigation into their robustness would be useful.

Also, in practice, it may be easier to find robust designs, for given b, t and block-size, by using an algorithmic search over a range of correlation values suggested from prior information.

12.2 EGVT designs

Designs for EGVTs, and the spatial analysis of field experiments, were reviewed in chapter 9. Also, some methods to speed up algorithmic searches for efficient EGVT designs were presented in this chapter.

Simulation studies to see if some simple criteria are useful for comparing different designs for EGVTs, when the aim is to select the highest yielding new varieties, were carried out in chapter 10. Simulations for model 1 (see section 9.2.1) suggest that the A-, A_{nn}-, A_{ns}- and tr($C_1^{(nn)}$)- values are well associated with selection probabilities.

Further suggested work in this area includes more thorough investigations under models 2 and 3 (see section 9.2.1) of the criteria considered. Also, the usefulness of other simple criteria (such as measures of the spread of the control varieties) could be examined.

The efficiency and robustness of some systematic designs for EGVTs were investigated in chapter 11 over models 1, 2 and 3, and different variance structures. For the 2 examples considered, knight's move designs (see section 11.2) were shown to be robust. More detailed conclusions are provided in section 11.4. Although the 2 examples considered gave useful results, an examination of additional, differently constituted, examples and designs, may provide extra insight into the properties of efficient systematic designs.

Martin *et al.* (2000) derived theoretical results for EGVT designs under model 1, by considering approximations to the A_{nn}- and A_{ns}- values. It would also be very useful to derive such approximations for models 2 and 3, which would then allow properties of efficient designs under these models to be determined.

In practice, the selection of high yielding new varieties is dependent on how close the fitted dependence structure is to the true structure. Therefore, it would be useful to examine criteria for comparing designs with respect to estimating variance parameters as well as possible. Also, an examination of designs which allow variance parameters to be estimated well, would be helpful.

The investigations in chapters 10 and 11 modelled the additional spatial error to be from an AR(1)*AR(1) process. Consideration of other dependence processes would also be of interest.

Improvements in the efficacy of the algorithmic search method used in chapters 10 and 11 to find efficient designs would be advantageous. Such improvements may be obtained by having better settings for the parameters of the algorithm used, or perhaps by using other search techniques, such as genetic algorithms.

A1   Appendix 1 - Some general results

A1.1   Frequently used vectors and matrices

A list of some frequently used vectors and matrices is provided here.

$\underline{1}_n$ is an $n \times 1$ vector of ones;

$\underline{0}_n = 0 \times \underline{1}_n$ is an $n \times 1$ vector of zeros;

I_n is the $n \times n$ identity matrix;

$J_n = \underline{1}_n \underline{1}_n'$ is an $n \times n$ vector of ones;

$E_n = I_n - n^{-1} J_n$.

A1.2   Generalised Inverses
(John & Williams, 1995, Appendix A)

Let A be an $n \times n$ matrix such that $r = \text{rank}(A)$. A^- is a *generalised inverse* of A if and only if

$$AA^-A = A. \tag{A1.1}$$

A^- is not unique.

For a scalar constant $a \neq 0$,

$$(aA)^- = a^{-1}A^-. \tag{A1.2}$$

The *Moore-Penrose generalised inverse* of A, denoted by A^+ is such that

$$AA^+A = A, \quad A^+AA^+ = A^+, \quad (AA^+)' = AA^+ \quad \text{and} \quad (A^+A)' = A^+A. \tag{A1.3}$$

A^+ is unique and satisfies (A1.1).

Let λ_1, λ_2,..., λ_n be the eigenvalues of A and let $\underline{x}_1$, $\underline{x}_2$,..., $\underline{x}_n$ be the corresponding orthogonal and normalized eigenvectors of A, such that

$$\underline{x}_i'\underline{x}_j = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{if } i \neq j \end{cases}.$$

Let the $\{\lambda_i\}$ be ordered so that λ_1, $\lambda_2,\ldots$, λ_r are the non-zero eigenvalues of A. Then the *spectral decomposition* of A is given by

$$A = \sum_{i=1}^{r} \lambda_i \underline{x}_i \underline{x}_i'$$

(A1.4)

and $\quad A^{+} = \sum_{i=1}^{r} \frac{1}{\lambda_i} \underline{x}_i \underline{x}_i'.$

(A1.5)

If A is symmetric with $r = n-1$ and $A\underline{1}_n = \underline{0}_n$, then

$$\underline{1}_n' A^{+} \underline{1}_n = 0.$$

(A1.6)

If A is symmetric and idempotent (i.e. $AA = A$) then

$$A^{+} = A$$

(A1.7)

A1.3 Kronecker Products

(John & Williams, 1995, Appendix A)

Let A be an $n_1 \times n_2$ matrix with $(i,j)^{\text{th}}$ element $a_{i,j}$ and let B be an $m_1 \times m_2$ matrix. The *Kronecker product* of A and B is the $n_1 m_1 \times n_2 m_2$ matrix

$$A \otimes B = \begin{pmatrix} a_{1,1}B & a_{1,2}B & \cdots & a_{1,n_2}B \\ a_{2,1}B & a_{2,2}B & \cdots & a_{2,n_2}B \\ \vdots & \vdots & \ddots & \vdots \\ a_{n_1,1}B & a_{n_1,2}B & \cdots & a_{n_1,n_2}B \end{pmatrix}.$$

So $\quad I_n \otimes I_m = I_{nm}$

(A1.8)

and $\quad \underline{1}_n \otimes \underline{1}_m = \underline{1}_{nm}.$

(A1.9)

Also,

$$(A \otimes B)' = A' \otimes B'$$

(A1.10)

and $\quad (A \otimes B)^{-} = A^{-} \otimes B^{-}.$

(A1.11)

Then, if the matrices are conformable

$$(A \otimes B)(C \otimes D) = AC \otimes BD \qquad \text{(A1.12)}$$

$$(A + B) \otimes C = A \otimes C + B \otimes C \qquad \text{(A1.13)}$$

If A and B are square matrices then

$$\text{tr}(A \otimes B) = \text{tr}(A)\text{tr}(B) \qquad \text{(A1.14)}$$

A1.4 Toeplitz and centro-symmetric matrices (Graybill, 1983, section 8)

Let A be an $n \times n$ matrix with $(i, j)^{\text{th}}$ element $a_{i,j}$. A is a *Toeplitz* matrix (also known as a *banded* matrix) if

$$a_{i,j} = a_{i-j}, \text{say}, \quad \forall\ 2 - n \le i - j \le n - 2.$$

A is *centro-symmetric* if

$$A = H_n A H_n,$$

where H_n is an $n \times n$ symmetric matrix with ones on the NE-SW diagonal, that is,

$$(H_n)_{i,j} = \begin{cases} 1 & \text{if } i + j - 1 = n \\ 0 & \text{otherwise} \end{cases}.$$

Therefore, for a centro-symmetric matrix,

$$a_{i,j} = a_{n+1-j, n+1-i} \quad \forall\ i, j.$$

Note that a symmetric Toeplitz matrix is centro-symmetric.   (A1.15)

The following are centro-symmetric matrices:

$$I_n, J_n, E_n. \qquad \text{(A1.16)}$$

If A is centro-symmetric,

$$A' \text{ is centro-symmetric,} \qquad \text{(A1.17)}$$

and if A is also non-singular,

$$A^{-1} \text{ is centro-symmetric.} \qquad \text{(A1.18)}$$

If A and B are centro-symmetric matrices then for scalars a and b

$$aA + bB, \qquad \text{(A1.19)}$$

$$AB, \quad \text{and} \qquad \text{(A1.20)}$$

$$A \otimes B \tag{A1.21}$$

are centro-symmetric.

A1.5 Inverse of a partitioned matrix
(Graybill, 1983, section 8)

Let X be a non-singular $n \times n$ matrix partitioned as

$$X = \left(\begin{array}{c|c} A & B \\ \hline B' & C \end{array} \right),$$

where A, B and C are $n_1 \times n_1$, $n_1 \times n_2$ and $n_2 \times n_2$ matrices, such that

$n_1 + n_2 = n$.

The inverse of X is

$$X^{-1} = \left(\begin{array}{c|c} A^{-1} + A^{-1}BD^{-1}B'A^{-1} & -A^{-1}BD^{-1} \\ \hline -D^{-1}B'A^{-1} & D^{-1} \end{array} \right), \tag{A1.22}$$

where $D = C - B'A^{-1}B$.

Equivalently,

$$X^{-1} = \left(\begin{array}{c|c} E^{-1} & -E^{-1}BC^{-1} \\ \hline -C^{-1}B'E^{-1} & C^{-1} + C^{-1}B'E^{-1}BC^{-1} \end{array} \right), \tag{A1.23}$$

where $E = A - BC^{-1}B'$.

Note that, for conformable matrices A, B, C and D,

$$\left(A + BD^{-1}C \right)^{-1} = A^{-1} - A^{-1}B\left(D + CA^{-1}B \right)^{-1}CA^{-1}. \tag{A1.24}$$

A1.6 Autoregressive integrated moving-average process.

Let $\underline{\varepsilon}$ be an m-vector with elements $\{\varepsilon_j\}$. These elements $\{\varepsilon_j\}$ are from an *autoregressive moving-average process* of autoregressive order p and moving-average order q (ARMA(p,q)) if

$$\varepsilon_j = \xi_j + \sum_{h=1}^{p} \eta_h \varepsilon_{j-h} + \sum_{h=1}^{q} \varphi_h \xi_{j-h},$$

where $\{\xi_j\}$ are independent random variables with zero mean and constant variance $\forall\, j$.

Let ∇_d be the $(m-d) \times m$ d-difference matrix corresponding to an m-vector $\underline{x}$, say. For example, when $m = 4$ and $d = 1$,

$$\nabla_1 = \begin{pmatrix} 1 & -1 & 0 & 0 \\ 0 & 1 & -1 & 0 \\ 0 & 0 & 1 & -1 \end{pmatrix},$$

so that if $\underline{x}' = (x_1, x_2, x_3, x_4)$,

$$\nabla_1 \underline{x} = \begin{pmatrix} x_1 - x_2 \\ x_2 - x_3 \\ x_3 - x_4 \end{pmatrix}$$

gives the first differences of $\underline{x}$. For second differences,

$$\nabla_2 = \begin{pmatrix} 1 & -2 & 1 & 0 \\ 0 & 1 & -2 & 1 \end{pmatrix},$$

and $\nabla_2 \underline{x} = \begin{pmatrix} (x_1 - x_2) - (x_2 - x_3) \\ (x_2 - x_3) - (x_3 - x_4) \end{pmatrix} = \begin{pmatrix} x_1 - 2x_2 + x_3 \\ x_2 - 2x_3 + x_4 \end{pmatrix}.$

If the elements of $\nabla_d \underline{\varepsilon}$ are from an ARMA(p,q) process, then the elements of $\underline{\varepsilon}$ are from an *autoregressive integrated moving-average process* of autoregressive order p, moving-average order q and differencing d (ARIMA(p,d,q)).

A1.7 Balanced block designs

Shah & Sinha (1989, chapter 2) gave the definition of a *balanced block design*. For a given (t, b, k), a design is a balanced block design if:
i)   the design is binary,
ii) the design is equi-replicate, and
iii) each pair of treatments occur equally often in a block.
When $V = I_{bk}$, a balanced block design is universally optimal among all connected designs under a fixed block effect model. When $k < t$, a balanced block design is a *Balanced Incomplete Block* (BIB) design.

A1.8 Positive definite and non-negative definite matrices

An $n \times n$ matrix A is defined to be positive definite if and only if

$$A = A'$$

and $\underline{x}' A \underline{x} > 0$ for all n-vectors $\underline{x} \neq \underline{0}_n$.

An $n \times n$ matrix A is defined to be non-negative definite if and only if

$$A = A'$$

and $\underline{x}' A \underline{x} \geq 0$ for all n-vectors $\underline{x} \neq \underline{0}_n$.

If A is a $n \times n$ non-negative definite matrix then for any $n \times n$ matrix P

$P' A P$ is a non-negative definite matrix. (A1.25)

A2 Appendix 2 - Additional material to chapters 3 to 7

A2.1 Upper bound on the number of different designs for the example in section 3.3

For the illustration in section 3.3, an upper bound for the number of different complete block designs is given as

$$n^* = \binom{\frac{1}{2}(k!) + b - 2}{b - 1}.$$

Assume here that the number of different designs equals n^*. For $k = 3$ and $b = 3, 4, 5$, the n^* different designs are listed below.

For $k = 3$, there are $\frac{1}{2}(3!) = 3$ different arrangements of the treatments within a block. These are

$\boxed{1\ 2\ 3}$, $\boxed{1\ 3\ 2}$ and $\boxed{2\ 1\ 3}$.

Let the blocks having these arrangements be called A_1, A_2 and A_3, respectively. A design is given as a series of b of these arrangements. Let the first block remain unchanged over all designs, and let it be A_1, say.

When there are 3 blocks, the 6 different designs are

1) A_1, A_1, A_1;

2) A_1, A_1, A_2;

3) A_1, A_1, A_3;

4) A_1, A_2, A_2;

5) A_1, A_2, A_3;

6) A_1, A_3, A_3.

For $b = 4$, there are 10 different designs:

1) A_1, A_1, A_1, A_1;

2) A_1, A_1, A_1, A_2;

3) A_1, A_1, A_1, A_3;

4) A_1, A_1, A_2, A_2;

5) A_1, A_1, A_2, A_3;

6) A_1, A_1, A_3, A_3;

7) A_1, A_2, A_2, A_2;

8) A_1, A_2, A_2, A_3;

9) A_1, A_2, A_3, A_3;

10) A_1, A_3, A_3, A_3.

For $b = 5$, the 15 different designs are:

1) A_1, A_1, A_1, A_1, A_1;

2) A_1, A_1, A_1, A_1, A_2;

3) A_1, A_1, A_1, A_1, A_3;

4) A_1, A_1, A_1, A_2, A_2;

5) A_1, A_1, A_1, A_2, A_3;

6) A_1, A_1, A_1, A_3, A_3;

7) A_1, A_1, A_2, A_2, A_2;

8) A_1, A_1, A_2, A_2, A_3;

9) A_1, A_1, A_2, A_3, A_3;

10) A_1, A_1, A_3, A_3, A_3;

11) A_1, A_2, A_2, A_2, A_2;

12) A_1, A_2, A_2, A_2, A_3;

13) A_1, A_2, A_2, A_3, A_3;

14) A_1, A_2, A_3, A_3, A_3;

15) A_1, A_3, A_3, A_3, A_3;

A2.2 Proof for part of the optimality result in section 6.2.1

Lemma A2.1

For $i \in \{2,3,4\}$ and $\{j_1, j_2\} = \{2,3,4\} \setminus \{i\}$,

$$w_i \geq 0 \Rightarrow \begin{cases} w_i \geq w_{j_1} \\ w_i \geq w_{j_2} \end{cases},$$

where

$$w_1 = \tfrac{1}{4}\left(\lambda_2^{-1} + \lambda_3^{-1} + \lambda_4^{-1}\right), \quad w_i = \tfrac{1}{2}\lambda_i^{-1} - w_1 \quad \text{and} \quad \lambda_i > 0.$$

<u>Proof</u>

Writing w_i as

$$w_i = \tfrac{1}{4}\left(\lambda_i^{-1} - \lambda_{j_1}^{-1} - \lambda_{j_2}^{-1}\right),$$

it follows that

$$w_i \geq 0 \;\Rightarrow\; \lambda_i^{-1} \geq \lambda_{j_1}^{-1} + \lambda_{j_2}^{-1} \geq \lambda_j^{-1} \quad \text{for } j = j_1 \text{ or } j_1,$$

since $\lambda_l > 0 \;\Rightarrow\; \lambda_l^{-1} > 0 \quad \text{for } l = 2,3,4.$

Thus

$$w_i - w_j = \tfrac{1}{2}\left(\lambda_i^{-1} - \lambda_{j_1}^{-1}\right) \geq 0. \qquad \blacksquare$$

A2.3 Elements of Ω^* for the separable process in chapter 7

Expressions for the elements of Ω^* for the separable process under model IV for blocks of size 3×2 are derived in this section. Recall (from Definition 7.6 in section 7.4) that

$$\vartheta_1 = \lambda_{2,2}\lambda_{2,3} = 1 + \rho_2 - 2\rho_1^2, \quad \vartheta_2 = 3 - 4\rho_1 + \rho_2, \quad \vartheta_3 = 1 - 2\rho_1 + \rho_2,$$

$$\vartheta_4 = 1 - \rho_1, \qquad\qquad \vartheta_5 = 1 + \rho_1, \qquad\qquad \vartheta^* = 2\lambda_{1,1}\lambda_{1,2}\lambda_{2,1}\vartheta_1\vartheta_2.$$

From the matrix Λ given in Definition 7.1 (in section 7.2) it follows that

$$\Lambda^{-1} = \Lambda_2^{-1} \otimes \Lambda_1^{-1}. \tag{A2.1}$$

The inverse of Λ_1 is

$$\Lambda_1^{-1} = \frac{1}{\lambda_{1,1}\lambda_{1,2}}\begin{pmatrix} 1 & -\rho_3 \\ -\rho_3 & 1 \end{pmatrix},$$

and the inverse of Λ_2 is

$$\Lambda_2^{-1} = \frac{1}{\lambda_{2,1}\vartheta_1}\begin{pmatrix} \vartheta_4\vartheta_5 & -\rho_1\lambda_{2,1} & -\rho_2+\rho_1^2 \\ -\rho_1\lambda_{2,1} & 1+\rho_2 & -\rho_1\lambda_{2,1} \\ -\rho_2+\rho_1^2 & -\rho_1\lambda_{2,1} & \vartheta_4\vartheta_5 \end{pmatrix}.$$

From equation (A2.1) it follows that

$$\lambda_{1,1}\lambda_{1,2}\lambda_{2,1}\vartheta_1\Lambda^{-1} =$$

$$\begin{pmatrix} \vartheta_4\vartheta_5 & -\rho_3\vartheta_4\vartheta_5 & -\rho_1\lambda_{2,1} & \rho_1\rho_3\lambda_{2,1} & -\rho_2+\rho_1^2 & \rho_3(\rho_2-\rho_1^2) \\ -\rho_3\vartheta_4\vartheta_5 & \vartheta_4\vartheta_5 & \rho_1\rho_3\lambda_{2,1} & -\rho_1\lambda_{2,1} & \rho_3(\rho_2-\rho_1^2) & -\rho_2+\rho_1^2 \\ -\rho_1\lambda_{2,1} & \rho_1\rho_3\lambda_{2,1} & (1+\rho_2)\lambda_{2,1} & -\rho_3(1+\rho_2)\lambda_{2,1} & -\rho_1\lambda_{2,1} & \rho_1\rho_3\lambda_{2,1} \\ \rho_1\rho_3\lambda_{2,1} & -\rho_1\lambda_{2,1} & -\rho_3(1+\rho_2)\lambda_{2,1} & (1+\rho_2)\lambda_{2,1} & \rho_1\rho_3\lambda_{2,1} & -\rho_1\lambda_{2,1} \\ -\rho_2+\rho_1^2 & \rho_3(\rho_2-\rho_1^2) & -\rho_1\lambda_{2,1} & \rho_1\rho_3\lambda_{2,1} & \vartheta_4\vartheta_5 & -\rho_3\vartheta_4\vartheta_5 \\ \rho_3(\rho_2-\rho_1^2) & -\rho_2+\rho_1^2 & \rho_1\rho_3\lambda_{2,1} & -\rho_1\lambda_{2,1} & -\rho_3\vartheta_4\vartheta_5 & \vartheta_4\vartheta_5 \end{pmatrix}$$

$$(A2.2)$$

Now consider

$$\Lambda^{-1}\underline{1}_6\underline{1}_6'\Lambda^{-1} = \Lambda_2^{-1}\underline{1}_3\underline{1}_3'\Lambda_2^{-1} \otimes \Lambda_1^{-1}\underline{1}_2\underline{1}_2'\Lambda_1^{-1},$$

where

$$\underline{1}_2'\Lambda_1^{-1} = \lambda_{1,1}^{-1}\underline{1}_2' \tag{A2.3}$$

and

$$\underline{1}_3'\Lambda_2^{-1} = \vartheta_1^{-1}\begin{pmatrix} \vartheta_4 & \vartheta_3 & \vartheta_4 \end{pmatrix}. \tag{A2.4}$$

It follows that

$$\Lambda_1^{-1}\underline{1}_2\underline{1}_2'\Lambda_1^{-1} = \lambda_{1,1}^{-2}\underline{1}_2\underline{1}_2'$$

and

$$\Lambda_2^{-1}\mathbf{1}_3\mathbf{1}_3'\Lambda_2^{-1} = \vartheta_1^{-2}\begin{pmatrix} \vartheta_4^2 & \vartheta_3\vartheta_4 & \vartheta_4^2 \\ \vartheta_3\vartheta_4 & \vartheta_3^2 & \vartheta_3\vartheta_4 \\ \vartheta_4^2 & \vartheta_3\vartheta_4 & \vartheta_4^2 \end{pmatrix}.$$

From equations (A2.3) and (A2.4), it follows that

$$\mathbf{1}_2'\Lambda_1^{-1}\mathbf{1}_2 = 2/\lambda_{1,1}$$

and $\mathbf{1}_3'\Lambda_2^{-1}\mathbf{1}_3 = (\vartheta_3 + 2\vartheta_4)/\vartheta_1 = \vartheta_2/\vartheta_1$.

