OPTIMAL PAIRED COMPARISON DESIGNS FOR FACTORIAL EXPERIMENTS

PROEFSCHRIFT

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Contents

Preface

The name of R.A. Bradley (together with that of M.E. Terry) is associated with a model that is widely employed in paired comparisons. Therefore, it seems appropriate to begin this thesis with a quotation from Bradley (1976).

> Consulting statisticians are familiar with the consultee who, after describing his proposed experiment in several sentences has only one question: "How many observations do I need ?".

In particular the consultee might be tempted to ask this question when paired comparisons are involved. In paired comparison experiments observations are made by presenting pairs of objects to one or more judges. This method is used extensively in experimental situations where objects can be judged only subjectively, that is to say, when it is impossible or impracticable to make relevant measurements in order to decide which of two objects is preferable. When all pairs are presented to each of n judges (round robin), then the number of paired comparisons is $n\ \binom{t}{2}$, where t is the number of objects. This number is often too large for practical purposes. Bradley and Terry postulate the existence of parameters, π_i for T_i, where T_i is the i-th object or treatment. In many cases these parameters are functions of quantities determining the objects and a linear model can be formulated. The information from this model can be used to construct designs, that are more efficient than the round robin design, i.e., less comparisons are needed to measure the parameters of the linear model with the same accuracy as the round robin design. The aim of this thesis is to construct such designs.

The method of paired comparisons provides a simple experimental technique. However, many models have been formulated for paired comparison experiments. Some of these models and procedures are discussed in section 1. These procedures yield covariance matrices of the estimators for the unknown parameters. These covariance matrices are in particular important with regard to the construction of optimal designs, because many criteria depend on the covariance matrix of the estimators. However, these matrices depend in general on the unknown parameters. Therefore, the assumption of no differences in treatment is made in order to construct optimal designs. In section 1 it is shown that in this case an ordinary linear model can be applied for constructing optimal designs. In section 2 a general approach for the construction of D-optimal designs for paired comparisons is given. This approach assumes an underlying structure. It uses the equivalence of the D-criterion and the G-criterion, when adapted to the situation of paired comparisons. This approach is more general than the above approach, where the objects are fixed. Now they may be chosen in a given experimental region. The concept of exact and discrete designs is introduced. The latter designs are useful in constructing optimal designs. A discrete design consists of, say, N pairs with weights p_i, such that $p_1 + \cdots + p_N = 1$. Exact designs can be used in practical applications. They can de defined as discrete designs with rational p_i .

Applications are given in sections 3, 4 and 5.
Section 3 deals with a factorial model with main effects and first-order interactions. Exact D-optimal designs are given both for the case of a hypersphere as experimental region and for the case of a hypercube as experimental region. Some of these results are known in the literature. Sections 4 and 5 deal with a quadratic model, in section 4 with a hypersphere as experimental region, in section 5 with a hypercube as experimental region. In both sections discrete D-optimal designs are presented. Some of these designs have a large number of pairs, in particular in the case of a hypercube of high dimension. Therefore discrete D-optimal designs are given for which the number of pairs is reduced considerably. Using these discrete designs we construct exact designs with a high efficiency and with a relatively small number of pairs. The robustness of the discrete designs is investigated, i.e. we discuss the efficiency of the designs when the assumption of no differences in treatment does not hold.

1. Formulation of models for paired comparisons

1.1. Introduction

In paired comparison experiments observations are made by presenting objects in pairs to one or more judges. The word "object" may stand for item, treatment, stimulus, and the like. The judge has to declare which object of the pair presented he prefers. In the simplest situation the observations are 0 or 1, indicating the preference for one of the two objects. More generally the preference may be recorded on some finer scale, for example a 7-points scale ($-3,-2,-1, 0, 1, 2, 3$), implicitly allowing ties to be declared. The method of paired comparisons may be used in cases where objects can be judged only subjectively. So, applications have been to taste testing, consumer tests, psychophysical analysis, and more generally to situations where quantification through measurement is difficult.
Many models have been formulated with regard to paired comparison experiments. Some of these will be discussed in the following sections.

1.2. The Bradley-Terry model

A model, which is widely employed, is the model provided by Bradley and Terry (1952). The paired comparison experiment has t objects, $T_1, \ldots, T_t$, with n_{ij} judgements or comparisons of T_i and T_j, $n_{ij} \geqslant 0$, $n_{ii} = 0$, $n_{ji} = n_{ij}$, $i, j = 1, \ldots, t$. Let $n_{i.ij}$ be the number of times T_i has been preferred to T_j when T_i and T_j were compared, $n_{i.ij} = n_{i.ji}$, $n_{i.ij} + n_{j.ij} = n_{ij}$ $(i \neq j)$. So in the model it is not allowed to declare ties.
Bradley and Terry postulate the existence of parameters, π_i for T_i, $\pi_i > 0$, such that the probability $\pi_{i.ij}$ of selecting T_i when compared with T_j is

$$\pi_{i.ij} = \frac{\pi_i}{\pi_i + \pi_j}, \ (i \neq j). \tag{1.2.1}$$

Since (1.2.1) is not dependent on parameter scale, convenient scale-determining constraints are formulated like

$$\sum_{i=1}^{t} \pi_i = 1 , \tag{1.2.2}$$

or

$$\sum_{i=1}^{t} \log \pi_i = 0 . \tag{1.2.3}$$

Likelihood methods can be used to estimate these parameters. On the assumption of independent selections, the likelihood function is

$$L(\pi) = \frac{\prod_i \pi_i^{a_i}}{\prod\prod_{i<j} (\pi_i + \pi_j)^{n_{ij}}} , \tag{1.2.4}$$

where

$$a_i = \sum_j n_{i.ij} \quad ,$$

and

$$\pi = (\pi_1, \ldots, \pi_t)' .$$

Maximizing (1.2.4), subject to (1.2.2), gives the likelihood equations

$$\frac{a_i}{p_i} - \sum_{j \neq i} \frac{n_{ij}}{p_i + p_j} = 0 \quad , i = 1, \ldots, t \quad , \tag{1.2.5}$$

$$\sum_{i=1}^{t} p_i = 1 \quad , \tag{1.2.6}$$

where p_i is the likelihood estimate of π_i.