Hence,

$$\left(\mathbf{1}_6'\Lambda^{-1}\mathbf{1}_6\right)^{-1} = \left\{\left(\mathbf{1}_2'\Lambda_1^{-1}\mathbf{1}_2\right)\left(\mathbf{1}_3'\Lambda_2^{-1}\mathbf{1}_3\right)\right\}^{-1} = \tfrac{1}{2}\lambda_{1,1}\vartheta_1/\vartheta_2.$$

Therefore,

$$\left(\mathbf{1}_6'\Lambda^{-1}\mathbf{1}_6\right)^{-1}\Lambda^{-1}\mathbf{1}_6\mathbf{1}_6'\Lambda^{-1}$$

$$= \frac{1}{2\lambda_{1,1}\vartheta_1\vartheta_2}\left(\begin{array}{cc|cc|cc} \vartheta_4^2 & \vartheta_4^2 & \vartheta_3\vartheta_4 & \vartheta_3\vartheta_4 & \vartheta_4^2 & \vartheta_4^2 \\ \vartheta_4^2 & \vartheta_4^2 & \vartheta_3\vartheta_4 & \vartheta_3\vartheta_4 & \vartheta_4^2 & \vartheta_4^2 \\ \hline \vartheta_3\vartheta_4 & \vartheta_3\vartheta_4 & \vartheta_3^2 & \vartheta_3^2 & \vartheta_3\vartheta_4 & \vartheta_3\vartheta_4 \\ \vartheta_3\vartheta_4 & \vartheta_3\vartheta_4 & \vartheta_3^2 & \vartheta_3^2 & \vartheta_3\vartheta_4 & \vartheta_3\vartheta_4 \\ \hline \vartheta_4^2 & \vartheta_4^2 & \vartheta_3\vartheta_4 & \vartheta_3\vartheta_4 & \vartheta_4^2 & \vartheta_4^2 \\ \vartheta_4^2 & \vartheta_4^2 & \vartheta_3\vartheta_4 & \vartheta_3\vartheta_4 & \vartheta_4^2 & \vartheta_4^2 \end{array}\right). \quad (A2.5)$$

The elements of the matrix $\Omega^* = \Lambda^{-1} - \left(\mathbf{1}_6'\Lambda^{-1}\mathbf{1}_6\right)^{-1}\Lambda^{-1}\mathbf{1}_6\mathbf{1}_6'\Lambda^{-1}$ can now be obtained easily from the matrices given in (A2.2) and (A2.5). For example, $\left(\Omega^*\right)_{1,1} = w_{1,1}$ is

$$w_{1,1} = \frac{\vartheta_4\vartheta_5}{\lambda_{1,1}\lambda_{1,2}\lambda_{2,1}\vartheta_1} - \frac{\vartheta_4^2}{2\lambda_{1,1}\vartheta_1\vartheta_2},$$

which can be re-written, with denominator $\vartheta^* = 2\lambda_{1,1}\lambda_{1,2}\lambda_{2,1}\vartheta_1\vartheta_2$, as

$$w_{1,1} = \vartheta_4\left(2\vartheta_2\vartheta_5 - \lambda_{1,2}\lambda_{2,1}\vartheta_4\right)/\vartheta^*.$$

The other elements of Ω^* can be obtained similarly, and are listed in Definition 7.7 (in section 7.4), with common denominator ϑ^*.

A2.4 Inadmissible types from Table 7.1

It is shown in Appendix A2.4 that 54 of the 72 different types in Table 7.1 are inadmissible under reflection symmetry. Let $c_W^{(e)}$ be the value of c_W for type e. Table A2.1 lists these inadmissible types, giving for each inadmissible type e,

types e_1 and e_2;

$c_W^{(e_1)} - c_W^{(e)}$ and $c_W^{(e_2)} - c_W^{(e)}$;

and

an inequality $\mathcal{X}$

such that if $\mathcal{X}$ is true then

type e_1 is better than type e, (i.e. $c_W^{(e_1)} \geq c_W^{(e)}$),

otherwise

type e_2 is better than type e, (i.e. $c_W^{(e_2)} \geq c_W^{(e)}$).

Therefore, type e is inadmissible since either type e_1 or e_2 is always better than type e. For example, consider $e = 21$. Here $\mathcal{X}$ is the inequality $w_{1,2} \geq 0$. If $w_{1,2} \geq 0$, then type $e_1 = 5$ is better than type 21 (since $c_W^{(e_1)} - c_W^{(e)} = 2w_{1,2} \geq 0$), and if $w_{1,2} < 0$, type $e_2 = 117$ is better than type 21 (since $c_W^{(e_2)} - c_W^{(e)} = -2(w_{1,2} - w_{3,3}) \geq 0$). Therefore type 21 is inadmissible.

If $c_W^{(e_1)} - c_W^{(e)}$ is always non-negative then type e_1 is always better than type e, and so only type e_1 is then given.

Table A2.1

List of inadmissible types for blocks of size 3×2 under reflection symmetry. For each inadmissible type e,

e_1, e_2, $c_W^{(e_1)} - c_W^{(e)}$, $c_W^{(e_2)} - c_W^{(e)}$ and $\mathcal{X}$ are given.

† indicates that $c_W^{(e_1)} - c_W^{(e)} \geq 0$ is always true.

‡ indicates that $c_W^{(e_2)} - c_W^{(e)} = -\left(c_W^{(e_1)} - c_W^{(e)}\right)$

†† indicates that $c_W^{(e_1)} - c_W^{(e)} \geq 0$ is always true by Lemma 7.1

e	e_1	e_2	$c_W^{(e_1)} - c_W^{(e)}$	$c_W^{(e_2)} - c_W^{(e)}$	$\mathcal{X}$
1	2		$2w_{1,1}$		†
2	117		$2(w_{1,1} + w_{3,3})$		†
4	117		$4w_{1,1}$		†
5	86		$2w_{3,3}$		†
6	87		$2w_{1,1}$		†
7	92		$2w_{1,1}$		†
8	99		$2w_{3,3}$		†
9	103		$2w_{3,3}$		†
14	86		$-4(w_{1,3} + w_{1,4})$		††
16	34		$w_{3,3} + w_{3,4}$		††
19	103		$-4(w_{1,3} + w_{1,4})$		††
21	5	117	$2w_{1,2}$	$-2(w_{1,2} - w_{3,3})$	$w_{1,2} \geq 0$
22	6	117	$2w_{1,3}$	$2(w_{1,1} - w_{1,3})$	$w_{1,3} \geq 0$
23	7	117	$2w_{1,4}$	$2(w_{1,1} - w_{1,4})$	$w_{1,4} \geq 0$
24	8	117	$2w_{1,5}$	$-2(w_{1,5} - w_{3,3})$	$w_{1,5} \geq 0$
25	9	117	$2w_{1,6}$	$-2(w_{1,6} - w_{3,3})$	$w_{1,6} \geq 0$
30	14	92	$2(w_{1,2} + w_{1,3})$	‡	$w_{1,2} + w_{1,3} \geq 0$
31	14	87	$2(w_{1,2} + w_{1,4})$	‡	$w_{1,2} + w_{1,4} \geq 0$
32	104		$w_{3,3} + w_{3,4}$		††
33	100		$w_{3,3} + w_{3,4}$		††
34	116	13	$2w_{1,1} - w_{3,3} - w_{3,4}$	‡	$2w_{1,1} - w_{3,3} - w_{3,4} \geq 0$
35	18	87	$2(w_{1,3} + w_{1,5})$	‡	$w_{1,3} + w_{1,5} \geq 0$
36	19	92	$2(w_{1,3} + w_{1,6})$	‡	$w_{1,3} + w_{1,6} \geq 0$
37	20	92	$2(w_{1,4} + w_{1,5})$	‡	$w_{1,4} + w_{1,5} \geq 0$
38	19	87	$2(w_{1,4} + w_{1,6})$	‡	$w_{1,4} + w_{1,6} \geq 0$
39	81		$w_{3,3} + w_{3,4}$		††
50	86		$-2(w_{1,3} + w_{1,4})$		††

e	e_1	e_2	$c_W^{(e_1)}-c_W^{(e)}$	$c_W^{(e_2)}-c_W^{(e)}$	α
51	29	96	$-2(w_{1,1}+w_{1,4})$ $+w_{3,3}+w_{3,4}$	‡	$-2(w_{1,1}+w_{1,4})$ $+w_{3,3}+w_{3,4} \geq 0$
52	18	99	$4w_{1,3}$	‡	$w_{1,3} \geq 0$
53	103		$-2(w_{1,3}+w_{1,4})$		††
54	29	87	$-2(w_{1,1}+w_{1,3})$ $+w_{3,3}+w_{3,4}$	‡	$-2(w_{1,1}+w_{1,3})$ $+w_{3,3}+w_{3,4} \geq 0$
56	20	99	$4w_{1,4}$	‡	$w_{1,4} \geq 0$
64	111		$-2(w_{1,3}+w_{1,4})$		††
71	30	82	$2w_{1,4}$	‡	$w_{1,4} \geq 0$
73	117	29	$2w_{1,1}-w_{3,3}-w_{3,4}$	‡	$2w_{1,1}-w_{3,3}-w_{3,4} \geq 0$
75	116		$w_{3,3}+w_{3,4}$		††
76	52	87	$2w_{1,5}$	‡	$w_{1,5} \geq 0$
77	36	88	$2w_{1,4}$	‡	$w_{1,4} \geq 0$
78	56	92	$2w_{1,5}$	‡	$w_{1,5} \geq 0$
81	60	116	$2w_{1,2}$	‡	$w_{1,2} \geq 0$
82	61	108	$2w_{1,3}$	‡	$w_{1,3} \geq 0$
83	62	108	$2w_{1,4}$	‡	$w_{1,4} \geq 0$
88	63	112	$2w_{1,3}$	‡	$w_{1,3} \geq 0$
89	35	111	$4w_{1,3}$	$-2w_{1,3}$	$w_{1,3} \geq 0$
90	87	96	$2(w_{1,3}-w_{1,4})$	‡	$w_{1,3}-w_{1,4} \geq 0$
93	65	112	$2w_{1,4}$	‡	$w_{1,4} \geq 0$
94	37	111	$4w_{1,4}$	$-2w_{1,4}$	$w_{1,4} \geq 0$
100	67	116	$2w_{1,5}$	‡	$w_{1,5} \geq 0$
104	70	116	$2w_{1,6}$	‡	$w_{1,6} \geq 0$
108	86	117	$2w_{1,2}$	‡	$w_{1,2} \geq 0$
109	87	117	$2w_{1,3}$	‡	$w_{1,3} \geq 0$
110	92	117	$2w_{1,4}$	‡	$w_{1,4} \geq 0$
111	99	117	$2w_{1,5}$	‡	$w_{1,5} \geq 0$
112	103	117	$2w_{1,6}$	‡	$w_{1,6} \geq 0$

A2.5 Proof of Corollary 7.4

It is shown in section 7.5.1 that

$$w_{1,2} \leq 0 \quad \text{if} \quad \rho_3 \geq -\frac{x_{1,2}}{z_{1,2}}$$

and

$$w_{1,5} \leq 0 \quad \text{if} \quad \rho_3 \leq \frac{x_{1,5}}{z_{1,5}}$$

where

$$x_{1,2} = \lambda_{2,1}\vartheta_4,$$

$$z_{1,2} = 5 - \rho_1 + 3\rho_2 + \rho_1\rho_2 - 8\rho_1^2 > 0,$$

$$x_{1,5} = 1 - 2\rho_1 + 5\rho_2 - 6\rho_1\rho_2 - 5\rho_1^2 + 2\rho_2^2 - 3\rho_1^2\rho_2 + 8\rho_1^3$$

and $z_{1,5} = \lambda_{2,1}\vartheta_4^2 > 0$.

Consider when
$$w_{1,5} \leq 0 \quad \Rightarrow \quad w_{1,2} \geq 0$$

i.e. $\quad \rho_3 \leq \dfrac{x_{1,5}}{z_{1,5}} \quad \Rightarrow \quad \rho_3 \leq -\dfrac{x_{1,2}}{z_{1,2}}$

i.e. $\quad x_{1,5}z_{1,2} \leq -x_{1,2}z_{1,5}$.

It can be shown, after some algebra, that this is true when

$$\rho_2 < \upsilon,$$

where

$$\upsilon = -\frac{(1 - \rho_1 - 4\rho_1^2)}{(3 + \rho_1)}.$$

The minimum value of υ, for $|\rho_1| < 1$, is at $\rho_1 = -3 + 2\sqrt{2}$, giving

$\upsilon = 16\sqrt{2} - 23$. Therefore, when $\rho_2 < 16\sqrt{2} - 23$, $w_{1,5} \leq 0 \Rightarrow w_{1,2} \geq 0$, so type 117 cannot be optimal.

A2.6 Proof of Theorem 7.5

Theorem 7.5 is proved in this section. First consider Lemma A2.2 and Lemma A2.3.

Lemma A2.2

$$c_W^{(13)} \geq c_W^{(60)} \Rightarrow \begin{cases} w_{1,3} \leq 0 \\ w_{1,5} \geq 0 \end{cases}.$$

<u>Proof</u>

Assume here that type 13 is better than type 60, (the condition in (7.13))

i.e. $\vartheta_3 \leq 0$.

Recall from the condition in (7.7) in section 7.5.1 that $w_{1,3} \leq 0$ when

$z_{1,3} = \vartheta_3 \vartheta_4 < 0$, which is clearly true here since $\vartheta_4 > 0$.

The inequality $x_{1,5} / z_{1,5} \leq -1$ is equivalent to $2\vartheta_1 \vartheta_3 \leq 0$, and is therefore true here. Recall from the condition in (7.9) that $w_{1,5} \geq 0$ when

$$\rho_3 \geq \frac{x_{1,5}}{z_{1,5}}.$$

It therefore follows that $w_{1,5} \geq 0$ here.   ∎

Lemma A2.3

$$c_W^{(13)} \geq c_W^{(67)} \Rightarrow \begin{cases} \rho_3 < 0 \\ w_{1,2} \geq 0 \\ w_{1,4} \leq 0 \\ w_{3,4} \geq 0 \end{cases}.$$

<u>Proof</u>

Assume here that type 13 is better than type 67:

i.e. $\rho_3 \leq -\dfrac{x_{13,67}}{z_{13,67}}.$

Since $x_{13,67}$ and $z_{13,67}$ are positive, it follows that $\rho_3 < 0$.

Now consider when

$$c_W^{(13)} \geq c_W^{(67)} \Rightarrow w_{1,2} \geq 0,$$

i.e. $\rho_3 \leq -\dfrac{x_{13,67}}{z_{13,67}} \Rightarrow \rho_3 \leq -\dfrac{x_{1,2}}{z_{1,2}},$

i.e. $\dfrac{x_{13,67}}{z_{13,67}} \geq \dfrac{x_{1,2}}{z_{1,2}},$

i.e. $x_{13,67} z_{1,2} \geq x_{1,2} z_{13,67}.$ (A2.6)

After some algebra, the inequality (A2.6) simplifies to

$$\vartheta_1 \vartheta_2 \geq 0,$$

which is clearly true.

Recall from (7.8) that $w_{1,4} \leq 0$ when $x_{1,3} < 0$. Consider when

$$c_W^{(13)} \geq c_W^{(67)} \Rightarrow w_{1,4} \leq 0 \quad \text{for } x_{1,3} > 0,$$

i.e. $\rho_3 \leq -\dfrac{x_{13,67}}{z_{13,67}} \Rightarrow \rho_3 \leq \dfrac{z_{1,3}}{x_{1,3}},$

i.e. $-x_{1,3} x_{13,67} \leq z_{1,3} z_{13,67}.$ (A2.7)

After some algebra, the inequality (A2.7) simplifies to

$$\vartheta_1 \vartheta_2 \vartheta_4 \geq 0,$$

which is true.

To show that $w_{3,4} \geq 0$ here, consider when

$$c_W^{(13)} \geq c_W^{(67)} \Rightarrow w_{3,4} \geq 0,$$

i.e. $\rho_3 \leq -\dfrac{x_{13,67}}{z_{13,67}} \Rightarrow \rho_3 \leq -\dfrac{x_{3,4}}{z_{3,4}},$

i.e. $x_{13,67} z_{3,4} \geq x_{3,4} z_{13,67}.$ (A2.8)

After some algebra, the inequality (A2.8) simplifies to

$$\lambda_{2,1} \vartheta_1 \vartheta_2 \geq 0,$$

which is true.   ∎

Assume that

$$c_W^{(13)} \geq c_W^{(e_1)} \quad \text{for } e_1 \in \{20, 60, 67\}.$$

Call this assumption χ_{13}. Let $\Xi_{13} = \Xi \setminus \{13, 20, 60, 67\}$, i.e.

$\Xi_{13} = \{18, 29, 61, 62, 63, 65, 70, 86, 87, 92, 99, 103, 116, 117\}$. In order to

prove Theorem 7.5, it is sufficient to show that, under χ_{13},

$$c_W^{(13)} \geq c_W^{(e)} \quad \text{for all } e \in \Xi_{13}.$$

In terms of $\{w_{i,j}\}$, Table A2.2 and Table A2.3 give $c_W^{(13)} \geq c_W^{(e_1)}$ for $e_1 \in \{20,$

$60, 67\}$ and $c_W^{(13)} \geq c_W^{(e)}$ for $e \in \Xi_{13}$, respectively. Table A2.4 gives the

condition when

$$c_W^{(13)} \geq c_W^{(e_i)} \implies c_W^{(13)} \geq c_W^{(e_j)} \quad \text{for } i, j \in \{1, 2, 3, 4\},$$

where e_1, e_2, e_3, e_4 are such that

$$c_W^{(13)} \geq c_W^{(e_1)} \implies c_W^{(13)} \geq c_W^{(e_2)} \implies c_W^{(13)} \geq c_W^{(e_3)} \implies c_W^{(13)} \geq c_W^{(e_4)}$$

$$\text{for } e_1 \neq e_2 \neq e_3 \neq e_4$$

and $\{e_2, e_3, e_4\} \subseteq \Xi_{13} \setminus \{63, 65\}$.