Ford (1957) describes an iterative solution of the likelihood equations. Bradley (1955) gives large sample results and the asymptotic distribution of the maximum likelihood estimators. These results will be discussed later.

1.3. Generalizations of the Bradley-Terry model

There are many generalizations of the Bradley-Terry model. Rao and Kupper (1967) generalize the model by introducing a threshold parameter $\eta_0 \geqslant 0$. This parameter is interpreted as the threshold of sensory perception for the judge. They model the probabilities of preference and no preference as

$$\begin{aligned}
\pi_{i.ij} &= \frac{\pi_i}{\pi_i + \theta\pi_j} \quad , \\
\pi_{0.ij} &= \frac{\pi_i\pi_j(\theta^2 - 1)}{(\pi_i + \theta\pi_j)(\pi_j + \theta\pi_i)} \quad , \\
\pi_{j.ij} &= \frac{\pi_j}{\pi_j + \theta\pi_i} \quad ,
\end{aligned} \tag{1.3.1}$$

where

$$\theta = e^{\eta_0} . \tag{1.3.2}$$

For $\theta = 1$ the Rao-Kupper model coincides with the Bradley-Terry model. Rao and Kupper show that the maximum likelihood estimates p_i $(i = 1, \ldots, t)$ and $\hat{\theta}$ of π_i $(i = 1, \ldots, t)$ and θ are the solutions of the equations

$$\frac{b_i}{p_i} - \sum_{j \neq i} \frac{n_{0.ij} + n_{i.ij}}{p_i + \hat{\theta}p_j} - \sum_{j \neq i} \frac{(n_{0.ij} + n_{j.ij})\hat{\theta}}{p_j + \hat{\theta}p_i} = 0 \quad , i = 1, \ldots, t \quad , \tag{1.3.3}$$

where

$$b_i = \sum_j (n_{0.ij} + n_{i.ij}) \ ,$$

and

$$\sum_{i=1}^{t} p_i = 1 \ .$$

Beaver and Gokhale (1975) generalize the model in order to incorporate within-pair order effects. They assume the existence of parameters $\delta_{ij},\ i,j=1,\ldots,t,\ \delta_{ij} = \delta_{ji}$, associated with the pair (i,j) such that the preference probabilities for the ordered pair (i,j) are

$$\pi_{i.ij} = \frac{\pi_i + \delta_{ij}}{\pi_i + \pi_j} \ ,$$

$$\pi_{j.ij} = \frac{\pi_i - \delta_{ij}}{\pi_i + \pi_j} \ , \qquad (1.3.4)$$

where

$$|\delta_{ij}| \leqslant \min\{\pi_i \ , \pi_j\} \ .$$

In this model the likelihood equations are rather complicated. We refer to Beaver and Gokhale (1975) who also describe an iterative technique to find solutions.

1.4. Weighted least squares approach

Beaver (1977) presents a general approach to the models defined above. His results concerning the covariance matrix of the estimators are used later on. Therefore, some results are given here. Beaver uses a method described by Grizzle, Starmer and Koch (1969), who present a unified approach to the analysis of data resulting from an experiment involving s multinomial populations, each having r categories.

Let $m_{i_1}, m_{i_2}, \ldots, m_{i_r}$ be the observed cell counts for the i-th multinomial population resulting from $m_{i.} = \sum_{j=1}^{r} m_{ij}$ observations, $i = 1,\ldots,s$.

Let

$$\bar{p}_i = (p_{i_1}, \ldots, p_{i_r})' \ , \qquad (1.4.1)$$

be the sample estimate of the cell probabilities

$$\bar{\pi}_i = (\pi_{i_1}, \ldots, \pi_{i_r})' \ , \qquad (1.4.2)$$

and let $V(\bar{p}_i)$ be the usual sample estimate of the covariance matrix of $\bar{p}_i$ $(i = 1,\ldots,s)$.

Define (1.4.3)

$\overline{\pi}$ $= (\overline{\pi}_1', \ldots, \overline{\pi}_s')'$,

$\bar{p}$ $= (\bar{p}_1', \ldots, \bar{p}_s')'$,

$\overline{V}(\bar{p})$ = block diagonal matrix of dimension rs x rs having $V(\bar{p}_i)$ as the i-th diagonal block,

$f_m(\overline{\pi})$ = any function of the elements of $\overline{\pi}$ having continuous partial derivatives up to second order with respect to the elements of $\overline{\pi}$, $m = 1, \ldots, u$, with $u \leqslant (r-1)s$,

$F(\overline{\pi})$ $= (f_1(\overline{\pi}), \ldots, f_u(\overline{\pi}))'$,

H = a matrix of dimension u x rs with

$$H_{kl} = \frac{\partial f_k(\overline{\pi})}{\partial \pi_{ij}} \text{ , where } i \text{ and } j \text{ are such that}$$

$$l = j \pmod r\ ,\ 0 \leqslant j < r\ ,\ i = (l-j)/r + 1\ ,$$

S $= H\ \overline{V}(\bar{p})\ H'$ of dimension u x u .

When the u parametric and possibly nonlinear functions f_m are functionally independent of one another and of the sums $\sum_{j=1}^{r} \pi_{ij}$ $(i = 1, \ldots, s)$, then both H and S are of rank u.

Let

$$F(\overline{\pi}) = X\beta \ , \tag{1.4.4}$$

where X is a known matrix of dimension u x v and of rank v, and β is a vector of unknown parameters. As Beaver (1977) points out, weighted regression produces the best asymptotic normal estimate of β given by

$$\hat{\beta} = (X'S^{-1}X)^{-1}X'S^{-1}F(\bar{p}) \ . \tag{1.4.5}$$

The elements of S are stochastic. If they are not stochastic, then the covariance matrix of $\hat{\beta}$ is equal to

$$var\,\hat{\beta} = (X'S^{-1}X)^{-1} \ . \tag{1.4.6}$$

Therefore, one can expect that equation (1.4.6) is asymptotically correct if the elements of S are stochastic. An important special case of $F(\overline{\pi})$ involves a loglinear function of $\overline{\pi}$. For a positive matrix A of dimension k x l we define $\log A$ by $(\log A)_{ij} = \log(A_{ij})$, for all $i = 1, \ldots, k$, $j = 1, \ldots, l$. When $F(\overline{\pi}) = K \log(A\,\overline{\pi})$ with K of dimension t x u and of rank $t < u$, then

$$H = K\ D_a^{-1} A \ ,$$

and

$$S = K\ D_a^{-1} A\ \overline{V}(\bar{p})\ [K\ D_a^{-1} A]' \ ,$$

where D_α is a diagonal matrix with the elements of $A\,\bar{p}$ on the diagonal. The use of $\log \pi_i$ instead of π_i will be discussed later.
The model of Beaver specializes to the Bradley-Terry model as follows.

Let

$$
\begin{aligned}
r &= 2, \\
\bar{\pi} &= (\pi_{1.12}, \pi_{2.12}, \pi_{1.13}, \pi_{3.13}, \ldots, \pi_{t-1.t-1\,t}, \pi_{t.t-1\,t})' , \\
\bar{p} &= (p_{1.12}, p_{2.12}, p_{1.13}, p_{3.13}, \ldots, p_{t-1.t-1\,t}, p_{t.t-1\,t})' ,
\end{aligned}
$$

where

$$
\begin{aligned}
p_{i.ij} &= n_{i.ij} \,/\, n_{ij} \text{ , an estimate of } \pi_{i.ij} \;; \\
f_{ij}(\bar{\pi}) &= \log (\pi_{i.ij} \,/\, \pi_{j.ij}) \;, \\
F(\bar{\pi}) &= (f_{12}, f_{13}, \ldots, f_{1t}, f_{23}, \ldots, f_{t-1t})' .
\end{aligned}
$$

Now, $\bar{V}(\bar{p})$ is a block diagonal matrix of dimension $2\binom{t}{2} \times 2\binom{t}{2}$ having as blocks the matrices

$$
\frac{1}{n_{ij}} \begin{vmatrix} p_{i.ij}p_{j.ij} & -p_{i.ij}p_{j.ij} \\ -p_{i.ij}p_{j.ij} & p_{i.ij}p_{j.ij} \end{vmatrix} ,
$$

and S is a diagonal matrix with diagonal elements $(n_{ij}\; p_{i.ij}\; p_{j.ij})^{-1}$.
Let, according to the Bradley-Terry model,

$$
\log (\pi_{i.ij}/\pi_{j.ij}) = \log \pi_i - \log \pi_j \quad ,
$$

and so

$$
F(\bar{\pi}) = K \;\log \pi \quad ,
$$

with

$$
K = \begin{bmatrix}
1 & -1 & 0 & 0 & \ldots & 0 & 0 \\
0 & 0 & 1 & -1 & \ldots & 0 & 0 \\
. & . & . & . & & . & . \\
. & . & . & . & & . & . \\
. & . & . & . & & . & . \\
0 & 0 & 0 & 0 & \ldots & 1 & -1
\end{bmatrix} .
$$

If we write $\alpha_i = \log \pi_i - \log \pi_t \quad (i = 1, \ldots, t-1)$,
then

$$F(\overline{\pi}) = \begin{bmatrix} 1 & -1 & 0 & \ldots & 0 & 0 \\ 1 & 0 & -1 & \ldots & 0 & 0 \\ \cdot & \cdot & \cdot & & \cdot & \cdot \\ \cdot & \cdot & \cdot & & \cdot & \cdot \\ \cdot & \cdot & \cdot & & \cdot & \cdot \\ 1 & 0 & 0 & \ldots & 0 & -1 \\ 1 & 0 & 0 & \ldots & 0 & 0 \\ 0 & 1 & -1 & \ldots & 0 & 0 \\ \cdot & \cdot & \cdot & & \cdot & \cdot \\ \cdot & \cdot & \cdot & & \cdot & \cdot \\ \cdot & \cdot & \cdot & & \cdot & \cdot \\ 0 & 0 & 0 & \ldots & 0 & 1 \end{bmatrix} \begin{bmatrix} \alpha_1 \\ \alpha_2 \\ \cdot \\ \cdot \\ \cdot \\ \alpha_{t-1} \end{bmatrix} .$$

Now, the α_i can be estimated by use of (1.4.5), and the estimates of the π_i are easily obtained from the estimates of the α_i with the constraint (1.2.6).

1.5. Response surface fitting

Springall (1973) assumes that the π_i $(i=1,\ldots,t)$ are functions of continuous independent variables $x_1,\ldots,x_s$. As in the classical regression situation, the most useful functions are those that are linear in the unknown parameters, i.e,

$$\log \pi_i = \sum_{k=1}^{s} x_{ik}\, \beta_k \quad . \tag{1.5.1}$$

Using a method similar to that of Rao and Kupper (1967), Springall obtains results concerning the covariance matrix $(\nu_{lr})^{-1}$ of his estimators $\hat{\theta}$ of θ and $\hat{\xi}_i$ of ξ_i, where

$$\xi_i = e^{\beta_i} \quad (i=1,\ldots,s) \quad ,$$

and

θ as defined in (1.3.1) .