By Lemma A2.2 and Lemma A2.3, all the conditions in Table A2.4 are

satisfied when $c_W^{(13)} \geq c_W^{(60)}$ and $c_W^{(13)} \geq c_W^{(67)}$. Therefore, $c_W^{(13)} \geq c_W^{(e)}$ for all

$e \in \Xi_{13} \setminus \{63, 65\}$.

It now remains to show that when $c_W^{(13)} \geq c_W^{(60)}$ and $c_W^{(13)} \geq c_W^{(67)}$,

$$c_W^{(13)} \geq c_W^{(e)} \quad \text{for all } e \in \{63, 65\}.$$

For $e \in \{63, 65\}$, $c_W^{(13)} \geq c_W^{(e)}$ involves $w_{1,6}$, which may be positive or negative.

However, the condition for

$$c_W^{(13)} \geq c_W^{(103)} \implies c_W^{(13)} \geq c_W^{(e)}$$

can be written without using $w_{1,6}$. This is given in Table A2.5. Then, it is

shown that the condition

$$c_W^{(13)} \geq c_W^{(87)} \implies (c_W^{(13)} \geq c_W^{(103)} \implies c_W^{(13)} \geq c_W^{(e)}).$$

is satisfied when $c_W^{(13)} \geq c_W^{(60)}$ and $c_W^{(13)} \geq c_W^{(67)}$. Since it has been shown in Table A2.4 that $c_W^{(13)} \geq c_W^{(87)}$ when $c_W^{(13)} \geq c_W^{(60)}$ and $c_W^{(13)} \geq c_W^{(67)}$, the proof is complete.

Table A2.2

$c_W^{(13)} \geq c_W^{(e_1)}$ for $e_1 \in \{20, 60, 67\}$.

e_1	$c_W^{(13)} \geq c_W^{(e_1)}$
20	$w_{3,3} + 2w_{3,4} \geq 2w_{1,1} + 4w_{1,4} + 2w_{1,5}$
60	$w_{3,3} + w_{3,4} \geq 2w_{1,1} + 2w_{1,2}$
67	$w_{3,3} + w_{3,4} \geq 2w_{1,1} + 2w_{1,5}$

Table A2.3

$c_W^{(13)} \geq c_W^{(e)}$ for $e \in \Xi_{13}$

e	$c_W^{(13)} \geq c_W^{(e)}$
18	$w_{3,3} + 2w_{3,4} \geq 2w_{1,1} + 4w_{1,3} + 2w_{1,5}$
29	$w_{3,4} \geq 0$
61	$w_{3,3} + 2w_{3,4} \geq 2w_{1,1} + w_{1,2} + 2w_{1,3}$
62	$w_{3,3} + 2w_{3,4} \geq 2w_{1,1} + w_{1,2} + 2w_{1,4}$
63	$w_{3,3} + 2w_{3,4} \geq 2w_{1,1} + 2w_{1,3} + w_{1,6}$
65	$w_{3,3} + 2w_{3,4} \geq 2w_{1,1} + 2w_{1,4} + w_{1,6}$
70	$w_{3,3} + w_{3,4} \geq 2w_{1,1} + 2w_{1,6}$
86	$w_{3,3} + 2w_{3,4} \geq 2w_{1,1} + 2w_{1,2}$
87	$w_{3,3} + 2w_{3,4} \geq 2w_{1,1} + 2w_{1,3}$
92	$w_{3,3} + 2w_{3,4} \geq 2w_{1,1} + 2w_{1,4}$
99	$w_{3,3} + 2w_{3,4} \geq 2w_{1,1} + 2w_{1,5}$
103	$w_{3,3} + 2w_{3,4} \geq 2w_{1,1} + 2w_{1,6}$
116	$w_{3,3} + w_{3,4} \geq 2w_{1,1}$
117	$w_{3,3} + 2w_{3,4} \geq 2w_{1,1}$

Table A2.4

The condition when $c_W^{(13)} \geq c_W^{(e_i)} \Rightarrow c_W^{(13)} \geq c_W^{(e_j)}$.

i	j	e_i	e_j	$c_W^{(13)} \geq c_W^{(e_i)} \Rightarrow c_W^{(13)} \geq c_W^{(e_j)}$ when
1	2	60	70	$\rho_3 \leq 0$
			86	$w_{3,4} \geq 0$
		67	29	$w_{3,4} \geq 0$
			99	$w_{3,4} \geq 0$
			116	$w_{1,5} \geq 0$
2	3	70	103	$w_{3,4} \geq 0$
		86	61	$w_{1,2} \geq 2w_{1,3}$
			62	$w_{1,2} \geq 2w_{1,4}$
		99	18	$w_{1,3} \leq 0$
			117	$w_{1,5} \geq 0$
3	4	117	87	$w_{1,3} \leq 0$
			92	$w_{1,4} \leq 0$

Table A2.5

The condition for when $c_W^{(13)} \geq c_W^{(87)} \Rightarrow (c_W^{(13)} \geq c_W^{(103)} \Rightarrow c_W^{(13)} \geq c_W^{(e)})$ for $e \in \{63, 65\}$

e	$c_W^{(13)} \geq c_W^{(103)} \Rightarrow c_W^{(13)} \geq c_W^{(e)}$ when	$c_W^{(13)} \geq c_W^{(87)} \Rightarrow (c_W^{(13)} \geq c_W^{(103)} \Rightarrow c_W^{(13)} \geq c_W^{(e)})$ when
63	$w_{3,3} + 2w_{3,4} \geq 2w_{1,1} + 4w_{1,3}$	$w_{1,3} \leq 0$
65	$w_{3,3} + 2w_{3,4} \geq 2w_{1,1} + 4w_{1,4}$	$w_{1,4} \leq 0$

A2.7 Proof of Theorem 7.6

A proof of Theorem 7.6 is given in this section.

Lemma A2.4

$$w_{1,3} \geq 0 \Rightarrow \begin{cases} \rho_1 < 0 \\ w_{1,4} \leq 0 \\ w_{1,2} + w_{1,6} \leq 0 \end{cases}.$$

<u>Proof</u>

Consider when

$$w_{1,3} \ge 0,$$

i.e. $2\rho_1\vartheta_2 + \lambda_{1,2}\vartheta_3\vartheta_4 \le 0$.

This inequality is equivalent to

$$(1+\rho_2)(1-\rho_3) + \rho_1(3+\rho_2)(1+\rho_3) - 2\rho_1^2(3+\rho_3) \le 0,$$

which is true when

i.e. $\rho_1 \le q_1(\rho_2,\rho_3)$ or $\rho_1 \ge q_2(\rho_2,\rho_3)$,

where

$$q_1(\rho_2,\rho_3) = \left(a_1 - \sqrt{a_2}\right)/a_3, \quad q_2(\rho_2,\rho_3) = \left(a_1 + \sqrt{a_2}\right)/a_3,$$

$$a_1 = (3+\rho_2)(1+\rho_3), \qquad a_2 = a_1^2 + 8(1+\rho_2)(1-\rho_3)(3+\rho_3)$$

and $a_3 = 4(3+\rho_3)$.

Recall that Λ is positive definite when

$$\vartheta_1 > 0,$$

i.e. $-\sqrt{a_4} < \rho_1 < \sqrt{a_4}$,

where

$$a_4 = \tfrac{1}{2}(1+\rho_2).$$

It can be shown, after some algebra, that

$$q_2(\rho_2,\rho_3) > \sqrt{a_4}$$

is equivalent to

$$a_1^2(1+\rho_2)(1-\rho_2)^2 > 0,$$

which is clearly true. Therefore, $w_{1,3} \ge 0$ when $\rho_1 \le q_1(\rho_2,\rho_3)$. However, it can be shown that the inequality

$$q_1(\rho_2,\rho_3) < 0$$

is equivalent to

$$(1+\rho_2)(1-\rho_3)(3+\rho_3) > 0,$$

which is true. Hence $w_{1,3} \geq 0 \Rightarrow \rho_1 < 0$.

Since $w_{1,3} + w_{1,4} \leq 0$ (see Lemma 7.1), clearly $w_{1,4} \leq 0$ here.

Now consider $w_{1,2} + w_{1,6} \leq 0$. From the expressions for $w_{1,2}$ and $w_{1,6}$ given in Definition 7.7, this inequality is equivalent to

$$2\rho_3(\rho_2 - \rho_1^2)\vartheta_2 - 2\rho_3\vartheta_2\vartheta_4\vartheta_5 - 2\lambda_{1,2}\lambda_{2,1}\vartheta_4^2 \leq 0,$$

i.e. $\rho_3(\vartheta_2 - \vartheta_4^2) + \vartheta_4^2 \geq 0$.

It can easily be shown that $\vartheta_2 - \vartheta_4^2 = \vartheta_1 + \vartheta_4^2$, which is positive. Hence $w_{1,2} + w_{1,6} \leq 0$ when

$$\rho_3 \geq -\frac{\vartheta_4^2}{(\vartheta_2 - \vartheta_4^2)}.$$

Now consider when

$$w_{1,3} \geq 0 \quad \Rightarrow w_{1,2} + w_{1,6} \leq 0,$$

i.e. $\rho_3 \geq \dfrac{x_{1,3}}{z_{1,3}} \Rightarrow \rho_3 \geq -\dfrac{\vartheta_4^2}{(\vartheta_2 - \vartheta_4^2)}$,

i.e. $\dfrac{x_{1,3}}{z_{1,3}} \geq -\dfrac{\vartheta_4^2}{(\vartheta_2 - \vartheta_4^2)}$,

i.e. $x_{1,3}(\vartheta_2 - \vartheta_4^2) \geq -z_{1,3}\vartheta_4^2$.

After some algebra, this simplifies to

$$\vartheta_1\vartheta_2\vartheta_5 \geq 0,$$

which is clearly true.   ∎

Lemma A2.5

$$c_W^{(18)} \geq c_W^{(87)} \Rightarrow \rho_1 + \rho_2 < 0.$$

<u>Proof</u>

From the inequality in (7.20), $c_W^{(18)} \geq c_W^{(87)}$ when

$$\rho_3 \geq \frac{x_{18,87}}{z_{18,87}},$$

where $z_{18,87} > 0$. Now consider

$$x_{18,87} / z_{18,87} < 1$$

i.e. $\quad 2(\rho_1 + \rho_2)\vartheta_2 < 0.$

Therefore $\rho_1 + \rho_2 < 0$ is needed for type 18 to be better than type 87. ∎

Assume that

$$c_W^{(18)} \geq c_W^{(e_1)} \quad \text{for } e_1 \in \{60, 61, 63, 67, 87, 99\}.$$

Call this assumption χ_{18}. For convenience, the conditions $c_W^{(18)} \geq c_W^{(e_1)}$, given in section 7.5.3, are reiterated here in Table A2.6. Let $\Xi_{18} = \Xi \setminus \{18, 60, 61, 63, 67, 87, 99\}$. To prove Theorem 7.6, it is sufficient to show that under χ_{18},

$$c_W^{(18)} \geq c_W^{(e)} \quad \text{for all } e \in \Xi_{18}.$$

Conditions for $c_W^{(18)} \geq c_W^{(e)}$, in terms of $\{w_{i,j}\}$, are given in Table A2.7. The condition $c_W^{(18)} \geq c_W^{(e)}$ is clearly satisfied for all $e \in \{13, 20, 29, 62, 65, 92, 117\}$ when $c_W^{(18)} \geq c_W^{(e_2)}$ for all $e_2 \in \Xi_{18}^{\bullet}$, where $\Xi_{18}^{\bullet} \subseteq \{60, 61, 63, 67, 87, 99\}$ is also given in Table A2.7.

Under χ_{18}, proving that $c_W^{(18)} \geq c_W^{(e)}$ for $e \in \{70, 86, 103, 116\}$ is more complicated, as shown in sections A2.7.1 to A2.7.4, for $e = 70, 86, 103$ and 116, respectively.

Table A2.6

$c_W^{(18)} \geq c_W^{(e_1)}$ for $e_1 \in \{60, 61, 63, 67, 87, 99\}$.

e_1	$c_W^{(18)} \geq c_W^{(e_1)}$
60	$4w_{1,3} + 2w_{1,5} \geq 2w_{1,2} + w_{3,4}$
61	$2w_{1,3} + 2w_{1,5} \geq w_{1,2}$
63	$2w_{1,3} + 2w_{1,5} \geq w_{1,6}$
67	$4w_{1,3} \geq w_{3,4}$
87	$w_{1,3} + w_{1,5} \geq 0$
99	$w_{1,3} \geq 0$

Table A2.7

$c_W^{(18)} \geq c_W^{(e)}$ for $e \in \Xi_{18}$

e	$c_W^{(18)} \geq c_W^{(e)}$	Ξ_{18}^*
13	$4w_{1,3} \geq 2w_{1,2} + 2w_{1,6} + w_{3,4}$ †	67, 99
20	$w_{1,3} \geq w_{1,4}$	99
29	$2w_{1,3} \geq w_{1,2} + w_{1,6}$	99
62	$4w_{1,3} + 2w_{1,5} \geq w_{1,2} + 2w_{1,4}$	61, 99
65	$4w_{1,3} + 2w_{1,5} \geq 2w_{1,4} + w_{1,6}$	63, 99
70	$4w_{1,3} + 2w_{1,5} \geq 2w_{1,6} + w_{3,4}$	87, 99 ‡
86	$2w_{1,3} + w_{1,5} \geq w_{1,2}$	60, 61, 99 ‡
92	$2w_{1,3} + w_{1,5} \geq w_{1,4}$	87, 99
103	$2w_{1,3} + w_{1,5} \geq w_{1,6}$	87, 99 ‡
116	$4w_{1,3} + 2w_{1,5} \geq w_{3,4}$	60, 87, 99 ‡
117	$2w_{1,3} + w_{1,5} \geq 0$	87, 99

† this inequality is equivalent to $2w_{1,1} + 4w_{1,3} + 2w_{1,5} \geq w_{3,3} + 2w_{3,4}$

(c.f. $c_W^{(13)} \geq c_W^{(18)}$ in Table A2.3).

‡ this is shown in sections A2.7.1 to A2.7.4.

A2.7.1 To show $c_W^{(18)} \geq c_W^{(70)}$ under χ_{18}

It is now shown that $c_W^{(18)} \geq c_W^{(70)}$ when $c_W^{(18)} \geq c_W^{(87)}$ and $c_W^{(18)} \geq c_W^{(99)}$. Firstly consider

$$c_W^{(18)} \geq c_W^{(70)}.$$

In terms of $\{w_{i,j}\}$, this inequality is given in Table A2.7. After some algebra, it can be shown to be equivalent to

$$\rho_3 \geq \frac{x_{18,70}}{z_{18,70}}, \tag{A2.9}$$

where

$$x_{18,70} = x_{18,60}$$

$$= 3 + 16\rho_1 + 11\rho_2 - 24\rho_1\rho_2 - 40\rho_1^2 + 24\rho_1^2\rho_2 + \rho_2^2 - 8\rho_1\rho_2^2 + 16\rho_1^3 + \rho_2^3$$

and $z_{18,70} = 9 - 16\rho_1 - 11\rho_2 + 24\rho_1\rho_2 + 16\rho_1^2 - 13\rho_2^2 + 8\rho_1\rho_2^2 - 16\rho_1^3 - \rho_2^3$.

It is assumed that $z_{18,70} > 0$, since $x_{18,70}/z_{18,70} < -1$ for $z_{18,70} < 0$.

Lemma A2.6

$$c_W^{(18)} \geq c_W^{(99)} \Rightarrow c_W^{(18)} \geq c_W^{(70)} \quad \text{when } \rho_2 \leq 0.$$

<u>Proof</u>

By the inequalities in (7.15) and (A2.9),

$$c_W^{(18)} \geq c_W^{(99)} \Rightarrow c_W^{(18)} \geq c_W^{(70)}$$

is equivalent to

$$\rho_3 \geq \frac{x_{1,3}}{z_{1,3}} \Rightarrow \rho_3 \geq \frac{x_{18,70}}{z_{18,70}}$$

i.e. $\quad x_{1,3}z_{18,70} \geq x_{18,70}z_{1,3}$.

In terms of $\{\rho_i\}$, this is

$$2\vartheta_1\vartheta_2(1 + 2\rho_1 - 4\rho_2 - 2\rho_1\rho_2 + 4\rho_1^2 - \rho_2^2) \geq 0$$

i.e. $\quad q_1(\rho_1) \leq \rho_2 \leq q_2(\rho_1), \tag{A2.10}$

where

$$q_1(\rho_1) = -(2 + \rho_1) - \sqrt{5 + 6\rho_1 + 5\rho_1^2}$$

and $\quad q_2(\rho_1) = -(2 + \rho_1) + \sqrt{5 + 6\rho_1 + 5\rho_1^2}$.

Clearly $q_1(\rho_1) < -1$, and it can be shown that $q_2(\rho_1) > 0$. Therefore, $\rho_2 \leq 0$ satisfies the inequality (A2.10). ∎

It is shown in Lemma A2.6 that $c_W^{(18)} \geq c_W^{(70)}$ when $c_W^{(18)} \geq c_W^{(99)}$ for $\rho_2 \leq 0$.
Hence only $\rho_2 > 0$ remains to be considered.

When $x_{18,70}/z_{18,70} \geq 1$, $c_W^{(70)} \geq c_W^{(18)}$ for $|\rho_3| < 1$. The inequality $x_{18,70}/z_{18,70} \geq 1$ is equivalent to

$$x_{18,70} \geq z_{18,70},$$

i.e. $\quad 2\vartheta_2(1 - 4\rho_1 - 4\rho_2 + 4\rho_1\rho_2 + 4\rho_1^2 - \rho_2^2) \leq 0,$

i.e. $\quad \rho_2 \leq q_3(\rho_1) \quad$ or $\quad \rho_2 \geq q_4(\rho_1),$

where

$$q_3(\rho_1) = -2(1 - \rho_1) - \sqrt{5 - 12\rho_1 + 8\rho_1^2}$$

and $\quad q_4(\rho_1) = -2(1 - \rho_1) + \sqrt{5 - 12\rho_1 + 8\rho_1^2}.$

Clearly $q_3(\rho_1) < 0$. Also, it can be shown that $q_4(\rho_1) > 0$. Therefore, for $\rho_2 > 0$, $c_W^{(70)} \geq c_W^{(18)}$ when $\rho_2 \geq q_4(\rho_1)$ (i.e. type 18 cannot be optimal when $\rho_2 \geq q_4(\rho_1)$ since type 70 is better than type 18). This means that only $0 < \rho_2 < q_4(\rho_1)$ remains to be considered; in which case, $c_W^{(18)} \geq c_W^{(70)}$ when $c_W^{(18)} \geq c_W^{(87)}$, as shown in Lemma A2.7.

Lemma A2.7
$$c_W^{(18)} \geq c_W^{(87)} \Rightarrow c_W^{(18)} \geq c_W^{(70)} \quad \text{when } 0 < \rho_2 < q_4(\rho_1).$$

<u>Proof</u>

Consider when

$$c_W^{(18)} \geq c_W^{(87)} \quad \Rightarrow c_W^{(18)} \geq c_W^{(70)}$$

i.e. $\quad \rho_3 \geq \dfrac{x_{18,87}}{z_{18,87}} \quad \Rightarrow \rho_3 \geq \dfrac{x_{18,70}}{z_{18,70}}$

i.e. $\quad x_{18,87} z_{18,70} \geq x_{18,70} z_{18,87}.$

After some algebra, this can be shown to be equivalent to

$$4\vartheta_1\vartheta_2(1 - \rho_1 - \rho_2 + \rho_1\rho_2 + 4\rho_1^2 - 4\rho_2^2) \geq 0$$

i.e. $\quad q_5(\rho_1) \le \rho_2 \le q_6(\rho_1),$ $\qquad\qquad\qquad\qquad\qquad$ (A2.11)

where $\quad q_5(\rho_1) = \tfrac{1}{8}\left\{-(1-\rho_1) - \sqrt{17 - 18\rho_1 + 65\rho_1^2}\right\}$

and $\quad q_6(\rho_1) = \tfrac{1}{8}\left\{-(1-\rho_1) + \sqrt{17 - 18\rho_1 + 65\rho_1^2}\right\}.$

Clearly $q_5(\rho_1) < 0$. It can be shown that $q_4(\rho_1) < q_6(\rho_1)$, therefore

$0 < \rho_2 < q_4(\rho_1)$ satisfies the inequality (A2.11). $\qquad\qquad\qquad\blacksquare$

A2.7.2 To show $c_W^{(18)} \ge c_W^{(86)}$ under χ_{18}

It is shown in this section that $c_W^{(18)} \ge c_W^{(86)}$ when $c_W^{(18)} \ge c_W^{(60)}$, $c_W^{(18)} \ge c_W^{(61)}$ and

$c_W^{(18)} \ge c_W^{(99)}$. Consider

$\qquad c_W^{(18)} \ge c_W^{(86)}.$

After some algebra, it can be shown that this is equivalent to

$\qquad \rho_3 \ge \dfrac{x_{18,86}}{z_{18,86}} \quad$ for $\rho_1 < 0$,

where

$\qquad x_{18,86} = 1 + 3\rho_1 + 3\rho_2 - 6\rho_1\rho_2 - 9\rho_1^2 + 5\rho_1^2\rho_2 - \rho_1\rho_2^2 + 4\rho_1^3$

and $\quad z_{18,86} = (1 - \rho_1)(4 - 3\rho_1 + \rho_2 + 3\rho_1\rho_2 - 4\rho_1^2 - \rho_2^2).$

Note that $z_{18,86} > 0$ for $\rho_1 < 0$.

Now consider the following lemmas, which show that:

- for $\rho_1 < 0$ $\qquad$ and $\rho_2 \ge q_1(\rho_1)$, $\quad c_W^{(18)} \ge c_W^{(61)} \Rightarrow c_W^{(18)} \ge c_W^{(86)}$;

- for $-\tfrac{1}{3} \le \rho_1 < 0$ and $\rho_2 \le q_1(\rho_1)$, $\quad c_W^{(18)} \ge c_W^{(99)} \Rightarrow c_W^{(18)} \ge c_W^{(86)}$;

- for $\rho_1 \le -\tfrac{1}{3}$ $\qquad$ and $\rho_2 \le q_1(\rho_1)$, $\quad c_W^{(18)} \ge c_W^{(60)} \Rightarrow c_W^{(18)} \ge c_W^{(86)}$.

This completes the proof that $c_W^{(18)} \ge c_W^{(86)}$ under χ_{18}. Note that the functions

$\{q_i\}$ considered in this section are not the same as the $\{q_i\}$ defined in section

A2.7.1.

Lemma A2.8

$$c_W^{(18)} \geq c_W^{(61)} \Rightarrow c_W^{(18)} \geq c_W^{(86)} \quad \text{when } \rho_2 \geq q_1(\rho_1) \text{ and } \rho_1 < 0,$$

where

$$q_1(\rho_1) = \tfrac{1}{4}\left\{(5+3\rho_1) - \sqrt{33 + 6\rho_1 - 23\rho_1^2}\right\}.$$

Proof

Consider when

$$c_W^{(18)} \geq c_W^{(61)} \Rightarrow c_W^{(18)} \geq c_W^{(86)}$$

i.e. $\quad \rho_3 \geq \dfrac{x_{18,61}}{z_{18,61}} \Rightarrow \rho_3 \geq \dfrac{x_{18,86}}{z_{18,86}}$

i.e. $\quad \vartheta_1 \vartheta_2 (1 - 3\rho_1 + 5\rho_2 + 3\rho_1\rho_2 - 4\rho_1^2 - 2\rho_2^2) \geq 0$

i.e. $\quad q_1(\rho_1) \leq \rho_2 \leq q_2(\rho_1),$ \hfill (A2.12)

where

$\quad q_1(\rho_1)$ is given above,

and $\quad q_2(\rho_1) = \tfrac{1}{4}\left\{(5+3\rho_1) + \sqrt{33 + 6\rho_1 - 23\rho_1^2}\right\}.$

It can be shown that $q_2(\rho_1) > 1$. Therefore the inequality (A2.12) is satisfied when $\rho_2 \geq q_1(\rho_1)$. ∎

Lemma A2.9

$$c_W^{(18)} \geq c_W^{(99)} \Rightarrow c_W^{(18)} \geq c_W^{(86)} \quad \text{when } \rho_2 \leq q_1(\rho_1) \text{ and } -\tfrac{1}{3} \leq \rho_1 < 0.$$

Proof

Consider when

$$c_W^{(18)} \geq c_W^{(99)} \Rightarrow c_W^{(18)} \geq c_W^{(86)}$$

i.e. $\quad \rho_3 \geq \dfrac{x_{1,3}}{z_{1,3}} \Rightarrow \rho_3 \geq \dfrac{x_{18,86}}{z_{18,86}}.$

After some algebra, this simplifies to

$$\rho_2 \leq 1 + 4\rho_1.$$ \hfill (A2.13)

It can be shown that $q_1(\rho_1) \leq 1 + 4\rho_1$ when $-\tfrac{1}{3} \leq \rho_1 < 0$, therefore satisfying (A2.13). ∎

Lemma A2.10

$$c_W^{(18)} \geq c_W^{(60)} \Rightarrow c_W^{(18)} \geq c_W^{(86)} \quad \text{when } \rho_2 \leq q_1(\rho_1) \text{ and } \rho_1 \leq -\tfrac{1}{3}.$$

<u>Proof</u>

Consider when

$$c_W^{(18)} \geq c_W^{(60)} \Rightarrow c_W^{(18)} \geq c_W^{(86)}$$

i.e. $\rho_3 \geq \dfrac{x_{18,60}}{z_{18,60}} \Rightarrow \rho_3 \geq \dfrac{x_{18,86}}{z_{18,86}}$

i.e. $-3 - 6\rho_2 + 8\rho_1\rho_2 + \rho_2^2 \geq 0$

i.e. $\rho_2 \leq q_3(\rho_1)$ $\hspace{5cm}$ (A2.14)

or $\rho_2 \geq q_4(\rho_1)$,

where

$$q_3(\rho_1) = (3 - 4\rho_1) - 2\sqrt{3 - 6\rho_1 + 4\rho_1^2}$$

and $q_4(\rho_1) = (3 - 4\rho_1) + 2\sqrt{3 - 6\rho_1 + 4\rho_1^2}$.

It can easily be shown that $q_4(\rho_1) > 1$. It can also be shown that

$q_1(\rho_1) < q_3(\rho_1)$ when $\rho_1 \leq -\tfrac{1}{3}$. Therefore $\rho_2 \leq q_1(\rho_1)$ satisfies the inequality

(A2.14) when $\rho_1 \leq -\tfrac{1}{3}$. $\hspace{5cm}$ ∎

A2.7.3 To show $c_W^{(18)} \geq c_W^{(103)}$ under χ_{18}

In this section it is shown that $c_W^{(18)} \geq c_W^{(103)}$ when $c_W^{(18)} \geq c_W^{(87)}$ and $c_W^{(18)} \geq c_W^{(99)}$.

First consider $c_W^{(18)} \geq c_W^{(103)}$.

This is equivalent to

$$\rho_3 \geq \frac{x_{18,103}}{z_{18,103}},$$

where

$$x_{18,103} = 1 + 3\rho_1 + 3\rho_2 - 6\rho_1\rho_2 - 9\rho_1^2 + 5\rho_1^2\rho_2 - \rho_1\rho_2^2 + 4\rho_1^3$$

and $z_{18,103} = 1 - 3\rho_1 - 3\rho_2 + 6\rho_1\rho_2 + 5\rho_1^2 - \rho_1^2\rho_2 - 2\rho_2^2 + \rho_1\rho_2^2 - 4\rho_1^3$.

It is assumed that $z_{18,103} > 0$, since $x_{18,103}/z_{18,103} < -1$ for $z_{18,103} < 0$.

Lemma A2.11

$$c_W^{(18)} \geq c_W^{(87)} \Rightarrow c_W^{(18)} \geq c_W^{(103)} \quad \text{when } \rho_1 < 0.$$

<u>Proof</u>

Consider when

$$c_W^{(18)} \geq c_W^{(87)} \Rightarrow c_W^{(18)} \geq c_W^{(103)}$$

i.e. $\quad \rho_3 \geq \dfrac{x_{18,87}}{z_{18,87}} \Rightarrow \rho_3 \geq \dfrac{x_{18,103}}{z_{18,103}}$

i.e. $\quad -2\vartheta_1\vartheta_2\vartheta_3(\rho_1 + \rho_2) \geq 0.$ $\hfill$ (A2.15)

It can easily be shown that

$$\vartheta_1 > 0 \Rightarrow \vartheta_3 > 0 \quad \text{when } \rho_1 < 0.$$

Therefore inequality (A2.15) simplifies to

$$(\rho_1 + \rho_2) \leq 0 \quad \text{for } \rho_1 < 0.$$ $\hfill$ (A2.16)

By Lemma A2.5, the inequality (A2.16) is satisfied when $c_W^{(18)} \geq c_W^{(87)}$ and

$\rho_1 < 0.$ $\hfill$ ∎

A2.7.4 To show $c_W^{(18)} \geq c_W^{(116)}$ under χ_{18}

To show that $c_W^{(18)} \geq c_W^{(116)}$ when $c_W^{(18)} \geq c_W^{(60)}$, $c_W^{(18)} \geq c_W^{(87)}$ and $c_W^{(18)} \geq c_W^{(99)}$, first

consider

$$c_W^{(18)} \geq c_W^{(116)},$$

i.e. $\quad \rho_3 \geq \dfrac{x_{18,116}}{z_{18,116}},$

where

$$x_{18,116} = 5 + 12\rho_1 + 9\rho_2 - 20\rho_1\rho_2 - 38\rho_1^2 + 22\rho_1^2\rho_2 + \rho_2^2 - 8\rho_1\rho_2^2 + 16\rho_1^3 + \rho_2^3$$

and

$$z_{18,116} = (1 - \rho_2)(11 - 20\rho_1 + 10\rho_2 - 8\rho_1\rho_2 + 6\rho_1^2 + \rho_2^2).$$

Note that $z_{18,116} > 0$ when $\rho_1 < 0$.

The following lemmas show that :

- for $\rho_2 \geq -\tfrac{1}{3}$, $\qquad\qquad\qquad c_W^{(18)} \geq c_W^{(87)} \Rightarrow c_W^{(18)} \geq c_W^{(116)}$;

- for $-\tfrac{1}{3} \leq \rho_1 < 0$ and $\rho_2 \leq -\tfrac{1}{3}$, $\quad c_W^{(18)} \geq c_W^{(99)} \Rightarrow c_W^{(18)} \geq c_W^{(116)}$;

- for $\rho_1 \leq -\tfrac{1}{3}$ $\quad$ and $\rho_2 \leq -\tfrac{1}{3}$, $\quad c_W^{(18)} \geq c_W^{(60)} \Rightarrow c_W^{(18)} \geq c_W^{(116)}$.

This completes the proof that $c_W^{(18)} \geq c_W^{(116)}$ under χ_{18}. The functions $\{q_i\}$ defined in this section are different to the $\{q_i\}$ previously defined.

Lemma A2.12
$$c_W^{(18)} \geq c_W^{(87)} \Rightarrow c_W^{(18)} \geq c_W^{(116)} \quad \text{when } \rho_2 \geq -\tfrac{1}{3}.$$

<u>Proof</u>

Consider when

$$c_W^{(18)} \geq c_W^{(87)} \Rightarrow c_W^{(18)} \geq c_W^{(116)}$$

i.e. $\quad \rho_3 \geq \dfrac{x_{18,87}}{z_{18,87}} \Rightarrow \rho_3 \geq \dfrac{x_{18,116}}{z_{18,116}}$

i.e. $\quad 4\vartheta_1\vartheta_2(1-\rho_2)(1+3\rho_2) \geq 0$

i.e. $\qquad\qquad\qquad \rho_2 \geq -\tfrac{1}{3}.$ $\qquad\qquad\qquad$ ∎

Lemma A2.13
$$c_W^{(18)} \geq c_W^{(99)} \Rightarrow c_W^{(18)} \geq c_W^{(116)} \quad \text{when } -\tfrac{1}{3} \leq \rho_1 < 0 \text{ and } \rho_2 \leq -\tfrac{1}{3}.$$

<u>Proof</u>

Consider when

$$c_W^{(18)} \geq c_W^{(99)} \Rightarrow c_W^{(18)} \geq c_W^{(116)}$$

i.e. $\quad \rho_3 \geq \dfrac{x_{1,3}}{z_{1,3}} \Rightarrow \rho_3 \geq \dfrac{x_{18,116}}{z_{18,116}}$

i.e. $\quad 2\vartheta_1\vartheta_2(1+4\rho_1-2\rho_2-2\rho_1^2-\rho_2^2) \geq 0$

i.e. $\quad q_1(\rho_2) \leq \rho_1 \leq q_2(\rho_2)$ $\qquad\qquad\qquad\qquad$ (A2.17)

where

$$q_1(\rho_2) = 1 - \tfrac{1}{2}\sqrt{2(3-2\rho_2+\rho_2^2)}$$

and $\quad q_2(\rho_2) = 1 + \tfrac{1}{2}\sqrt{2(3-2\rho_2+\rho_2^2)}.$

Clearly $q_2(\rho_2) > 1$, and it can be shown that $q_1(\rho_2) \le -\frac{1}{3}$ when $\rho_2 \le -\frac{1}{3}$.

Hence $\rho_2 \le -\frac{1}{3}$ and $-\frac{1}{3} \le \rho_1 < 0$ satisfy the inequality (A2.17). ∎

Lemma A2.14

$$c_W^{(18)} \ge c_W^{(60)} \Rightarrow c_W^{(18)} \ge c_W^{(116)} \quad \text{when } \rho_1 \le -\frac{1}{3} \text{ and } \rho_2 \le -\frac{1}{3}.$$

<u>Proof</u>

Consider when

$$c_W^{(18)} \ge c_W^{(60)} \Rightarrow c_W^{(18)} \ge c_W^{(116)}$$

i.e. $\quad \rho_3 \ge \dfrac{x_{18,60}}{z_{18,60}} \Rightarrow \rho_3 \ge \dfrac{x_{18,116}}{z_{18,116}}$

i.e. $\quad -8\vartheta_1\vartheta_2(1-\rho_1)(3+6\rho_1-6\rho_1\rho_2-4\rho_1^2+\rho_2^2) \ge 0$

i.e. $\quad \rho_1 \le q_3(\rho_2)$ $\hfill$ (A2.18)

or $\quad \rho_1 \ge q_4(\rho_2)$,

where

$$q_3(\rho_2) = \tfrac{1}{4}\Big\{3(1-\rho_2) - \sqrt{21-18\rho_2+13\rho_2^2}\Big\}$$

and $\quad q_4(\rho_2) = \tfrac{1}{4}\Big\{3(1-\rho_2) + \sqrt{21-18\rho_2+13\rho_2^2}\Big\}.$

It can be shown that $q_4(\rho_2) > 1$. Also, $q_3(\rho_2) \ge -\frac{1}{3}$ when $\rho_2 \le -\frac{1}{3}$, so $\rho_1, \rho_2 \le -\frac{1}{3}$ satisfies the inequality (A2.18). ∎

A2.8 Proof of Theorem 7.7

Assume that

$$c_W^{(20)} \ge c_W^{(e_1)} \quad \text{for } e_1 \in \{65, 67, 92, 99\}.$$

Let this assumption be called χ_{20}. Conditions for $c_W^{(20)} \ge c_W^{(e_1)}$, in terms of $\{w_{i,j}\}$, are given in Table A2.8. Let $\Xi_{20} = \Xi \setminus \{20, 65, 67, 92, 99\}$. Theorem 7.7 is proved here by showing that, under χ_{20}

$$c_W^{(20)} \ge c_W^{(e)} \quad \text{for all } e \in \Xi_{20}.$$

First consider the following lemmas.

Lemma A2.15

$$w_{1,4} \geq 0 \Rightarrow \begin{cases} \rho_1 > 0 \\ w_{1,3} \leq 0 \\ w_{1,2} + w_{1,6} \leq 0 \end{cases}.$$

Proof

By Lemma 7.1, it is clear that $w_{1,3} \leq 0$ when $w_{1,4} \geq 0$. Similarly to the proof

of Lemma A2.4 in Appendix A2.7, it can be shown that when $w_{1,4} \geq 0$, $\rho_1 > 0$

and $w_{1,2} + w_{1,6} \leq 0$. ∎

Lemma A2.16

$$c_W^{(20)} \geq c_W^{(92)} \Rightarrow w_{1,5} \geq w_{1,2} \quad \text{when } \rho_1 > 0.$$

Proof

First consider

$$w_{1,5} \geq w_{1,2}$$

i.e. $\quad \rho_3 \geq \dfrac{(\rho_2 - \rho_1^2)}{(1 - \rho_1^2)}$.

Now consider when

$$c_W^{(20)} \geq c_W^{(92)} \Rightarrow w_{1,5} \geq w_{1,2}$$

i.e. $\quad \rho_3 \geq \dfrac{x_{20,92}}{z_{20,92}} \Rightarrow \rho_3 \geq \dfrac{(\rho_2 - \rho_1^2)}{(1 - \rho_1^2)}$

i.e. $\quad \vartheta_1(2 - 5\rho_1 + \rho_2 + \rho_1^2 - 5\rho_1^2\rho_2 + \rho_2^2 + \rho_1\rho_2^2 + 4\rho_1^3) \geq 0$ (A2.19)

It can be shown that the inequality (A2.19) is true when $\rho_1 > 0$. ∎

Conditions for $c_W^{(20)} \geq c_W^{(e)}$ for $e \in \Xi_{20}$, in terms of $\{w_{i,j}\}$, are given in Table

A2.9, and are clearly satisfied under χ_{20} for

$e \in \{13, 18, 29, 60, 61, 62, 63, 86, 87, 117\}$ when $c_W^{(20)} \geq c_W^{(e_2)}$ for all $e_2 \in \Xi_{20}^*$,

where $\Xi_{20}^* \subseteq \{65, 67, 92, 99\}$.

Table A2.8

$c_W^{(20)} \geq c_W^{(e_1)}$ for $e_1 \in \{65, 67, 92, 99\}$.

e_1	$c_W^{(20)} \geq c_W^{(e_1)}$
65	$2w_{1,4} + 2w_{1,5} \geq w_{1,6}$
67	$4w_{1,4} \geq w_{3,4}$
92	$w_{1,4} + w_{1,5} \geq 0$
99	$w_{1,4} \geq 0$

Table A2.9

$c_W^{(20)} \geq c_W^{(e)}$ for $e \in \Xi_{20}$

e	$c_W^{(20)} \geq c_W^{(e)}$	$\Xi_{20}^{\bullet}$	
13	$4w_{1,4} \geq 2w_{1,2} + 2w_{1,6} + w_{3,4}$	67, 99	
18	$w_{1,4} \geq w_{1,3}$	99	
29	$2w_{1,4} \geq w_{1,2} + w_{1,6}$	99	
60	$4w_{1,4} + 2w_{1,5} \geq 2w_{1,2} + w_{3,4}$	67, 92, 99	
61	$4w_{1,4} + 2w_{1,5} \geq w_{1,2} + 2w_{1,3}$	92, 99	
62	$2w_{1,4} + 2w_{1,5} \geq w_{1,2}$	92, 99	
63	$4w_{1,4} + 2w_{1,5} \geq 2w_{1,3} + w_{1,6}$	65, 99	
70	$4w_{1,4} + 2w_{1,5} \geq 2w_{1,6} + w_{3,4}$	92, 99	‡
86	$2w_{1,4} + w_{1,5} \geq w_{1,2}$	92, 99	
87	$2w_{1,4} + w_{1,5} \geq w_{1,3}$	92, 99	
103	$2w_{1,4} + w_{1,5} \geq w_{1,6}$	92, 99	‡
116	$4w_{1,4} + 2w_{1,5} \geq w_{3,4}$	92, 99	‡
117	$2w_{1,4} + w_{1,5} \geq 0$	92, 99	

‡ this is shown in sections A2.8.1 to A2.8.3.