His results are listed as

$$\nu_{00} = 2n_0 \frac{\theta^2+1}{(\theta^2-1)^2} - \sum_{i<j}\sum n_{ij}\, \phi^*_{ij}\, \theta^{-1} \quad ,$$

$$\nu_{0r} = \frac{1}{\xi_r \theta} \sum_{i<j}\sum n_{ij}\, \phi^*_{ij}\, (x_{jr} - x_{ir}) \qquad r=1,\ldots,s \quad ,$$

$$\nu_{rq} = \frac{1}{\xi_r \xi_q} \sum_{i<j}\sum n_{ij}\, \phi^*_{ij}\, (x_{ir} - x_{jr})(x_{iq} - x_{jq}) \qquad r,q=1,\ldots,s \, , \tag{1.5.2}$$

where

$$\phi^*_{ij} = \frac{\theta^2 \pi_i \pi_j \left[\theta\,(\pi_i^2 + \pi_j^2) + 2\pi_i\pi_j\right]}{(\pi_i + \theta\pi_j)^2\,(\pi_j + \theta\pi_i)^2} \; .$$

These results contain some mistakes, even when the random variable n_0 is replaced by its expectation. They should read

$$\nu_{00} = \sum\sum_{i<j} n_{ij} \left[\frac{\theta^2+3}{\theta^2(\theta^2-1)} \phi_{ij}^{*} + \frac{4\pi_i^2\pi_j^2}{(\pi+\theta\pi_j)^2(\pi_j+\theta\pi_i)^2} \right] ,$$

$$\nu_{0r} = \frac{1}{\xi_r} \sum\sum_{i<j} n_{ij} \frac{\pi_i\,\pi_j\,\theta^2(\pi_j^2-\pi_i^2)(x_{ir}-x_{jr})}{(\pi_i+\theta\pi_j)^2(\pi_j+\theta\pi_i)^2} , \tag{1.5.3}$$

ν_{rq} as above.

In deriving the covariance matrix $(\lambda_{rq})^{-1}$ of the estimators of β Springall uses

$$\lambda_{0r} = \nu_{0r}/\xi_{0r} \quad ,$$

$$\lambda_{rq} = \nu_{rq}/(\xi_r\,\xi_q) .$$

This is not correct, it should be

$$\lambda_{rq} = \xi_r\;\xi_q\;\nu_{rq} .$$

When the Bradley-Terry model is used without the threshold parameter η_0 the results concerning the covariance matrix $(\lambda_{rq})^{-1}$ of the estimators $\hat{\beta}_l$ of β are

$$\lambda_{rq} = \sum\sum_{i<j} n_{ij}\;\phi_{ij}\;(x_{ir}-x_{jr})(x_{iq}-x_{jq}) \quad , \tag{1.5.4}$$

where

$$\phi_{ij} = \pi_i\;\pi_j/(\pi_i+\pi_j)^2 = \pi_{i.ij}\;\pi_{j.ij} . \tag{1.5.5}$$

1.6. The covariance matrices of the estimators

For convenience we formulate (1.5.4) in a different fashion. Let X be a matrix of dimension $t \times s$, the elements of which are the x_{ik} from (1.5.1). This matrix plays the role of design matrix in the standard experimental situation with $\log \pi_i$ as observations.

Define

$$G = \begin{bmatrix} 1 & -1 & 0 & \dots & 0 & 0 \\ 1 & 0 & -1 & \dots & 0 & 0 \\ \cdot & \cdot & \cdot & & \cdot & \cdot \\ \cdot & \cdot & \cdot & & \cdot & \cdot \\ \cdot & \cdot & \cdot & & \cdot & \cdot \\ 1 & 0 & 0 & \dots & 0 & -1 \\ 0 & 1 & -1 & \dots & 0 & 0 \\ \cdot & \cdot & \cdot & & \cdot & \cdot \\ \cdot & \cdot & \cdot & & \cdot & \cdot \\ \cdot & \cdot & \cdot & & \cdot & \cdot \\ 0 & 0 & 0 & \dots & 1 & -1 \end{bmatrix} , \tag{1.6.1}$$

a matrix of dimension $\binom{t}{2} \times t$ having one +1, one -1, and $t-2$ zeroes in each row, such that

$$(G'G)_{ij} = \begin{cases} -1 & ,if \;\; i \neq j \;, \\ t-1 & ,if \;\; i = j \;. \end{cases}$$

The matrix G corresponds to a design where every two items are compared just once ($n_{ij} = 1; i, j = 1, \ldots, t, \; i \neq j$).
Define

$$D = G\,X \quad , \tag{1.6.2}$$

$$\Phi(\pi) = \operatorname{diag}(n_{12}\phi_{12}, n_{13}\phi_{13}, \ldots, n_{1t}\phi_{1t}, n_{23}\phi_{23}, \ldots, n_{t-1\,t}\phi_{t-1\,t}), \tag{1.6.3}$$

a matrix of dimension $\binom{t}{2} \times \binom{t}{2}$. It is easily verified that (1.5.4) may be rewritten as follows:

$$\begin{aligned} \lambda_{rq} &= -\sum_{i<j}\sum x_{ir}\, n_{ij}\,\phi_{ij}\, x_{jq} - \sum_{i<j}\sum x_{jr}\, n_{ij}\,\phi_{ij}\, x_{iq} \\ &\quad + \sum_{i<j}\sum x_{ir}\, n_{ij}\,\phi_{ij}\, x_{iq} + \sum_{i<j}\sum x_{jr}\, n_{ij}\,\phi_{ij}\, x_{jq} \\ &= \sum_{i\neq j}\sum x_{ir}(-n_{ij}\phi_{ij})x_{jq} + \sum_{i} x_{ir}\Big(\sum_{j\neq i} n_{ij}\phi_{ij}\Big)x_{iq} \\ &= \sum_{i\neq j}\sum x_{ir}(G'\Phi(\pi)G)_{ij}\,x_{jq} + \sum_{i} x_{ir}(G'\Phi(\pi)G)_{ii}\,x_{iq} \;. \end{aligned}$$

Hence

$$(\lambda_{rq})^{-1} = (D'\,\Phi(\pi)\,D)^{-1} \;. \tag{1.6.4}$$

The methods of Beaver and Bradley-Terry can also be used to estimate the parameters of the model (1.5.1). Actually, El-Helbawy and Bradley(1978) analyse factorial models and give large-sample results. Asymptotically, the covariance matrix of the estimators of the parameters coincides with the matrix given in (1.6.4). This is to be expected since the methods are based on maximum likelihood estimation of the parameters. It may also be verified as follows.