In sections A2.8.1 to A2.8.3, it is shown that, under χ_{20},

$$c_W^{(20)} \geq c_W^{(e)} \quad \text{for } e \in \{70, 103, 116\}.$$

Since $\rho_1 > 0$ under χ_{20} (Lemma A2.15), it is assumed henceforth in this section that $\rho_1 > 0$.

A2.8.1 To show $c_W^{(20)} \geq c_W^{(70)}$ under χ_{20}

It is shown here that $c_W^{(20)} \geq c_W^{(70)}$ when $c_W^{(20)} \geq c_W^{(92)}$ and $c_W^{(20)} \geq c_W^{(99)}$. First consider

$$c_W^{(20)} \geq c_W^{(70)}.$$

This can be written as

$$\rho_3 \geq \frac{x_{20,70}}{z_{20,70}},$$

where

$$x_{20,70} = 3 - 8\rho_1 + 11\rho_2 - 8\rho_1\rho_2 - 8\rho_1^2 - 8\rho_1^2\rho_2 + \rho_2^2 + 16\rho_1^3 + \rho_2^3$$

and $\quad z_{20,70} = 9 + 8\rho_1 - 11\rho_2 + 8\rho_1\rho_2 - 16\rho_1^2 + 32\rho_1^2\rho_2 - 13\rho_2^2 - 16\rho_1^3 - \rho_2^3.$

It is assumed that $z_{20,70} > 0$, since for $z_{20,70} < 0$, $x_{20,70}/z_{20,70} < -1$.

For $c_W^{(20)} \geq c_W^{(70)}$, $x_{20,70}/z_{20,70} < 1$ is required, since $|\rho_3| < 1$. This occurs when

$$x_{20,70} < z_{20,70}$$

i.e. $\quad 2\vartheta_2(1 + 4\rho_1 - 4\rho_2 - 4\rho_1\rho_2 + 4\rho_1^2 - \rho_2^2) > 0$

i.e. $\quad q_1(\rho_1) < \rho_2 < q_2(\rho_1)$

where

$$q_1(\rho_1) = -2(1 + \rho_1) - \sqrt{5 + 12\rho_1 + 8\rho_1^2}$$

and $\quad q_2(\rho_1) = -2(1 + \rho_1) + \sqrt{5 + 12\rho_1 + 8\rho_1^2}.$

Clearly, $q_1(\rho_1) < -1$, so $\rho_2 < q_2(\rho_1)$ is needed for type 20 to be optimal.

Lemma A2.17 and Lemma A2.18 show that for $\rho_2 < q_2(\rho_1)$, $c_W^{(20)} \geq c_W^{(70)}$ under χ_{20}.

Lemma A2.17

$$c_W^{(20)} \geq c_W^{(92)} \Rightarrow c_W^{(20)} \geq c_W^{(70)} \quad \text{when } q_3(\rho_1) \leq \rho_2 < q_2(\rho_1) \text{ and } \rho_1 > 0,$$

where

$$q_3(\rho_1) = \frac{1}{4(2+\rho_1)}\left\{-(1+\rho_1)(1-7\rho_1) - (1-\rho_1)\sqrt{17+30\rho_1+17\rho_1^2}\right\}.$$

Proof

Consider when

$$c_W^{(20)} \geq c_W^{(92)} \Rightarrow c_W^{(20)} \geq c_W^{(70)}$$

i.e. $\rho_3 \geq \dfrac{x_{20,92}}{z_{20,92}} \Rightarrow \rho_3 \geq \dfrac{x_{20,70}}{z_{20,70}}$

i.e. $4\vartheta_1\vartheta_2(1-\rho_2+6\rho_1\rho_2-3\rho_1^2+7\rho_1^2\rho_2-4\rho_2^2-2\rho_1\rho_2^2-4\rho_1^3) \geq 0$

i.e. $q_3(\rho_1) \leq \rho_2 \leq q_4(\rho_1),$ \hfill (A2.20)

where

$q_3(\rho_1)$ is given above

and $q_4(\rho_1) = \dfrac{1}{4(2+\rho_1)}\left\{-(1+\rho_1)(1-7\rho_1) + (1-\rho_1)\sqrt{17+30\rho_1+17\rho_1^2}\right\}.$

It can be shown that $q_2(\rho_1) < q_4(\rho_1)$ when $\rho_1 > 0$. Hence,

$q_3(\rho_1) \leq \rho_2 < q_2(\rho_1)$ satisfies the inequality (A2.20). ∎

Lemma A2.18

$$c_W^{(20)} \geq c_W^{(99)} \Rightarrow c_W^{(20)} \geq c_W^{(70)} \quad \text{when } \rho_2 \leq q_3(\rho_1) \text{ and } \rho_1 > 0.$$

Proof

Consider when

$$c_W^{(20)} \geq c_W^{(99)} \Rightarrow c_W^{(20)} \geq c_W^{(70)}$$

i.e. $\rho_3 \geq \dfrac{z_{1,3}}{x_{1,3}} \Rightarrow \rho_3 \geq \dfrac{x_{20,70}}{z_{20,70}}$

i.e. $2\vartheta_1\vartheta_2(1-2\rho_1-4\rho_2+2\rho_1\rho_2+4\rho_1^2-\rho_2^2) \geq 0$

i.e. $q_5(\rho_1) \leq \rho_2 \leq q_6(\rho_1),$ \hfill (A2.21)

where

$$q_5(\rho_1) = -2 + \rho_1 - \sqrt{5 - 6\rho_1 + 5\rho_1^2}$$

and $\quad q_6(\rho_1) = -2 + \rho_1 + \sqrt{5 - 6\rho_1 + 5\rho_1^2}$.

Clearly, $q_5(\rho_1) < -1$. Also, it can be shown that $q_3(\rho_1) < q_6(\rho_1)$ when $\rho_1 > 0$. Therefore $\rho_2 \le q_3(\rho_1)$ satisfies the inequality (A2.21).　∎

A2.8.2 To show $c_W^{(20)} \ge c_W^{(103)}$ under χ_{20}

It is shown in this section that $c_W^{(20)} \ge c_W^{(103)}$ under χ_{20}.

Lemma A2.19

$$c_W^{(20)} \ge c_W^{(99)} \Rightarrow c_W^{(20)} \ge c_W^{(103)} \quad \text{when } \rho_1^2 \ge \rho_2.$$

Proof

Consider when

$$c_W^{(20)} \ge c_W^{(99)} \Rightarrow c_W^{(20)} \ge c_W^{(103)}$$

i.e.　　　$w_{1,4} \ge 0 \Rightarrow 2w_{1,4} + w_{1,5} \ge w_{1,6}$

i.e.　　　　$w_{1,5} \ge w_{1,6}$

i.e.　　　　$\rho_1^2 \ge \rho_2$　　　　　　　　　　　　　　∎

Lemma A2.20

$$c_W^{(20)} \ge c_W^{(92)} \Rightarrow c_W^{(20)} \ge c_W^{(103)} \quad \text{when } 0 < \rho_2 \le \rho_1 \text{ and } \rho_3 \ge 0.$$

Proof

Consider when

$$c_W^{(20)} \ge c_W^{(92)} \Rightarrow c_W^{(20)} \ge c_W^{(103)}$$

i.e.　　　　　$w_{1,4} + w_{1,5} \ge 0 \Rightarrow 2w_{1,4} + w_{1,5} \ge w_{1,6}$

i.e.　　　　　　$w_{1,4} \ge w_{1,6}$

i.e.　$\rho_3(5 - \rho_1 + 3\rho_2 + \rho_1\rho_2 - 8\rho_1^2)(\rho_1 - \rho_2) \ge -(1 - \rho_1)(1 - \rho_2)(\rho_1 - \rho_2)$

$$(A2.22)$$

Clearly, (A2.22) is true when $\rho_1 = \rho_2$. If $\rho_1 > \rho_2$ then (A2.22) can be written as

$$\rho_3 \geq -\frac{(1-\rho_1)(1-\rho_2)}{(5-\rho_1+3\rho_2+\rho_1\rho_2-8\rho_1^2)}, \qquad (A2.23)$$

since $(5-\rho_1+3\rho_2+\rho_1\rho_2-8\rho_1^2)$ can be shown to be positive for Λ positive definite. This also means that the right-hand side of the inequality in (A2.23) is negative, so $\rho_3 \geq 0$ and $0 < \rho_2 \leq \rho_1$ satisfy the inequality (A2.22). ∎

This means that the regions $\mathcal{R}_1$ and $\mathcal{R}_2$, defined below, are not covered by Lemma A2.19 and Lemma A2.20:

$$\mathcal{R}_1 = \{(\rho_1,\rho_2,\rho_3): 0 < \rho_1 \leq \sqrt{\rho_2}, \ \rho_2 > 0 \text{ and } \rho_3 \leq 0\}$$

and $\mathcal{R}_2 = \{(\rho_1,\rho_2,\rho_3): 0 < \rho_1 < \rho_2 \text{ and } \rho_3 > 0\}$.

It is now shown that, for these two regions, $c_W^{(103)} \geq c_W^{(20)}$.

Consider

$$c_W^{(20)} \geq c_W^{(103)}.$$

This can be written as

$$\rho_3 \geq \frac{x_{20,103}}{z_{20,103}},$$

where

$$x_{20,103} = 1 - 3\rho_1 + 3\rho_2 - 2\rho_1\rho_2 - \rho_1^2 - 3\rho_1^2\rho_2 + \rho_1\rho_2^2 + 4\rho_1^3$$

and $z_{20,103} = 1 + 3\rho_1 - 3\rho_2 + 2\rho_1\rho_2 - 3\rho_1^2 + 7\rho_1^2\rho_2 - 2\rho_2^2 - \rho_1\rho_2^2 - 4\rho_1^3$.

It is assumed that $z_{20,103} > 0$, since for $z_{20,103} < 0$, $x_{20,103}/z_{20,103} < -1$.

When $x_{20,103}/z_{20,103} \geq 0$, $c_W^{(103)} \geq c_W^{(20)}$ for $\rho_3 \leq 0$. The inequality $x_{20,103}/z_{20,103} \geq 0$ simplifies to $x_{20,103} \geq 0$, and for $\rho_1 > 0$, this is equivalent to

$$\rho_2 \leq q_1(\rho_1) \quad \text{or} \quad \rho_2 \geq q_2(\rho_1), \qquad (A2.24)$$

where

$$q_1(\rho_1) = \frac{1}{(2\rho_1)}\left\{-3 + 2\rho_1 + 3\rho_1^2 - (1-\rho_1)\sqrt{(1+\rho_1)(9-7\rho_1)}\right\}$$

and

$$q_2(\rho_1) = \frac{1}{(2\rho_1)}\left\{-3 + 2\rho_1 + 3\rho_1^2 + (1-\rho_1)\sqrt{(1+\rho_1)(9-7\rho_1)}\right\}.$$

For Λ positive definite, $\rho_2 > q_1(\rho_1)$, so (A2.24) simplifies to $\rho_2 \geq q_2(\rho_1)$.

Also, it can be shown that $\rho_1^2 > q_2(\rho_1)$ when $\rho_1 > 0$. Therefore, (A2.24) is satisfied by the region $\mathcal{R}_1$.

Also, $c_W^{(103)} \geq c_W^{(20)}$ when

$$x_{20,103} / z_{20,103} > 1,$$

i.e.
$$x_{20,103} > z_{20,103}$$

i.e. $\vartheta_2(1 + \rho_1)(\rho_2 - \rho_1) > 0$

i.e.
$$\rho_1 < \rho_2.$$

This is clearly satisfied by the region $\mathcal{R}_2$.

A2.8.3 To show $c_W^{(20)} \geq c_W^{(116)}$ under χ_{20}

Now to show that $c_W^{(20)} \geq c_W^{(116)}$ under χ_{20}, first consider

$$c_W^{(20)} \geq c_W^{(116)}.$$

After some algebra, this can be written as

$$\rho_3 \geq \frac{x_{20,116}}{z_{20,116}},$$

where

$$x_{20,116} = 5 - 12\rho_1 + 9\rho_2 - 4\rho_1\rho_2 - 6\rho_1^2 - 10\rho_1^2\rho_2 + \rho_2^2 + 16\rho_1^3 + \rho_2^3$$

and $z_{20,116} = (1 - \rho_2)(11 + 4\rho_1 + 10\rho_2 - 26\rho_1^2 + \rho_2^2).$

Note that $z_{20,116} > 0$ is assumed, since for $z_{20,116} < 0$, $x_{20,116} / z_{20,116} < -1$.

By Lemma A2.21 and Lemma A2.22, $c_W^{(20)} \geq c_W^{(116)}$ when $c_W^{(20)} \geq c_W^{(92)}$ and $c_W^{(20)} \geq c_W^{(99)}$.

Lemma A2.21

$$c_W^{(20)} \geq c_W^{(92)} \Rightarrow c_W^{(20)} \geq c_W^{(116)} \quad \text{when } \rho_2 \geq q_1(\rho_1),$$

where

$$q_1(\rho_1) = -\frac{(1-\rho_1-4\rho_1^2)}{(3+\rho_1)}.$$

<u>Proof</u>

Consider when

$$c_W^{(20)} \geq c_W^{(92)} \Rightarrow c_W^{(20)} \geq c_W^{(116)}$$

i.e. $\quad \rho_3 \geq \dfrac{x_{20,92}}{z_{20,92}} \Rightarrow \rho_3 \geq \dfrac{x_{20,116}}{z_{20,116}}$

i.e. $\quad 4\vartheta_1\vartheta_2(1-\rho_2)(1-\rho_1+3\rho_2+\rho_1\rho_2-4\rho_1^2) \geq 0$

i.e. $\qquad\qquad\qquad\qquad\qquad \rho_2 \geq q_1(\rho_1) \qquad\qquad\qquad\qquad \blacksquare$

Lemma A2.22

$$c_W^{(20)} \geq c_W^{(99)} \Rightarrow c_W^{(20)} \geq c_W^{(116)} \quad \text{when } \rho_2 \leq q_1(\rho_1).$$

<u>Proof</u>

Consider when

$$c_W^{(20)} \geq c_W^{(99)} \Rightarrow c_W^{(20)} \geq c_W^{(116)}$$

i.e. $\quad \rho_3 \geq \dfrac{z_{1,3}}{x_{1,3}} \Rightarrow \rho_3 \geq \dfrac{x_{20,116}}{z_{20,116}}$

i.e. $\quad 2\vartheta_1\vartheta_2(1-4\rho_1-2\rho_2+6\rho_1^2-\rho_2^2) \geq 0$

i.e. $\quad q_2(\rho_1) \leq \rho_2 \leq q_3(\rho_1),$ $\qquad\qquad\qquad\qquad\qquad$ (A2.25)

where

$$q_2(\rho_1) = -1 - \sqrt{2(1-2\rho_1+3\rho_1^2)}$$

and $\quad q_3(\rho_1) = -1 + \sqrt{2(1-2\rho_1+3\rho_1^2)}.$

Clearly, $q_2(\rho_1) < -1$. Also, it can be shown that $q_1(\rho_1) < q_3(\rho_1)$, so $\rho_2 \leq q_1(\rho_1)$ satisfies (A2.25). ∎

A2.9 Proof of Theorem 7.8

Let the assumption that

$$c_W^{(60)} \geq c_W^{(e_1)} \quad \text{for } e_1 \in \{13, 67, 86, 116\}.$$

be called χ_{60}. Let $\Xi_{60} = \Xi \setminus \{13, 60, 67, 86, 116\}$. In order to prove Theorem 7.8, it is shown that, under χ_{60}

$$c_W^{(60)} \geq c_W^{(e)} \quad \text{for all } e \in \Xi_{60}.$$

Conditions for $c_W^{(60)} \geq c_W^{(e_1)}$ and $c_W^{(60)} \geq c_W^{(e)}$ for $e \in \Xi_{60}$ are given in Table A2.10 and Table A2.11, respectively. For $e \in \{29, 99, 117\}$, $c_W^{(60)} \geq c_W^{(e)}$ is clearly satisfied for all $e_2 \in \Xi_{60}^*$, where $\Xi_{60}^* \subseteq \{13, 67, 86, 116\}$. For $e \in \{18, 20, 61, 62, 63, 65, 70, 87, 82, 103\}$, it is shown below that under χ_{60}, $c_W^{(60)} \geq c_W^{(e)}$.

Table A2.10
$c_W^{(60)} \geq c_W^{(e_1)}$ for $e_1 \in \{13, 67, 86, 116\}$.

e_1	$c_W^{(60)} \geq c_W^{(e_1)}$	
13	$2w_{1,1} + 2w_{1,2} \geq w_{3,3} + w_{3,4}$	†
67	$w_{1,2} \geq w_{1,5}$	
86	$w_{3,4} \geq 0$	
116	$w_{1,2} \geq 0$	

† this inequality is equivalent to $w_{1,5} + w_{1,6} \leq 0$, since row/column sums of W are zero

Table A2.11

$c_W^{(60)} \geq c_W^{(e)}$ for $e \in \Xi_{60}$

e	$c_W^{(60)} \geq c_W^{(e)}$	Ξ_{60}^*	
18	$2w_{1,2} + w_{3,4} \geq 4w_{1,3} + 2w_{1,5}$	67, 86	↕
20	$2w_{1,2} + w_{3,4} \geq 4w_{1,4} + 2w_{1,5}$	67, 86	↕
29	$w_{3,4} \geq 2w_{1,5} + 2w_{1,6}$	13, 86	
61	$w_{1,2} + w_{3,4} \geq 2w_{1,3}$	86, 116	↕
62	$w_{1,2} + w_{3,4} \geq 2w_{1,4}$	86, 116	↕
63	$2w_{1,2} + w_{3,4} \geq 2w_{1,3} + w_{1,6}$	86, 116	↕
65	$2w_{1,2} + w_{3,4} \geq 2w_{1,4} + w_{1,6}$	86, 116	↕
70	$w_{1,2} \geq w_{1,6}$	116	↕
87	$2w_{1,2} + w_{3,4} \geq 2w_{1,3}$	86, 116	↕
92	$2w_{1,2} + w_{3,4} \geq 2w_{1,4}$	86, 116	↕
99	$2w_{1,2} + w_{3,4} \geq 2w_{1,5}$	67, 86	
103	$2w_{1,2} + w_{3,4} \geq 2w_{1,6}$	86, 116	↕
117	$2w_{1,2} + w_{3,4} \geq 0$	86, 116	

↕ this is shown below.