Let n be the number of factors, the i-th factor has b_i levels, so that $t = \prod_{i=1}^{n} b_i$.

The general problem in the model of El-Helbawy and Bradley is to estimate the parameters μ_i, $i = 1, \ldots, t$ under the conditions

$$\begin{bmatrix} 1_t' \\ B_m \end{bmatrix} \mu = 0 \;, \tag{1.6.5}$$

where

$$\mu \quad = (\mu_1, \ldots, \mu_t)' \;,$$

$\mu_i \quad = \log \pi_i$,

$1_t \quad = (1, \ldots, 1)'$,

$1_t'\mu$ is the constraint (1.2.3),

$B_m \mu = 0$ means that m specified orthonormal contrasts are zero.

This problem is solved by estimating the other $t-m-1$ orthonormal contrasts; these can be written as linear combinations of the μ_i :

$$\theta_1 = B_m^* \mu \ , \tag{1.6.6}$$

where B_m^* is a $(t-m-1) \times t$ matrix, and

$$\begin{bmatrix} 1_t'/\sqrt{t} \\ B_m \\ B_m^* \end{bmatrix} [\, 1_t/\sqrt{t} \quad B_m' \quad B_m^{*\prime} \,] = I$$

It follows that

$$\mu = B_m^{*\prime} \, \theta_1 \, .$$

The result is

Asymptotically $(\hat{\theta}_1 - \theta_1)$ *has the asymptotic* $(t-m-1)$ *variate normal distribution with zero expectations and covariance matrix* $(B_m^* \, \Lambda(\pi) \, B_m^{*\prime})^{-1}$, *where* (1.6.7)

$$\Lambda(\pi) = \begin{cases} -n_{ij}\phi_{ij} & ,if \ \ i \neq j \ , \\ \sum\limits_{k \neq i} n_{ik}\phi_{ik} & ,if \ \ i = j \ . \end{cases}$$

We can reformulate these results as follows.
If

$$X = \sqrt{t} \ B_m^{*\prime} \ ,$$

then X can be regarded as the design matrix in the standard experimental situation with an appropriate model of type (1.5.1). Hence (1.6.6) is equivalent to

$$\mu = X \beta \ ,$$

and the estimator of β is $\hat{\beta} = \hat{\theta}_1/\sqrt{t}$.
Now

$$var \ (\hat{\theta}_1/\sqrt{t}\,) = (tB_m^* \, \Lambda(\pi) \, B_m^{*\prime})^{-1} = (X'\,G'\,\Phi(\pi)\,G\,X\,)^{-1} \, .$$

So, (1.6.7) may be rewritten as

$$var \ \hat{\beta} = (D'\,\Phi(\pi)\,D\,)^{-1} \ , \tag{1.6.8}$$

which coincides with (1.6.4).
The estimation procedure of Beaver is asymptotically equivalent to maximum

likelihood, so we may expect both procedures to lead to the same asymptotic covariance matrix when applied to the parameters of model (1.5.1). It can be shown that the results given in (1.4.3) and (1.4.6) can be rewritten as follows.

$$F(\overline{\pi}) = G \log \pi = G X \beta = D \beta . \qquad (1.6.9)$$

In section 1.4 we have seen that

$$S^{-1} = \Phi(\hat{\pi}) ,$$

where $\Phi(\hat{\pi})$ is the matrix $\Phi(\pi)$ in which the $\pi_{i.ij}$ have been replaced by the estimates $p_{i.ij}$. Substituting this in (1.4.6) we find

$$var\,\hat{\beta} = (D'\,\Phi(\hat{\pi})\,D)^{-1} . \qquad (1.6.10)$$

1.7. Generalized linear models

Generalized linear models provide a unified approach and computational framework for analysing data. McCullagh and Nelder (1983) give an extensive account of the applications generalized linear models have. Computer packages have been designed for analysing data by means of generalized linear models. One of them, GLIM, is widely used now.

McCullagh and Nelder formulate the generalized linear model in the following tripartite form.

i) *The random component:* a vector of observations y of lenght N is assumed to be a realization of a random vector Y with stochastically independent components. The components of Y have a distribution of an exponential family. These distributions are of the same form (e.g. all normal, or all binomial, etc.). The vector of expectations is $m = (m_1, \ldots, m_N)'$.

ii) *The systematic component:* the independent variables (or covariates) $x_1, x_2, \ldots, x_s$ produce a linear predictor η given by (1.7.1)

$$\eta = X \beta ,$$

where X is the design matrix with elements x_{ij}.

iii) *The link function* between the random component and the systematic component

$$\eta_i = g(m_i) .$$

This link function g may be any monotonic differentiable function.

The Bradley-Terry model may be formulated as a generalized linear model. Let N be the number of pairs for which $n_{ij} > 0$. Let N be the i-th row of the matrix X be denoted by x_{i*}' and the k-th column of X by x_{*k}. An object can be characterized by its row in the design matrix. Let y_l be the observation related to the pair characterized by x_{i_1*} and x_{i_2*}. Now, the observation y_l is a realization of a random variable Y_l, having a binomial distribution with parameters $n_{i_1 i_2}$ and $\pi_{i_1.i_1i_2}$. We choose the logit function $g(x) = \log(x/(1-x))$ as

the link function. This function maps the unit interval (0,1) onto the real line $(-\infty, \infty)$. So, we have

$$\eta_l = g(\pi_{i_1 \cdot i_1 i_2}) = \log \left[\frac{\pi_{i_1}}{\pi_{i_1} + \pi_{i_2}} / (1 - \frac{\pi_{i_1}}{\pi_{i_1} + \pi_{i_2}}) \right] = \log \frac{\pi_{i_1}}{\pi_{i_2}} \quad ,$$

or

$$\eta_l = \log \pi_{i_1} - \log \pi_{i_2} \, . \tag{1.7.2}$$

The independent variables produce the η_l given by

$$\eta_l = \sum_{l=1}^{s} z_{il} \, \beta_l \quad ,$$

where

$$z_{il} = x_{i_1 l} - x_{i_2 l} \, .$$

Substituting this in (1.7.2), we obtain

$$\log \pi_{i_1} - \log \pi_{i_2} = \sum_{l=1}^{s} (x_{i_1 l} - x_{i_2 l}) \, \beta_l \quad , \tag{1.7.3}$$

in which we can recognize the model (1.5.1).
Now, the advantage of using $\log \pi_i$ instead of π_i is becoming clear. The use of $\log \pi_i$ will be discussed also when dealing with Thurstone's model in section 1.9 .

Fienberg and Larntz (1976) give a log linear representation for paired comparisons (and for multiple comparisons). They reformulate the model and show that it coincides with a log linear model of quasisymmetry for a $t \times t$ contingency tabel. The likelihood equations for this model can be solved using a version of the general iterative scaling technique described by Darrock and Ratcliff (1972).

1.8. Ordinary linear model

It is possible to formulate an ordinary linear model by choosing an appropriate distribution and link function in (1.7.1).
If the assumption is made that

i) The Y_i in (1.7.1) are independent and normally distributed with constant variance σ^2 and expectation m_i, (1.8.1)
ii) The link function is the identity function,

then the generalized linear model coincides with an ordinary model.
We have

$$Y = D^t \beta + e \quad , \tag{1.8.2}$$

where

$Y \quad = (Y_1, Y_2, \ldots, Y_{N_1})'$,

$Y_l \quad =$ a random variable indicating difference or preference,

$N_1 = \sum\sum_{i<j} n_{ij}$,

$D^* \;=$ the design matrix of dimension $N_1 \times s$,

$\beta \quad = (\beta_1, \ldots, \beta_s)'$,

$e \quad =$ the disturbance vector with $Ee = 0$, $var\ e = \sigma^2 I$.

In general the assumption $var\ e = \sigma^2 I$ does not hold when paired comparisons are made. The matrix D^* may be written as follows

$$D^* = G^* X \quad , \tag{1.8.3}$$

where X is the usual design matrix in a classical experiment, G^* is a matrix analogous to G. It has in each row one +1, one -1 and t-2 zeroes; a row is repeated n_{ij} times, when the objects T_i and T_j are compared n_{ij} times.
The least squares estimator for β is

$$\hat{\beta} = (D^{*\prime} D^*)^{-1} D^{*\prime} Y \quad ,$$

and

$$var\ \hat{\beta} = (D^{*\prime} D^*)^{-1} \sigma^2 . \tag{1.8.4}$$

This may be rewritten as:

$$D^{*\prime} D^* = X' G^{*\prime} G^* X = 4(X' G' \Phi(1_t) G X) = 4D' \Phi(1_t) D .$$

Hence

$$var\ \hat{\beta} = \frac{1}{4}\sigma^2 (D' \Phi(1_t) D)^{-1} . \tag{1.8.5}$$

The matrix (1.8.5) is proportional to the matrix in (1.6.4), if

$$\pi = (1, \ldots, 1)'. \tag{1.8.6}$$

Quenouille and John (1971) use the ordinary linear model when constructing designs for 2^n-factorials. However, if one uses the generalized linear model when constructing optimal designs, then the covariance matrix depends on the unknown parameters. In general there are no estimates of the parameters, since the parameters should be estimated from the experiment which is being designed. Therefore, assumption (1.8.6) is made very often. But in that case the generalized linear model coincides with the ordinary linear model. Actually the designs given by Springall (1973) and El-Helbawy and Bradley (1978) for 2^n-factorials may be found by using the method developed by Quenouille and John. Hence, the ordinary linear model is very useful in constructing optimal designs for paired comparison experiments.

1.9. Thurstone's model

The method of paired comparisons has applications in the fields of psychophysics and its use has been stimulated especially by the work of L.L.Thurstone. The method of paired comparisons is very useful in these fields, since the objects or the effect of stimuli can be judged only subjectively. A problem which has attracted much attention in phychophysics is: how is the subjective sensation in the consciousness of the subject related to the intensity of a continuously varying stimulus. Thurstone (1927) called the processes by which the subject discriminates or reacts to stimuli "discriminal processes", and he formulated the following model.

Each stimulus gives rise to a subjective value in a so-called sensory continuum. This subjective value is interpreted as the realization of a random variable which is real-valued and normally distributed. Following Bock and Jones (1968) in formulating this, one may represent the discriminal process associated with a stimulus T_i as a random variable v_i:

$$v_i = \mu_i + e_i \quad , \tag{1.9.1}$$

where μ_i is the fixed component and e_i is the random component. For T_j we have $v_j = \mu_j + e_j$, so

$$v_i - v_j = (\mu_i - \mu_j) + (e_i - e_j) \; . \tag{1.9.2}$$

The joint distribution of e_i and e_j is assumed to be bivariate normal with expectations 0, variances σ_i^2 and σ_j^2 , and correlation coefficient ρ_{ij} .