Now consider the following lemmas, which show that, under χ_{60},

$$c_W^{(60)} \geq c_W^{(e)} \text{ for } e \in \{18, 20, 61, 62, 70\}.$$

Lemma A2.23

$$c_W^{(60)} \geq c_W^{(116)} \Rightarrow c_W^{(60)} \geq c_W^{(70)}.$$

<u>Proof</u>

Consider

$$c_W^{(60)} \geq c_W^{(70)},$$

i.e. $w_{1,2} \geq w_{1,6}$

i.e. $-\rho_3 \vartheta_4 \vartheta_5 \geq \rho_3(\rho_2 - \rho_1^2)$

i.e. $\rho_3 \leq 0.$

Recall that for $c_W^{(60)} \geq c_W^{(116)}$, $\rho_3 \leq -x_{1,2}/z_{1,2}$ is needed. Since $x_{1,2}, z_{1,2} > 0$, it follows that, $-x_{1,2}/z_{1,2} < 0$, which completes the proof. ∎

Lemma A2.24

$$\{\, c_W^{(60)} \geq c_W^{(67)} \text{ and } c_W^{(60)} \geq c_W^{(86)} \,\} \Rightarrow \{\, c_W^{(60)} \geq c_W^{(18)} \text{ and } c_W^{(60)} \geq c_W^{(20)} \,\}.$$

<u>Proof</u>

By adding both sides of the inequalities for $e = 18$ and 20 in Table A2.11, it follows that when $c_W^{(60)} \geq c_W^{(18)}$ and $c_W^{(60)} \geq c_W^{(20)}$,

$$2w_{1,2} + w_{3,4} \geq 2w_{1,3} + 2w_{1,4} + 2w_{1,5}$$

i.e. $\qquad 2w_{1,2} + w_{3,4} \geq -(w_{3,3} + w_{3,4}) + 2w_{1,5}$

i.e. $\quad 2w_{1,2} + w_{3,3} + 2w_{3,4} \geq 2w_{1,5},$

which is true when $c_W^{(60)} \geq c_W^{(67)}$ and $c_W^{(60)} \geq c_W^{(86)}$. ∎

Lemma A2.25

$$\{\, c_W^{(60)} \geq c_W^{(86)} \text{ and } c_W^{(60)} \geq c_W^{(116)} \,\} \Rightarrow \{\, c_W^{(60)} \geq c_W^{(61)} \text{ and } c_W^{(60)} \geq c_W^{(62)} \,\}.$$

<u>Proof</u>

When $c_W^{(60)} \geq c_W^{(61)}$ and $c_W^{(60)} \geq c_W^{(62)}$, the following inequality is true:

$$2w_{1,2} + 2w_{3,4} \geq 2w_{1,3} + 2w_{1,4}$$

i.e. $\qquad 2w_{1,2} + 2w_{3,4} \geq -(w_{3,3} + w_{3,4})$

i.e. $\quad 2w_{1,2} + w_{3,3} + 3w_{3,4} \geq 0$.

This inequality is true when $c_W^{(60)} \geq c_W^{(86)}$ and $c_W^{(60)} \geq c_W^{(116)}$. ∎

It now follows that for $e \in \{63, 65, 87, 92, 103\}$, $c_W^{(60)} \geq c_W^{(e)}$ when $c_W^{(60)} \geq c_W^{(e_2)}$ and $c_W^{(60)} \geq c_W^{(e_3)}$, where e, e_2 and e_3 are listed in Table A2.12.

Table A2.12
e, e_2 and e_3

e	e_2	e_3
63	61	70
65	62	70
87	61	116
92	62	116
103	70	86

A2.10 Proof of Theorem 7.9

Assume that

$$c_W^{(67)} \geq c_W^{(e_1)} \quad \text{for } e_1 \in \{13, 18, 20, 60, 99, 116\}.$$

Let this assumption be called χ_{67}, and let $\Xi_{67} = \Xi \setminus \{13, 18, 20, 60, 67, 99, 116\}$. Theorem 7.9 is proved by showing that under χ_{67},

$$c_W^{(67)} \geq c_W^{(e)} \quad \text{for all } e \in \Xi_{67}.$$

Conditions for $c_W^{(67)} \geq c_W^{(e_1)}$ are given in Table A2.13, and conditions for $c_W^{(67)} \geq c_W^{(e)}$ are given in Table A2.14.

Table A2.13 $c_W^{(67)} \geq c_W^{(e_1)}$ for $e_1 \in \{13, 18, 20, 60, 99, 116\}$.

e_1	$c_W^{(67)} \geq c_W^{(e_1)}$
13	$2w_{1,1} + 2w_{1,5} \geq w_{3,3} + w_{3,4}$
18	$w_{3,4} \geq 4w_{1,3}$
20	$w_{3,4} \geq 4w_{1,4}$
60	$w_{1,5} \geq w_{1,2}$
99	$w_{3,4} \geq 0$
116	$w_{1,5} \geq 0$

Table A2.14 $c_W^{(67)} \geq c_W^{(e)}$ for $e \in \Xi_{67}$

e	$c_W^{(67)} \geq c_W^{(e)}$	Ξ_{67}^*
29	$2w_{1,1} + 2w_{1,5} \geq w_{3,3}$	13, 99
61	$4w_{1,5} + 2w_{3,4} \geq 2w_{1,2} + 4w_{1,3}$	18, 60, 99, 116
62	$4w_{1,5} + 2w_{3,4} \geq 2w_{1,2} + 4w_{1,4}$	20, 60, 99, 116
63	$4w_{1,5} + 2w_{3,4} \geq 4w_{1,3} + 2w_{1,6}$	18, 60, 99, 116 ‡
65	$4w_{1,5} + 2w_{3,4} \geq 4w_{1,4} + 2w_{1,6}$	20, 60, 99, 116 ‡
70	$w_{1,5} \geq w_{1,6}$	60, 99 †
86	$2w_{1,5} + w_{3,4} \geq 2w_{1,2}$	60, 99
87	$4w_{1,5} + 2w_{3,4} \geq 4w_{1,3}$	18, 99, 116
92	$4w_{1,5} + 2w_{3,4} \geq 4w_{1,4}$	20, 99, 116
103	$2w_{1,5} + w_{3,4} \geq 2w_{1,6}$	60, 99 ‡
117	$2w_{1,5} + w_{3,4} \geq 0$	99, 116

† shown in Lemma A2.26.

‡ clearly satisfied when $c_W^{(67)} \geq c_W^{(70)}$.

Note that under χ_{67}, $c_W^{(67)} \geq c_W^{(99)}$, which means that $\rho_3 < 0$ since $x_{3,4}$, $z_{3,4} > 0$. Now consider the following lemma.

Lemma A2.26

$$c_W^{(67)} \geq c_W^{(60)} \Rightarrow c_W^{(67)} \geq c_W^{(70)} \quad \text{when } \rho_3 < 0.$$

<u>Proof</u>

First consider

$$c_W^{(67)} \geq c_W^{(70)}$$

i.e. $\qquad w_{1,5} \geq w_{1,6}$.

This inequality simplifies to

$$\rho_2 - \rho_1^2 \leq 0.$$

Now consider when

$$c_W^{(67)} \geq c_W^{(60)} \Rightarrow c_W^{(67)} \geq c_W^{(70)}$$

i.e. $\quad \rho_2 - \rho_1^2 \leq \rho_3(1 - \rho_1^2) \Rightarrow \rho_2 - \rho_1^2 \leq 0$

i.e. $\qquad \rho_3(1 - \rho_1^2) \leq 0,$

which is true when $\rho_3 < 0$. ∎

The conditions for $c_W^{(67)} \geq c_W^{(e)}$ for $e \in \{29, 61, 62, 86, 87, 92, 117\}$ are clearly satisfied for all $e_2 \in \Xi_{67}^*$, where $\Xi_{67}^* \subseteq \{13, 18, 20, 60, 99, 116\}$. Lemma A2.26 means that $w_{1,5} \geq w_{1,6}$, so $c_W^{(67)} \geq c_W^{(e)}$ is also satisfied for $e \in \{63, 65, 103\}$

A3 Appendix 3

Additional material for chapters 9 to 11

A3.1 Equivalent expressions for the BLUEs and BLUPs for model 2

It is shown here that the BLUE of $\underline{c}_s'\underline{\tau}_s$ and the BLUP of $\underline{c}_n'\underline{\tau}_n$ are given by $\underline{c}_s'\hat{\underline{\tau}}_s$ and $\underline{c}_n'\tilde{\underline{\tau}}_n$, respectively, where

$$\hat{\underline{\tau}}_s = (X_s'V_2^*X_s)^{-1}X_s'V_2^*\underline{y} \tag{A3.1}$$

and $\quad \tilde{\underline{\tau}}_n = \sigma_n^2 G_n X_n'V_2^*(\underline{y} - X_s\hat{\underline{\tau}}_s),$ (A3.2)

are equivalent to $\hat{\underline{\tau}}_s$ given by

$$(\hat{\mu}, \hat{\underline{\tau}}_s') = (X_{1,s}'V_2^{-1}X_{1,s})^{-1}X_{1,s}'V_2^{-1}\underline{y} \tag{A3.3}$$

and $\quad \tilde{\underline{\tau}}_n = \sigma_n^2 G_n X_n'V_2^{-1}(\underline{y} - X_{1,s}(\hat{\mu}, \hat{\underline{\tau}}_s')').$ (A3.4)

First consider the equation in (A3.3), which can be re-written as

$$\begin{pmatrix} \hat{\mu} \\ \hat{\underline{\tau}}_s \end{pmatrix} = \begin{pmatrix} C^{(11)} & C^{(1s)} \\ \hline C^{(s1)} & C^{(ss)} \end{pmatrix} \begin{pmatrix} \underline{1}_m' \\ X_s' \end{pmatrix} V_2^{-1}\underline{y},$$

where

$$\begin{pmatrix} C^{(11)} & C^{(1s)} \\ \hline C^{(s1)} & C^{(ss)} \end{pmatrix} = (X_{1,s}'V_2^{-1}X_{1,s})^{-1} = \begin{pmatrix} \underline{1}_m'V_2^{-1}\underline{1}_m & \underline{1}_m'V_2^{-1}X_s \\ \hline X_s'V_2^{-1}\underline{1}_m & X_s'V_2^{-1}X_s \end{pmatrix}^{-1}.$$

Therefore

$$\hat{\underline{\tau}}_s = (C^{(s1)}\underline{1}_m' + C^{(ss)}X_s')V_2^{-1}\underline{y}. \tag{A3.5}$$

The sub-matrices $C^{(11)}$, $C^{(1s)}$, $C^{(s1)}$ and $C^{(ss)}$ are determined using (A1.22), which gives the inverse of a partitioned matrix. This gives

$$C^{(11)} = (\underline{1}_m'V_2^{-1}\underline{1}_m)^{-1} + (\underline{1}_m'V_2^{-1}\underline{1}_m)^{-2}\underline{1}_m'V_2^{-1}X_s C^{(ss)}X_s'V_2^{-1}\underline{1}_m,$$

$$C^{(1s)} = C^{(s1)'} = -(\underline{1}_m'V_2^{-1}\underline{1}_m)^{-1}\underline{1}_m'V_2^{-1}X_s C^{(ss)}$$

and $\quad C^{(ss)} = (X_s'V_2^*X_s')^{-1}.$

From the equation in (A3.5) it follows that

$$\hat{\underline{t}}_s = \left\{ -(1_m'V_2^{-1}1_m)^{-1}C^{(ss)}X_s'V_2^{-1}J_mV_2^{-1} + C^{(ss)}X_s'V_2^{-1} \right\}\underline{y}$$

$$= C^{(ss)}X_s'V_2^*\underline{y}$$

giving the equation in (A3.1).

Now consider $V_2^{-1}\left(\underline{y} - X_{1,s}(\hat{\mu}, \hat{\underline{t}}_s')'\right)$ from the equation in (A3.4).

This is equal to

$$V_2^{-1}\left(\underline{y} - (1_m \mid X_s)\left(\begin{array}{c|c} C^{(11)} & C^{(1s)} \\ \hline C^{(s1)} & C^{(ss)} \end{array}\right)\left(\begin{array}{c} 1_m' \\ X_s' \end{array}\right)V_2^{-1}\underline{y} \right)$$

$$= V_2^{-1}\left(V_2 - 1_m C^{(11)}1_m' - 1_m C^{(1s)}X_s' - X_s C^{(s1)}1_m' - X_s C^{(ss)}X_s' \right)V_2^{-1}\underline{y}$$

$$= \left\{ V_2^{-1} - (1_m'V_2^{-1}1_m)^{-1}V_2^{-1}J_mV_2^{-1} \right.$$

$$- (1_m'V_2^{-1}1_m)^{-2}V_2^{-1}J_mV_2^{-1}X_s C^{(ss)}X_s'V_2^{-1}J_mV_2^{-1}$$

$$+ (1_m'V_2^{-1}1_m)^{-1}V_2^{-1}J_mV_2^{-1}X_s C^{(ss)}X_s'V_2^{-1}$$

$$\left. + (1_m'V_2^{-1}1_m)^{-1}V_2^{-1}X_s C^{(ss)}X_s'V_2^{-1}J_mV_2^{-1} - V_2^{-1}X_s C^{(ss)}X_s'V_2^{-1} \right\}\underline{y}$$

$$= \left\{ V_2^* + (1_m'V_2^{-1}1_m)^{-1}V_2^{-1}J_mV_2^{-1}X_s C^{(ss)}X_s'V_2^* \right.$$

$$\left. - V_2^{-1}X_s C^{(ss)}X_s'V_2^* \right\}\underline{y}$$

$$= V_2^*\underline{y} - V_2^*X_s\hat{\underline{t}}_s$$

$$= V_2^*\left(\underline{y} - X_s\hat{\underline{t}}_s \right),$$

giving the equation in (A3.2).

A3.2 Expressions for the sub-matrices of C_2^{-1}

Expressions are derived here for the sub-matrices of C_2^{-1} (given in section 9.2). Recall that

$$C_2 = \left(\begin{array}{c|c} X_s'V_1^*X_s & X_s'V_1^*X_n \\ \hline X_n'V_1^*X_s & X_n'V_1^*X_n + \sigma_n^{-2}G_n^{-1} \end{array}\right),$$

First to simplify the notation, let

$$\underline{a} = X_n'V_1^{-1}\underline{1}_m; \qquad \underline{b} = V_1^{-1}\underline{1}_m; \qquad A = X_n'V_1^{-1}X_n + \sigma_n^{-2}G_n^{-1};$$

$$\omega = \left(\underline{1}_m'V_1^{-1}\underline{1}_m\right)^{-1}; \qquad \upsilon = \underline{a}'A^{-1}\underline{a}$$

and $\quad C_{2,nn} = X_n'V_1^*X_n + \sigma_n^{-2}G_n^{-1} = A - \omega\underline{a}\underline{a}'.$

Now consider the following Lemmas.

Lemma A3.1

$$C_{2,nn}^{-1} = A^{-1} + \omega(1-\omega\upsilon)^{-1}A^{-1}\underline{a}\underline{a}'A^{-1}.$$

<u>Proof</u>

The proof follows from the formula in (A1.24) in Appendix A1.5. ∎

Lemma A3.2

$$V_2^* = V_1^* - V_1^*X_nC_{2,nn}^{-1}X_n'V_1^* \tag{A3.6}$$

<u>Proof</u>

First consider V_2^*. The matrix V_2 is defined as $V_1 + \sigma_n^2X_nG_nX_n'$. From the formula in (A1.24), it follows that

$$V_2^{-1} = V_1^{-1} - V_1^{-1}X_nA^{-1}X_n'V_1^{-1}.$$

Then it can easily be shown that

$$\left(\underline{1}_m'V_2^{-1}\underline{1}_m\right)^{-1} = \omega/(1-\omega\upsilon)$$

and $\quad V_2^{-1}\underline{1}_m = \underline{b} - V_1^{-1}X_nA^{-1}\underline{a}.$

Hence, V_2^* can be written in terms of V_1^{-1} as

$$V_2^* = V_1^{-1} - V_1^{-1}X_nA^{-1}X_n'V_1^{-1}$$

$$- \omega(1-\omega\upsilon)^{-1}\left(\underline{b}\underline{b}' - \underline{b}\underline{a}'A^{-1}X_n'V_1^{-1} - V_1^{-1}X_nA^{-1}\underline{a}\underline{b}'\right.$$

$$\left. + V_1^{-1}X_nA^{-1}\underline{a}\underline{a}'A^{-1}X_n'V_1^{-1}\right). \tag{A3.7}$$

Now consider the right hand side of the equation in (A3.6). The matrix V_1^* can be written as

$$V_1^* = V_1^{-1} - \omega \underline{b}\underline{b}'.$$

Also,

$$X_n'V_1^* = X_n'V_1^{-1} - \omega \underline{a}\underline{b}'.$$

It then follows from Lemma A3.1 that $V_1^* - V_1^* X_n C_{2,nn}^{-1} X_n'V_1^*$ is equal to the right hand side of the equation in (A3.7). ∎

Lemma A3.3

$$\sigma_n^2 A^{-1} X_n'V_1^{-1}X_n G_n = \sigma_n^2 G_n - A^{-1}. \tag{A3.8}$$

Proof

The proof follows by substituting $A - \sigma_n^{-2}G_n^{-1}$ for $X_n'V_1^{-1}X_n$ in the left hand side of the equation in (A3.8). ∎

Lemma A3.4

$$\sigma_n^2 V_2^* X_n G_n = V_1^* X_n C_{2,nn}^{-1}. \tag{A3.9}$$

Proof

The proof involves writing both sides of (A3.9) in terms of V_1^{-1}. First consider $\sigma_n^2 V_2^* X_n G_n$. Substituting the expression for V_2^* given by (A3.7) into $\sigma_n^2 V_2^* X_n G_n$ and replacing $\sigma_n^2 A^{-1} X_n'V_1^{-1}X_n G_n$ by $\sigma_n^2 G_n - A^{-1}$ (Lemma A3.3) gives

$$V_1^{-1}X_n A^{-1} - \omega(1-\omega\upsilon)^{-1}\left(\underline{b}\underline{a}' A^{-1} - V_1^{-1}X_n A^{-1}\underline{a}\underline{a}A^{-1}\right). \tag{A3.10}$$

Now consider $V_1^* X_n C_{2,nn}^{-1}$. From the expression for $C_{2,nn}^{-1}$ given in Lemma A3.1, it follows that $V_1^* X_n C_{2,nn}^{-1}$ is equal to the expression given by (A3.10).