The probability that T_i will be preferred to T_j is given by

$$P(T_i > T_j) = \frac{1}{\sqrt{2\pi}\sigma_{ij}} \int_0^\infty \exp\left| -\frac{1}{2}\left(\frac{y-\mu_{ij}}{\sigma_{ij}} \right)^2 \right| dy \; , \tag{1.9.3}$$

where

$$\sigma_{ij}^2 = \sigma_i^2 + \sigma_j^2 - 2\rho_{ij}\sigma_i\sigma_j \quad ,$$

and

$$\mu_{ij} = \mu_i - \mu_j \; .$$

So

$$P(T_i > T_j) = \Phi_0\left(\frac{\mu_{ij}}{\sigma_{ij}} \right) \; , \tag{1.9.4}$$

where Φ_0 is the standardnormal distribution function. Usually, the following assumption is made

$$\sigma_{ij} = 1 \quad , i,j = 1, \ldots , t \quad \text{(Thurstone's case 5).} \tag{1.9.5}$$

Then the model coincides with the generalized linear model of (1.7.1) with the observations coming from a binomial distribution and the probit function as the link function. Note that there is only one difference with the Bradley-Terry

model: the link function. The relation between the Bradley-Terry model and Thurstone's model can also be formulated as follows. If we substitute the "logistic" density function for the normal density function, then we have

$$P(T_i > T_j) = \frac{1}{4} \int_{-\mu_{ij}}^{\infty} sech^2 \frac{z}{2} \, dz \ . \tag{1.9.6}$$

This yields

$$P(T_i > T_j) = \frac{1}{2} \left| 1 + \frac{e^{\frac{1}{2}\mu_{ij}} - e^{-\frac{1}{2}\mu_{ij}}}{e^{\frac{1}{2}\mu_{ij}} + e^{-\frac{1}{2}\mu_{ij}}} \right| = \frac{e^{\mu_{ij}}}{1 + e^{\mu_{ij}}}. \tag{1.9.7}$$

If we define $\mu_i = \log \pi_i$, then $e^{\mu_{ij}} = \pi_i / \pi_j$ and (1.9.7) gives

$$P(T_i > T_j) = \frac{\pi_i / \pi_j}{1 + \pi_i / \pi_j} = \frac{\pi_i}{\pi_i + \pi_j} \ , \tag{1.9.8}$$

which we recogninize as the Bradley-Terry model. So values $\log \pi_i$ correspond to values μ_i on a subjective continuum. This yields another argument in favour of model (1.5.1).

Bock and Jones (1968) discuss procedures for estimating the parameters in the Thurstonian model. The results concerning the covariance matrix of the estimators are analogous to the results of section 1.6. When, analogous to (1.8.6), the assumption is made that the μ_i have the same value, then the covariance matrix coincides with the matrix given in (1.8.5). Hence the designs constructed under this assumption are also useful in the Thurstonian concept.

Remark

The models discussed in this chapter assume a unidimensional continuum. Davidson and Bradley (1969) derive a model for multivariate paired comparisons. In this model t objects are to be compared on p attributes. However, it is not always possible to examine a priori whether a certain attribute is unidimensional or not. Gokhale, Beaver and Sirotnik (1983) provide a model-robust approach to the analysis of paired comparison experiments. Their approach makes it possible to examine the assumption of unidimensionality.

2. A method to construct optimal designs and an adapted criterium

2.1. Introduction

In chapter 1 we have seen that the design of a paired comparison experiment may be indicated by its t objects and the n_{ij}, where n_{ij} is the number of comparisons of the i-th and j-th object. When n_{ij} is constant for all i and j, the experiment is called a balanced paired comparison experiment. It is also called a round robin design. This name refers to a round robin tournament as used in many sports where each of the t teams plays every other team a fixed number of times. The experiment may also be seen as an experiment designed for the standard experimental situation, since the problem of design is the same whether we have for two objects an expression of preference or two separate values. In the standard experimental situation the experiment is known as a balanced incomplete block design (BIB), the block size being two. A balanced incomplete block design is a design with the properties:

i) all objects occur equally frequently,

ii) all pairs of objects occur in each block equally frequently.

The number of observations of a round robin design depends on the number of objects. When the number of the objects is 50 and all objects are compared once, the number of observations amounts to $\binom{50}{2}$, or 1225. This gives a practical difficulty in paired comparison experiments. Therefore many incomplete paired comparison designs have been constructed. These are designs in which not all possible pairs occur. There is a relation between these designs and designs in the standard experimental situation. The partially balanced incomplete block designs (PBIB) of the standard experimental situation can be used to design experiments in the situation of paired comparisons. David (1963) gives a survey of the results obtained in this area and gives references.

2.2. The use of underlying information on the objects when constructing optimal designs; some results in the literature

In the design of experiments discussed above one does not use any information on the underlying structure of the objects. Sometimes there is no information available. However, if a model of type (1.5.1) can be formulated, then it gives information on the objects. This information can be used in the design of experiments. Using this information it is possible to design experiments which are more efficient, according to some criterion, in estimating the parameters of the model than the round robin design. In this area only a few results are available. The results obtained are by Quenouille and John (1971), Springall (1973) and El-Helbawy and Bradley (1978). These results will be discussed in the next sections.

2.2.1. The results of Quenouille and John for 2^n-factorials

Quenouille and John (1971) present 2^n-factorial paired comparison designs, which can be constructed in order to reduce the number of pairs required by ignoring information on higher-order interactions. Following Quenouille and John we illustrate the method by considering designs for 2^2-experiments. In a 2^2-experiment there are four objects (1), a , b and ab in the usual notation. In a round robin design we have 6 comparisons or blocks in terms of the standard experimental situation. These 6 blocks can be broken up into three sets of blocks

(a) : ((1),ab) , (a, b);
(b) : ((1), a) , (b,ab);
(c) : ((1), b) , (a,ab).