∎

Lemma A3.5

$$C_{2,nn}^{-1} = \sigma_n^2\left(G_n - \sigma_n^2 G_n X_n'V_2^* X_n G_n\right). \tag{A3.11}$$

<u>Proof</u>

Consider the right hand side of the equation in (A3.11). Substituting the expression for $\sigma_n^2 V_2^* X_n G_n$ from (A3.10) gives

$$\sigma_n^2 G_n - \sigma_n^2 G_n X_n'V_1^{-1} X_n A^{-1}$$
$$+ \omega(1-\omega\upsilon)^{-1}\left(\sigma_n^2 G_n \underline{a}\underline{a}'A^{-1} - \sigma_n^2 G_n X_n'V_1^{-1} X_n A^{-1}\underline{a}\underline{a}'A^{-1}\right).$$

Then Lemma A3.3 gives the expression for $C_{2,nn}^{-1}$ in Lemma A3.1. ∎

From the formula (A1.23) for the inverse of a partitioned matrix, it follows that:

$$C_2^{(ss)} = \left(X_s'V_1^* X_s - X_s'V_1^* X_n C_{2,nn}^{-1} X_n'V_1^* X_s\right)^{-1}$$
$$= \left(X_s'V_2^* X_s\right)^{-1} \quad \text{(from Lemma A3.2)};$$
$$C_2^{(sn)} = -C_2^{(ss)} X_s'V_1^* X_n C_{2,nn}^{-1}$$
$$= -\sigma_n^2 C_2^{(ss)} X_s'V_2^* X_n G_n \quad \text{(by Lemma A3.4)};$$
$$C_2^{(nn)} = C_{2,nn}^{-1} + C_{2,nn}^{-1} X_n'V_1^* X_s C_2^{(ss)} X_s'V_1^* X_n C_{2,nn}^{-1}$$
$$= \sigma_n^2\left(G_n - \sigma_n^2 G_n X_n'V_2^* X_n G_n + \sigma_n^2 G_n X_n'V_2^* X_s C_2^{(ss)} X_s'V_2^* X_n G_n\right)$$

$$\text{(by Lemma A3.4 and Lemma A3.5).}$$

A3.3 Derivation of $\text{var}(\hat{\underline{\tau}}_s)$, $\text{var}(\tilde{\underline{\tau}}_n - \underline{\tau}_n)$ and
$\text{cov}(\hat{\underline{\tau}}_s, \tilde{\underline{\tau}}_n - \underline{\tau}_n)$ under model 2

From the equation in (2.16) in section 2.4.3.1, it follows that

$$\text{var}(\hat{\underline{\tau}}_s) = \left(X_s'V_2^* X_s\right)^{-1} = C_2^{(ss)}.$$

Recall from equation (9.7) in section 9.2 that

$$\begin{pmatrix} \hat{\underline{\tau}}_s \\ \widetilde{\underline{\tau}}_n \end{pmatrix} = \begin{pmatrix} C_2^{(ss)} & \vline & C_2^{(sn)} \\ \hline C_2^{(ns)} & \vline & C_2^{(nn)} \end{pmatrix} \begin{pmatrix} X_s' \\ X_n' \end{pmatrix} V_1^* \underline{y}$$

$$= \begin{pmatrix} R_s' \\ R_n' \end{pmatrix} \underline{y},$$

where

$$R_s' = C_2^{(ss)} X_s' V_1^* + C_2^{(sn)} X_n' V_1^*$$

and $R_n' = C_2^{(ns)} X_s' V_1^* + C_2^{(nn)} X_n' V_1^*.$

Now consider

$$\begin{pmatrix} R_s' \\ R_n' \end{pmatrix} (X_s \mid X_n)$$

$$= \begin{pmatrix} C_2^{(ss)} & \vline & C_2^{(sn)} \\ \hline C_2^{(ns)} & \vline & C_2^{(nn)} \end{pmatrix} \begin{pmatrix} X_s' \\ X_n' \end{pmatrix} V_1^* (X_s \mid X_n)$$

$$= \begin{pmatrix} C_2^{(ss)} & \vline & C_2^{(sn)} \\ \hline C_2^{(ns)} & \vline & C_2^{(nn)} \end{pmatrix} \left[\begin{pmatrix} X_s' V_1^* X_s & \vline & X_s' V_1^* X_n \\ \hline X_n' V_1^* X_s & \vline & X_n' V_1^* X_n + \sigma_n^{-2} G_n^{-1} \end{pmatrix} - \begin{pmatrix} 0 & \vline & 0 \\ \hline 0 & \vline & \sigma_n^{-2} G_n^{-1} \end{pmatrix} \right]$$

$$= \begin{pmatrix} I_c & \vline & 0 \\ \hline 0 & \vline & I_t \end{pmatrix} - \begin{pmatrix} 0 & \vline & \sigma_n^{-2} C_2^{(sn)} G_n^{-1} \\ \hline 0 & \vline & \sigma_n^{-2} C_2^{(nn)} G_n^{-1} \end{pmatrix},$$

i.e.

$$\begin{pmatrix} R_s' X_s & \vline & R_s' X_n \\ \hline R_n' X_s & \vline & R_n' X_n \end{pmatrix} = \begin{pmatrix} I_c & \vline & -\sigma_n^{-2} C_2^{(sn)} G_n^{-1} \\ \hline 0 & \vline & I_t - \sigma_n^{-2} C_2^{(nn)} G_n^{-1} \end{pmatrix}. \tag{A3.12}$$

To derive $\mathrm{var}(\widetilde{\underline{\tau}}_n - \underline{\tau}_n)$ and $\mathrm{cov}(\hat{\underline{\tau}}_s, \widetilde{\underline{\tau}}_n - \underline{\tau}_n)$ the equation in (A3.12) is useful (as in Appendix A of Henderson, 1975). First consider

$$\mathrm{var}(\widetilde{\underline{\tau}}_n) = R_n' \mathrm{var}(\underline{y}) R_n$$

$$= \sigma_n^2 R_n' X_n G_n X_n' R_n + R_n' V_1 R_n.$$

Substituting $R_n' X_n = I_t - \sigma_n^{-2} C_2^{(nn)} G_n^{-1}$ gives

$$\mathrm{var}(\widetilde{\underline{\tau}}_n) = \sigma_n^2 G_n - 2 C_2^{(nn)} + \sigma_n^{-2} C_2^{(nn)} G_n^{-1} C_2^{(nn)} + R_n' V_1 R_n.$$

It can easily be shown that $R_n'V_1R_n = C_2^{(nn)} - \sigma_n^{-2}C_2^{(nn)}G_n^{-1}C_2^{(nn)}$. It then follows

that $\quad \text{var}(\widetilde{\underline{\tau}}_n) = \sigma_n^2 G_n - C_2^{(nn)}$. $\qquad\qquad$ (A3.13)

Now consider

$$\begin{aligned}
\text{cov}(\widetilde{\underline{\tau}}_n, \underline{\tau}_n) &= E(\widetilde{\underline{\tau}}_n \underline{\tau}_n') \\
&= R_n'E(\underline{y}\underline{\tau}_n') \\
&= R_n'X_nE(\underline{\tau}_n\underline{\tau}_n') \\
&= R_n'X_n\text{var}(\underline{\tau}_n) \\
&= \sigma_n^2 G_n - C_2^{(nn)}.
\end{aligned}$$
$\qquad\qquad$ (A3.14)

Hence,

$$\begin{aligned}
\text{var}(\widetilde{\underline{\tau}}_n - \underline{\tau}_n) &= \text{mse}(\widetilde{\underline{\tau}}_n) \\
&= \text{var}(\widetilde{\underline{\tau}}_n) - 2\text{cov}(\widetilde{\underline{\tau}}_n, \underline{\tau}_n) + \text{var}(\underline{\tau}_n) \\
&= C_2^{(nn)} \qquad \text{(by (A3.13) and (A3.14)).}
\end{aligned}$$

Finally consider

$$\begin{aligned}
\text{cov}(\hat{\underline{\tau}}_s, \widetilde{\underline{\tau}}_n - \underline{\tau}_n) &= E\{\hat{\underline{\tau}}_s(\widetilde{\underline{\tau}}_n - \underline{\tau}_n)'\} \\
&= E(\hat{\underline{\tau}}_s\widetilde{\underline{\tau}}_n') - E(\hat{\underline{\tau}}_s\underline{\tau}_n') \\
&= R_s'E(\underline{y}\underline{y}')R_n - R_s'E(\underline{y}\underline{\tau}_n').
\end{aligned}$$

The term

$$\begin{aligned}
R_s'E(\underline{y}\underline{y}')R_n &= \mu R_s'\underline{1}_m E(\underline{y}')R_n + R_s'X_s\underline{\tau}_s E(\underline{y}')R_n \\
&\quad + R_s'X_nE(\underline{\tau}_n\underline{\tau}_n')X_n'R_n + R_s'V_1R_n.
\end{aligned}$$

Since $R_s'\underline{1}_m = \underline{0}_c$ and $R_s'X_s = I_c$, this simplifies to

$$R_s'E(\underline{y}\underline{y}')R_n$$

$$\begin{aligned}
&= \mu\underline{\tau}_s\underline{1}_m'R_n + \underline{\tau}_s\underline{\tau}_s'X_s'R_n + \sigma_n^2 R_s'X_nG_nX_n'R_n + R_s'V_1R_n \\
&= \sigma_n^2 R_s'X_nG_nX_n'R_n + R_s'V_1R_n
\end{aligned}$$

$\qquad\qquad$ (since $\underline{1}_m'R_n = \underline{0}_t'$ and $X_s'R_n = 0$).

Note that $R_s'V_1R_n = C_2^{(sn)} - \sigma_n^{-2}C_2^{(sn)}G_n^{-1}C_2^{(nn)}$.

Now consider the term

$$R_s'E(\underline{y}\underline{\tau}_n') = R_s'X_nE(\underline{\tau}_n\underline{\tau}_n')$$

$$= \sigma_n^2R_s'X_nG_n.$$

Hence, it follows that

$$\text{cov}(\hat{\underline{\tau}}_s,\tilde{\underline{\tau}}_n - \underline{\tau}_n) = C_2^{(sn)}.$$

A3.4 Simulating correlated values

A method to generate an n-vector $\underline{x}$ from a $N(\underline{0}_n,\Lambda)$ distribution is outlined in this section, where Λ is a positive definite $n \times n$ matrix.

A vector $\underline{x}$ with a $N(\underline{0}_n,\Lambda)$ distribution can be given as

$$\underline{x} = A\underline{e},$$

where A is a $n \times n$ matrix, such that $\Lambda = AA'$, and $\underline{e}$ is a n-vector, such that $\underline{e}$ has a $N(\underline{0}_n,I_n)$ distribution.

For a separable process, i.e. when $\Lambda = \Lambda_2 \otimes \Lambda_1$, where Λ_i ($i = 1,2$) is a $n_i \times n_i$ matrix ($n = n_1n_2$), A can be taken as

$$A = A_2 \otimes A_1,$$

where $\Lambda_i = A_iA_i'$ ($i = 1,2$).

Using MATLAB, the function chol can be applied to the matrix Λ to give A, and a vector $\underline{e}$ can be generated using the function randn.

A3.5 Best designs found for Example 11.1 under model 1

(ρ_r,ρ_c)	Ψ_1		Ψ_2		Ψ_3	
	A_{ns}	A_{nn}	A_{ns}	A_{nn}	A_{ns}	A_{nn}
$(\frac{1}{2},\frac{1}{2})$	Case 1		Case 2		Case 3	
$(\frac{1}{5},\frac{3}{5})$	Case 4		Case 5		Case 6	
$(\frac{1}{10},\frac{9}{10})$	Case 7		Case 8		Case 9	

Case 1 (Ψ_1)

A_{ns}:
```
• • • • •
• 1 • 2 •
2 • • • •
• • • • 1
• 2 • •
1 • • • •
• • 1 • •
• 2 • • •
• • • • 2
• • 1 • •
```

A_{nn}:
```
• • • • 1
• 2 • • •
• • • • 2
1 • • • •
• • • 1 •
• 2 • • •
• • • • 2
1 • • • •
• • • 1 •
• 2 • • •
```

Case 2 (Ψ_2)

A_{ns}:
```
• • • • •
• 1 • 2 •
2 • • • 1
• • • • •
• • 2 • •
• • • 1 •
1 • • • •
• • • • 2
• 2 1 • •
• • • • •
```

A_{nn}: D_{11}

Case 3 (Ψ_3)

A_{ns}:
```
• 1 • • •
• • 2 • •
• • • 1 •
2 • • • •
• 1 • • •
• 2 • • •
• • • 1 •
• • • • 2
1 • • • •
• • 2 • •
```

A_{nn}:
```
• 1 • • •
• • • • 2
• • 1 • •
2 • • • •
• • • 1 •
• 2 • • •
• • • • 1
1 • • • •
• • 2 • •
```

Case 4 (Ψ_1)

A_{ns}:
```
• • • • •
• • • 1 •
2 1 • • 2
• • 2 • •
• • • • •
• • • • •
1 • • 2 •
• 2 • • 1
• • 1 • •
• • • • •
```

A_{nn}: D_{11}

Case 5 (Ψ_2)

A_{ns}:
```
• • • • •
• • • • 1
• 2 1 • •
1 • 2 • •
• • • • •
• • • • •
• 1 • • 2
• • 2 1 •
2 • • • •
• • • • •
```

A_{nn}: D_{11}

Case 6 (Ψ_3)

A_{ns}:
```
• • • • •
• • 1 • •
• • • • 2
1 2 • • •
• • • 1 •
• • 2 • •
2 • • • 1
• 1 • • •
• • • 2 •
• • • • •
```

A_{nn}: D_{10}

Case 7 (Ψ_1)

A_{ns}: D_{11}

A_{nn}: D_{11}

Case 8 (Ψ_2)

A_{ns}:
```
• • 1 2 •
1 2 • 1
• • • • •
• • • • •
• • • • •
• 1 2 • •
2 • 1 •
• • • • 2
• • • • •
```

A_{nn}:
```
• • • • •
1 1 1 1 1
• • • • •
• • • • •
• • • • •
• • • • •
• • • • •
2 2 2 2 2
• • • • •
```

Case 9 (Ψ_3)

A_{ns}:
```
• • • • •
• 1 • • •
• • • 1 2
1 2 • • •
• • • • •
• • • • •
2 • • • 1
• • 1 2 •
• 2 • • •
• • • • •
```

A_{nn}: D_{10}

Ψ_4	
A_{ns}	A_{nn}
Case 10	

Case 10 (Ψ_4)

A_{ns}:
```
• 1 2 • •
2 • 1 • •
1 • • • •
• • • • •
• • • • •
• • • 2 •
• • • • 1
• • • • 2
• • • 1 •
• 2 • • •
```

A_{nn}:
```
• • • • 1
• • 2 1 •
2 1 • • •
1 • • 2 •
• • • • •
• • • • •
• 2 1 • •
• • • • 2
• • • • •
```

A3.6 Best designs found for Example 11.1 under model 2

Model 2, $\sigma_n^2 = \frac{1}{10}$, with respect to A_{ns}-criterion

(ρ_r, ρ_e)	Ψ_1	Ψ_2	Ψ_3
	Case 1	Case 2	Case 3

$(\frac{1}{2}, \frac{1}{2})$	<pre>• • • • •
	• • • 1 •
	• • 1 • •
	• 1 • 1 •
	• • 1 • •
	• • 2 • •
	• 2 • 2 •
	• • 2 • •
	• 2 • • •
	• • • • •</pre>
		<pre>• • • • •
		• 2 • • •
		• • • 2 •
		• • 2 • •
		• 1 • • 2
		1 • • 2 •
		• • 1 • •
		• 1 • • •
		• • • 1 •
		• • • • •</pre>
			<pre>• • • • •
			1 • • • •
			• • 1 • •
			• • • • 1
			• 1 • • •
			2 • • 1 •
			• • 2 • •
			• • • • 2
			• 2 • • •
			• • • 2 •</pre>

	Case 4	Case 5	Case 6

$(\frac{1}{3}, \frac{2}{3})$	<pre>• • • • •
	• • • • •
	• 2 • • •
	2 • 2 • •
	• 2 • 2 •
	• • 1 • 1
	• 1 • 1 •
	• • 1 • •
	• • • • •
	• • • • •</pre>
		<pre>• • • • •
		• 2 • • •
		2 • • • •
		• • 2 • •
		• 1 • • 2
		1 • • 2 •
		• • 1 • •
		• • • • 1
		• • • 1 •
		• • • • •</pre>
			<pre>• • • • •
			1 • • • •
			• • • 1 •
			• 1 • • •
			2 • • • 1
			• • 1 2 •
			• 2 • • •
			• • • • 2
			• • 2 • •
			• • • • •</pre>

	Case 7	Case 8	Case 9

$(\frac{1}{10}, \frac{9}{10})$	<pre>• • • • • •
	• • 2 • •
	2 • • 2 •
	• 2 • • •
	• • • • 1
	• • 1 • •
	1 • 2 1 •
	• 1 • • •
	• • • • •
	• • • • •</pre>
		<pre>• • • • •
		• • 1 • •
		1 • • • •
		• • • 1 •
		• 1 • • 2
		• • 2 • 1
		2 • • • •
		• • • 2 •
		• 2 • • •
		• • • • •</pre>
			<pre>• • • • •
			• • 1 • •
			1 • • • •
			• • • 1 •
			• 1 • • 2
			• • 2 • 1
			2 • • • •
			• • • 2 •
			• 2 • • •
			• • • • •</pre>

The systematic design D_6 is the A_{nn}-best design found for all the above cases.

Model 2, $\sigma_n^2 = \tfrac{1}{2}$, with respect to A_{ns}-criterion

(ρ_r, ρ_e)	Ψ_1	Ψ_2	Ψ_3
	Case 11	Case 12	Case 13
$(\tfrac{1}{2}, \tfrac{1}{2})$	<see grid below>	<see grid below>	<see grid below>
	Case 14	Case 15	Case 16
$(\tfrac{1}{5}, \tfrac{3}{5})$	<see grid below>	<see grid below>	<see grid below>
	Case 17	Case 18	Case 19
$(\tfrac{1}{10}, \tfrac{9}{10})$	<see grid below>	<see grid below>	<see grid below>

Case 11:
```
.  .  .  .  .  .
.  .  .  1  .
.  1  2  .  .
.  2  1  .  .
.  .  .  2  .
2  .  .  .  .
.  .  2  .  .
.  1  .  .  .
.  .  .  .  1
.  .  .  .  .
```

Case 12:
```
.  .  .  .  .  .
.  .  1  .  .
1  .  .  .  .
.  .  .  1  .
.  1  .  .  2
.  .  2  .  1
2  .  .  .  .
.  .  .  2  .
.  2  .  .  .
.  .  .  .  .
```

Case 13:
```
.  .  1  .  .
.  .  .  .  1
1  .  .  .  .
.  .  .  1  .
.  1  2  .  .
.  .  .  .  2
2  .  .  .  .
.  .  .  2  .
.  2  .  .  .
.  .  .  .  .
```

Case 14:
```
.  .  .  .  .  .
.  .  2  .  .
.  2  .  .  .
.  .  .  2  .
2  .  1  .  .
.  .  2  .  1
.  1  .  .  .
.  .  .  1  .
.  .  1  .  .
.  .  .  .  .
```

Case 15:
```
.  .  .  .  .  .
.  .  .  1  .
.  1  .  .  .
.  .  .  .  1
2  .  1  .  .
1  .  .  2  .
.  2  .  .  .
.  .  .  .  2
.  .  2  .  .
.  .  .  .  .
```

Case 16:
```
.  .  .  .  .  .
1  .  .  .  .
.  .  .  1  .
.  1  .  .  .
.  .  2  .  1
2  .  1  .  .
.  .  .  2  .
.  2  .  .  .
.  .  .  .  2
.  .  .  .  .
```

Case 17:
```
.  .  .  .  .  .
.  1  .  .  2
2  .  .  1  .
.  .  .  .  .
.  .  2  .  .
.  .  1  .  .
.  .  .  .  .
.  2  .  .  1
1  .  .  2  .
.  .  .  .  .
```

Case 18:
```
.  .  .  .  .  .
.  .  .  1  .
1  .  .  .  .
.  .  1  .  .
.  2  .  .  1
.  1  .  .  2
.  .  .  2  .
2  .  .  .  .
.  .  2  .  .
.  .  .  .  .
```

Case 19:
```
.  .  .  .  .  .
.  1  .  .  .
.  .  .  .  1
.  .  .  1  .
1  .  2  .  .
2  .  1  .  .
.  .  .  .  2
.  2  .  .  .
.  .  .  2  .
.  .  .  .  .
```

For $(\rho_r, \rho_e) = (\tfrac{1}{2}, \tfrac{1}{2})$ and Ψ_1, Ψ_3 the A_{nn}-best designs found are:

(ρ_r, ρ_e)	Ψ_1	Ψ_3
	Case 11	Case 13
$(\tfrac{1}{2}, \tfrac{1}{2})$	<see grid below>	<see grid below>

Case 11:
```
2  .  1  .  2
.  .  .  .  .
.  .  .  .  .
.  .  .  .  1
1  .  .  .  .
.  .  .  .  .
.  .  .  .  .
.  .  .  .  2
2  .  .  .  .
.  .  .  .  .
1  .  2  .  1
```
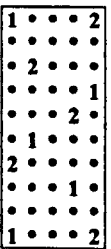
Case 13:
```
.  .  .  .  1
.  .  .  .  1
.  .  .  .  1
.  .  .  .  1
.  .  .  .  1
.  .  .  .  2
.  .  .  .  2
.  .  .  .  2
.  .  .  .  2
.  .  .  .  2
```

For $(\rho_r, \rho_e) = (\frac{1}{10}, \frac{9}{10})$ and Ψ_1 (case 17), D_9 is the A_{nn}-best design found.

For the other cases D_6 is the A_{nn}-best design found.

Model 2, $\sigma_n^2 = 1$, with respect to A_{ns}-criterion

(ρ_r, ρ_e)	Ψ_1	Ψ_2	Ψ_3
	Case 21	Case 22	Case 23

$(\frac{1}{2}, \frac{1}{2})$	<pre>. . . . . .
	. . 2 1 . .
	. . 1 2 . .
	. 2 . . . .
	 1
	. . 2 . . .
	2 . . . . .
	. . . 1 . .
	. 1 . . . .
	. . . . . .</pre>
		<pre>. . . . . .
		. 2 . . . .
		 2
		. . 2 . . .
		2 . . 1 . .
		. 1 . 2 . .
		 1
		1 . . . . .
		. . 1 . . .
		. . . . . .</pre>
			<pre>. . 1 . . .
			1 . . . . .
			 1
			. 1 . . . .
			. . 2 1 . .
			 2
			2 . . . . .
			. . . 2 . .
			. 2 . . . .
			. . . . . .</pre>

	Case 24	Case 25	Case 26

$(\frac{1}{5}, \frac{3}{5})$	<pre>. . . . . .
	. . 1 . . .
	 1
	. 1 . 2 . .
	. . . 1 . .
	1 . 2 . . .
	 2
	. 2 . . . .
	. . . 2 . .
	. . . . . .</pre>
		<pre>. . . . . .
		. . . 2 . .
		2 . . . . .
		. . 2 . . .
		. . 1 . 2 .
		. 2 . 1 . .
		1 . . . . .
		. . 1 . . .
		 1
		. . . . . .</pre>
			<pre>. . 1 . . .
			1 . . . . .
			 1
			. 1 . . . .
			. . . 1 2 .
			. . 2 . . .
			2 . . . . .
			. . . 2 . .
			. 2 . . . .
			. . . . . .</pre>

	Case 27	Case 28	Case 29

$(\frac{1}{10}, \frac{9}{10})$	D_{11}	<pre>. . . . . .
		. . . 1 . .
		. 1 . . . .
		1 . . . . .
		. . 2 . 1 .
		. . 1 . 2 .
		. 2 . . . .
		. . . 2 . .
		2 . . . . .
		. . . . . .</pre>
			<pre>. . . . . .
			. . 1 . . .
			 1
			1 . . . . .
			. 2 . 1 . .
			. 1 . 2 . .
			. . 2 . . .
			 2
			2 . . . . .
			. . . . . .</pre>

Model 2, $\sigma_n^2 = 1$, with respect to A_{nn}-criterion

(ρ_r, ρ_c)	Ψ_1	Ψ_2	Ψ_3
	Case 21	Case 22	Case 23
$(\frac{1}{2}, \frac{1}{2})$		D_7	D_2
	Case 24	Case 25	Case 26
$(\frac{1}{3}, \frac{2}{3})$	D_7	D_6	D_6
	Case 27	Case 28	Case 29
$(\frac{1}{10}, \frac{9}{10})$	D_9	D_6	D_6

Model 2, Ψ_4:

Any design with one check plot in each row and with two different control varieties in each column (for example, designs D_1 to D_5) seems to be A_{ns}-optimal for $\sigma_n^2 = \frac{1}{10}, \frac{1}{2}, 1$, and A_{nn}-optimal for $\sigma_n^2 = 1$.

Any design with the check plots in two rows and with two different control varieties in each column (for example, designs D_6 to D_{13}) seems to be A_{nn}-optimal for $\sigma_n^2 = \frac{1}{10}, \frac{1}{2}$.

A3.7 Best designs found for Example 11.2 under model 1

Best designs found with respect to A_{nn}-criterion

(ρ_r, ρ_c)	Ψ_1	Ψ_2	Ψ_3
	Case 1	Case 2	Case 3
$(\frac{1}{2}, \frac{1}{2})$	<pre>. . 4 . . . . 2 . 3 . . 1 . . . . 4 . . . . . 3 . . . 2 . 2 . . . . 1 . . . . . 4 . . . 3 . . . . 1 . . 2 . . . . 4 . . . 3 . . . . 1 . . . 2 . . . . . 3 . . . 4 . . . . 5 . . . . . 2 . . . 1 . . . . 3 . . . . 4 . . . . 1 . . . . 5 . . . .</pre>	<pre>. . . . . 1 5 . . . . 2 . . . 4 . 1 . . . . 4 . 3 . 2 . 3 . . . . 4 . 1 . . 3 1 . . . . . 2 . . . . 2 . . . 4 . . . . 3 . . . . 3 . . 1 . . . . 4 . . 2 2 4 1 . . . . 5 3 . . . .</pre>	<pre>. . . . 3 . . . . . 5 . . 2 . . . . . 4 . . . . 1 . . . . . . 3 . 2 . . . . 1 . . . . . 3 . . . . 2 . . . 1 . . . . . 3 . . . . 4 . . . 4 . . . . 2 . . . . . . 3 . . . . 4 . . . . . 1 . . 3 . . . . . 1 . . . . 4 . . . . . 2 . . 5 . . . . 4 . . 1 . . . . 2 . . . .</pre>
	Case 4	Case 5	Case 6
$(\frac{1}{3}, \frac{1}{3})$	<pre>. . . . . 5 . 3 . . 1 . . . . 3 . 2 . 4 . . . . 2 . 4 . . . . 1 . 5 . . . . 3 . . . . 2 . 4 . 2 . . . . 4 . 1 . . . . 3 . 1 . . . . 2 . . . . 4 . 2 . 4 . . . . 1 . 3 . 1 . 3 . . . .</pre>	<pre>. . . . . 3 2 3 1 2 3 1 3 . . . . 5 . 1 . . . 2 4 . 2 4 . 4 2 . . . . 1 . . 5 . . . . 4 3 2 4 1 4 3 1 . . . .</pre>	<pre>. . . 3 . . . . . 2 . . . . 5 . . . 1 . 4 . . . 2 . . . . . . 4 . . . . 1 . . . . 5 . . . . 2 . . . . 4 . . . . 3 . 1 . . . . 4 . . . . . 3 . . . 2 . . . . . 3 . . . . 4 . . . . . 1 . . . . . 3 . . . . . 4 . . . . 1 . . . . . . 3 . . 2 . 1 . . . . 2 . . . .</pre>

Best designs found with respect to A_{ns}-criterion

(ρ_r, ρ_c)	Ψ_1	Ψ_2	Ψ_3
	Case 1	Case 2	Case 3
$(\tfrac{1}{2}, \tfrac{1}{2})$			
	Case 4	Case 5	Case 6
$(\tfrac{1}{3}, \tfrac{1}{3})$			

Best designs found for Ψ_4 (Case 10),

A_{nn}-best design found	A_{ns}-best design found

<pre>· · · · 4 · · ·
· · 1 5 · · · ·
· 2 · · · · · ·
· 3 · · · · · ·
· · 2 · · · · ·
· · · 3 · 2 · ·
· 4 · · · · · ·
· · · · · · · 3
· · · · · · 1 ·
· 1 · · · · · ·
4 · · · 3 · ·
1 · · · · · 4 ·
3 · · · · · · 1
· · · · · · · ·
· · · · · · · 3
· · · 2 4 · ·
· · · · · 1 ·
· 2 · · · · ·
· · · 4 · · ·
· · 5 2 · · ·</pre>
	<pre>· · 2 · · · · ·
	· 3 · · 2 · · ·
	1 · · 4 · · · ·
	· · · · 4 · · ·
	· · · · · · 1 ·
	· · · · 3 · · 2
	· · · · · · 4 ·
	· · · 5 · 3 · ·
	· · · · · · 2 ·
	· · · · · 1 · 3
	· · · · · · 3 ·
	· · 1 · · · · ·
	· · · · · · · ·
	2 · · · · · 1
	· · 1 · 5 · ·
	· · 4 · · · · ·
	· 4 · 3 · · · ·
	4 2 · · · · · ·
	· · · · · · · ·
	· · · · · · · ·</pre>

A3.8 Best designs found for Example 11.2 under model 3

Best designs found with respect to A_{mn}-criterion, for $\sigma_n^2 = \frac{1}{10}$

(ρ_r, ρ_e)	Ψ_1	Ψ_3	Ψ_4
	Case 1	Case 3	Case 10
$(\frac{1}{2}, \frac{1}{2})$	<pre>4 • 3 • 1 • 2 4 • • • • • • • • 3 • • • • • • 2 • • • • • • • • 1 • • • • • • • • • • • • • • 3 • • • • • • • • 3 • • • • • • • • • • • • • • 1 2 • • • • • • • • • • • • • • 2 1 • • • • • • • • • • • • • • 3 • • • • • • • • 3 • • • • • • • • • • • • • • 1 2 • • • • • • • • • • • • • • 4 5 • • • • • • 4 5 • 1 • 4 4 • 2</pre>	<pre>5 • • • • • • 1 5 • • • • • • 1 1 • • • • • • 3 3 • • • • • • 1 • • • • • • • 3 • • • • • • • 3 • • • • • • • 3 • • • • • • • 3 • • • • • • • 4 • • • • • • • 4 • • • • • • • 4 • • • • • • • 4 • • • • • • • 4 • • • • • • • 4 • • • • • • • 2 • • • • • • • 2 • • • • • • • 2 • • • • • • • 2 2 • • • • • • 1 1 • • • • • • 2</pre>	<pre>• 1 • 2 • 4 • 2 • 3 • 1 4 • 4 • • • 2 1 • 4 3 1 1 3 5 2 3 • 1 5 2 4 4 3 3 2</pre>
	Case 4	Case 6	
$(\frac{1}{3}, \frac{2}{3})$	<pre>4 4 3 3 3 3 3 3 • • • • • • • • • • • • • • • • 1 • • • • • • 1 • • • • • • • • • • • • • • • • 4 • • • • • • 4 • • • • • • • • • • • • • • • • 1 • • • • • • • • • • • • • • 1 • • • • • • • • • • • • • • • • 4 • • • • • • 4 • • • • • • • • • • • • • • • • 1 • • • • • • 1 • • • • • • • • • • • • • • • • 5 5 2 2 2 2 2 2</pre>	<pre>5 1 1 1 1 1 1 4 4 • • • • • • 3 • • • • • • • 3 • • • • • • • 3 • • • • • • • 3 • • • • • • • 4 • 3 • • • • • • 4 4 • • • • • • 3 4 2 2 2 2 2 2 5</pre>	

Best designs found with respect to A_{ns}-criterion, for $\sigma_n^2 = \frac{1}{16}$

(ρ_r, ρ_c)	Ψ_1	Ψ_3	Ψ_4
	Case 1	Case 3	Case 10
$(\frac{1}{2}, \frac{1}{2})$	<pre>• • • • • • • • • • • • 3 • • • • • 3 • • • • • • 3 2 • • • • • 3 • • 2 • • • 3 • 2 • • • • • • 2 • 2 • • • • • • 2 • • • • • • • • • • • • • • • • • 4 • • • • • • 4 • 4 • • • • • • 4 • 4 • • • • • • 4 • • • • • • • • • • • • 1 • • • • • 1 • 1 • • • • • • • 1 3 5 • • • • • 5 1 • • • • • • • 1 • • • • • • • • •</pre>	<pre>• • • • • • • • • • • • 4 • • • • • 4 • • • • • • • • • • 4 • • • • 4 • • • • • • • 3 4 • • • 4 • • • • 3 • • • 3 2 • • • • • • • • • 3 2 • • 3 • 2 • • • • • • • 3 • • 2 • 1 • • 2 • • • • 2 • • 1 • • • • • 1 • • • • • • • • • • 1 • • • • • • 1 • • • • 1 • 5 • • • • • 5 •</pre>	<pre>• • • • • • 5 • • 3 • • • • • • • 1 • • • • • • • 4 • 1 • • • • • • 4 2 • • • • • 4 • • 3 • • • • 1 • • 2 • • • • • • • • • • 4 • • • • • • 2 • • • • • • • • • • • 5 • • • 4 • • • • • • • • • 3 • • 4 • 3 • • • • • • • 2 • • • • • 3 1 • • • • • • • • 1 • • • 1 • • • 1 • • • 2 • • • • • 3 • • • • • 2 • • • •</pre>
	Case 4	Case 6	
$(\frac{1}{3}, \frac{1}{3})$	<pre>• • • • • • • • • • • • • • • • • • • 2 • • • • • • 2 • 2 4 • • • 2 • 2 4 • 4 • • • 2 • • 4 • 4 • • • • • • 4 • • • • • • 3 • • • • • 3 • • • • • • 3 • • • • • • 3 • • • • • • 3 • • • • • • 3 • 5 • • • • • • • • 5 • • • • • • • 1 • • • • • • 1 • 1 • • • • 1 • 1 • • • • • • 1 •</pre>	<pre>• • • • • • • • • • • • • 1 • • • • • 1 • • • • • • 4 • • 1 • • 1 • • • • 4 • • • • 4 1 • • • • • 1 • • • • 4 • 5 • • 4 • • • • 2 • 5 • 4 • • • • • • • 2 • • • • • • • 2 • • • • 2 • • • • • • • • • • • 2 • • • • 2 • • 3 • • 3 • • • • • • • • • • 3 • • • • • 3 • • • • • • • • • • 3 • • • • • 3 • • • • • • • • • • • •</pre>	

Best designs found with respect to A_{nn}-criterion, for $\sigma_n^2 = 1$

(ρ_r, ρ_e)	Ψ_1	Ψ_3	Ψ_4
	Case 21	Case 23	Case 30
$(\frac{1}{2}, \frac{1}{2})$	(grid below)	(grid below)	(grid below)
	Case 24	Case 26	
$(\frac{1}{3}, \frac{2}{3})$	(grid below)	(grid below)	

Case 21 (Ψ_1):
```
5 • • 3 • • 2 •
• 1 • • • • • 3
• • • • • • • •
3 • • • • • • •
• • • • • • • 2
• 4 • • • • • •
• • • • • • 3 •
1 • • • • • • •
• • 3 • • • • 1
• • • • • • • •
• • • • • 2 • •
3 • • • • • • •
• • • • • • • 4
• 4 • • • • • •
• • • • • • 1 •
1 • • • • • • •
• • 4 • • • • 2
• 2 • • • • • •
• • 1 • • • 4 •
4 • • • 2 • • 5
```

Case 23 (Ψ_3):
```
5 • • • • • • 2
• • 1 • • • 4 •
• 4 • • • • • 1
• • • • • 2 • •
2 • • • • • • •
• • • • 1 • • •
• • • • • • • 4
4 • • • • • • •
• • • • • • 3 •
• 1 • • • • • •
• • • • • • • 3
3 • • • • • • •
• • 4 • • • • •
• • • 3 • • • •
2 • • • • • • •
• • • • • • • 3
• • • • • 2 • •
• • • 4 • • • •
• 2 • • • • 1 •
1 • • • 3 • • 5
```

Case 30 (Ψ_4):
```
• 2 • • • • • •
• • • • 1 • • •
• 3 • • • • 4 •
• • • • 2 • • •
5 • • 1 • • • •
• • • • • 1 • •
• • • • 4 • • 2
• • • • • • • 4
• • 1 2 • • • •
1 • • • • 3 • •
• • • • • • 3 •
• • • • • • • 3
• • 4 • • • • •
• 4 • • • • • •
• • • • • 2 • •
3 • • 5 • • • •
• • • • • • 1 •
• • 2 • • • • •
4 • • • • • • •
• • • 3 • • • •
```

Case 24 (Ψ_1):
```
• 4 • 3 • 4 • 5
3 • 1 • 2 • 3 •
• • • • • • • •
• • • • • • • •
• • • • 3 • • •
• • • • • • • •
1 • • 3 • • • 3
• • 3 • • • • •
• • • • • • 2 •
• • • • • • • •
• • • • • • • •
• 1 • • • • • •
• • • • • • • 4
2 • • • • 2 • •
• • • 1 • • • •
• • • • • • • •
• • • • • • • •
• 2 • • 2 • 4 •
4 • 1 4 • 1 • 5
```

Case 26 (Ψ_3):
```
5 • 3 • • 4 • 1
• 2 • • • • • •
• • • • 1 • • •
• • • • • • 3 •
• • • • • • • 2
3 • • • • • • •
• • • 4 • • • •
• • 2 • • • • •
• • • • • • • 3
• • • • • • 2 •
• • • • • 3 • •
• • • • 2 • • •
1 • • • • • • •
• • • • • • • 4
• • • 1 • • • •
• • 4 • • • • •
• 1 • • • • • •
• • • • 3 • • •
• • • 2 • • 4 •
4 • • • • 1 • 5
```

Best designs found with respect to A_{ns}-criterion, for $\sigma_n^2 = 1$

(ρ_r, ρ_e)	Ψ_1	Ψ_3	Ψ_4
	Case 21	Case 23	Case 30
$(\frac{1}{2}, \frac{1}{2})$	(see grid below)	(see grid below)	(see grid below)
	Case 24	Case 26	
$(\frac{1}{3}, \frac{2}{3})$	(see grid below)	(see grid below)	

Case 21 (Ψ_1, $(\frac{1}{2}, \frac{1}{2})$):

```
. . . . . . . . .
. . . 4 . . . . .
. . . . . . 4 .
. . 1 . . . . .
. . . 4 1 . .
. . . 1 4 . .
. 1 . . . . . .
. . . . . . 1 .
. . . 3 . . . .
. . . 4 3 . .
. . 2 . 3 1 2 .
. . . . 2 5 4 .
. . . . 5 3 . .
. 2 . . . . . .
. . . 3 . . . .
. . . . . 3 .
. . 2 . . . . .
. . . . 2 . .
. . . . . . . .
```

Case 23 (Ψ_3, $(\frac{1}{2}, \frac{1}{2})$):

```
. . . . . . . .
. 4 . . . . . .
. . . . 4 . . .
. . . . . . 3 .
. . 3 . . . . .
. . . 4 . . . .
4 . . . . . . .
. 3 1 . . 4 . .
. . 4 . 1 5 . .
. . . 2 5 3 . .
. . . 3 . 2 . .
. . . . . . . 3
2 . . . . . . .
. . . . . . 2 .
. . 2 . . . . .
. . . . 2 . 1 .
. . . 1 . . . .
. 1 . . . . . .
. . . . . 1 . .
```

Case 30 (Ψ_4, $(\frac{1}{2}, \frac{1}{2})$):

```
. . . . 2 . . .
. . 3 5 . . 2 .
. 4 . . . . . .
. 1 . . . . . .
. . . 3 . . . 1
. . 2 . . . . .
. . . . . 2 4 .
. . . . . . 1 2
4 . . . . . . .
2 . . . . . . .
. . . . 3 . . .
. 3 . . . 4 . .
. . . . 4 . . .
. . . . . . . 3
. . 1 . . . . .
. . . . . . . .
. . . . . 3 . .
1 . . 4 . . . .
. . . 1 . . 5 .
. . . . . . . .
```

Case 24 (Ψ_1, $(\frac{1}{3}, \frac{2}{3})$):

```
. . . . . . . .
. . . . . 2 . .
. . . 2 . . . .
. . . . . . 2 .
. . . . 3 . . .
. . . . . . . .
. . 2 4 . 3 . .
. 1 4 3 2 . . .
. 3 1 5 . . . .
. . 5 2 3 . . .
1 . 4 . . . 3 .
. . . . . . . .
. 1 . . . 4 . .
. . . 1 . . . .
. . . . . . . .
. . . . 4 . . .
. . 1 . . . 4 .
. . . . . . . .
. . . . $\Psi_1$ . . .
```

Case 26 (Ψ_3, $(\frac{1}{3}, \frac{2}{3})$):

```
. . . . . . . .
. . . . . 2 . .
. . . 2 . . . .
. . . . . . . 2
2 . . . . . . .
. . . . 2 . 4 .
. 2 5 . 4 . . .
. 5 4 . . . . .
. . . 3 . 4 . .
. 3 . 4 . . . .
4 . . . . 3 . .
. . . . . . . 3
. . 1 . 3 . . .
. . 3 . 1 . . .
. 1 . . . . . .
. . . . 1 . . .
. . . . . . 1 .
1 . . . . . . .
. . . . . . . .
```

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