If one is not interested in the interaction AB, then it is better to use the set (a) only. Set (a) measures the main effects A and B, but gives no information on the interaction AB. Sets (b) and (c) both measure the interaction AB and a main effect. So, in a round robin a main effect is measured in 4 out of 6 blocks. In the design consisting of set (a) a main effect is measured in 2 out of 2 blocks. Therefore, the set (a) gives 50 percent more information on A and B than the round robin design. Now, in a 2^n-experiment the $\frac{1}{2}2^n(2^n-1)$ paired comparisons can be broken up into 2^n-1 sets of 2^{n-1} blocks. Each set may be generated from an initial block consisting of object (1) and another object. Now, depending on the effects on which information may be ignored, a design can be composed of one or more of these sets. When considering the efficiency, Quenouille and John compare the new design with a round robin design for each effect to be estimated. For a specified effect the efficiency is defined to be the ratio of the accuracy with which the same effect is measured in a round robin design. Some of the designs constructed by Quenouille and John will be given in chapter 3 where these designs will be discussed in a more general context. In computing the accuracy with which an effect is measured Quenouille and John assume that the observations in the paired comparison experiment have the same variance. Their analysis of paired comparison experiments can be described by the ordinary linear model (1.8.2). A drawback of the criterion Quenouille and John use is that the design constructed is compared with the round robin design. Therefore, it is only possible to give relative efficiencies. When a more efficient design is found, it only may be claimed that the new design is better than the round robin design. However, there might be a design which is better than the new design. Another disadvantage of the criterion is that the efficiency of the design must be given for each effect separately. In the 2^2-factorial mentioned above the efficiency of a main effect for the design consisting of the pairs ((1),ab) and (a, b) is 1.5, whereas the efficiency of the interaction is zero.

2.2.2. Analogue designs

Springall (1973) obtained some results in the design of paired comparison experiments. As we have seen in section 1.5 Springall uses model (1.5.1). When constructing designs Springall considers properties based on the elements of the covariance matrix. He introduces the concept of analogue designs. Analogue designs are designs for which the covariance matrix of the estimators is proportional to the covariance matrix in the standard experimental situation with the same designpoints. Without mentioning it explicitly, Springall uses in this context a slightly adapted model for the standard experimental situation:

$$\log \pi_i = \beta_0 + \sum_{k=1}^{s} x_{ik} \beta_k \quad . \tag{2.2.1}$$

Compared to the model (1.5.1) the parameter β_0 has been added. If one does not assume the model (2.2.1) for the standard experiment, then the results of Springall are not correct. However, there seems to be no clear argument for comparing the paired comparison experiment in the case of model (1.5.1) with the standard experiment in the case of model (2.2.1).
The main result is

Theorem 2.2.1
An -approximate- analogue design may be found by choosing

$$n_{ij} = [N \, (\phi^*_{ij} \sum_{k<l}\sum (\phi^*_{kl})^{-1}) + 0.5] \ , \tag{2.2.2}$$

where $[x]$ *denotes the integral part of* x *and* $N = \sum_{i<j}\sum n_{ij}$ *(N should be chosen in advance), and* ϕ^*_{ij} *as defined in (1.5.2).*

Of course, the n_{ij} depend on the ϕ^*_{ij} , which are unknown. The n_{ij} give an exact analogue design, if all n_{ij} are integers before the integerization stage. The covariance matrix of the estimators is, when the n_{ij} from (2.2.2) are chosen, proportional to the matrix in (1.8.5). It can easily be seen that this matrix is proportional to the covariance matrix in the standard experimental situation in the case of model (2.2.1). It follows that, when (1.8.6) holds, the round robin design is an analogue design. The analogue design obtained by use of (2.2.2) is -as Springall points out- one out of many and does not necessarily yield the covariance matrix with the smallest elements. Therefore, linear programming methods are used to obtain analogue designs with the smallest elements. However, the objective functions in this linear programming problem depend on the ϕ^*_{ij} and when giving an example Springall makes the assumption (1.8.6).
The concept of analogue designs has the advantage that it enables certain desirable properties -for example rotatibility- to be readily reproduced. However, other properties are not reproduced, for example D-optimality, a criterion which will be defined in the next section. Actually, these designs are in general not efficient with regard to D-optimality. Starting from a more general concept in

the design of paired comparison experiments D-optimal designs can be constructed. This concept will be given in section 2.3.

2.2.3. Results of El-Helbawy and Bradley

El-Helbawy and Bradley (1978) consider some optimality criteria for designs and some applications to factorials. First, they consider the situation where some specified null hypothesis is tested. They construct designs for which the asymptotic power of the test is maximized. The asymptotic power depends on π, and assumption (1.8.6) is made. This assumption is -as they point out- consistent with the null hypothesis that some specified effects are zero and the concept that any other effects present are of the same order of magnitude relative to N as the factorial effects or interactions under test. They give three examples of a null hypothesis for a 2^3-factorial and construct the appropriate designs. The designs found can also be constructed by the method of Quenouille and John.

They further discuss a method to construct D- , A- and E-optimal designs for factorials. D-optimal designs minimize the generalized variance or the determinant of the covariance matrix, A-optimal designs minimize the average variance, E-optimal designs minimize the largest eigenvalue of the covariance matrix. They give results for one example: a 2^3-factorial, where one is interested only in the three interactions involving a specified factor. The criteria mentioned above depend on the covariance matrix, which is a function of the unknown parameters. Again, assumption (1.8.6) is made, and El-Helbawy and Bradley find a design which is A-, D- and E-optimal. The design coincides with the design they obtained before when maximizing the asymptotic power in testing the null hypothesis that the three interactions are zero. This idea can be used in a more general context, as will be seen in section 2.3.

2.3. A general concept for the design of paired comparison experiments

For convenience we reformulate model (1.5.1):

$$\log \pi = f_1(x)\beta_1 + \cdots + f_k(x)\beta_k \quad , \tag{2.3.1}$$

where

$x \in X$,

$X \subset \mathbf{R}^n$,

$f_j : X \to \mathbf{R}$, continuous on the experimental region X .

In Fedorov's (1972) notation for designs in the standard experimental situation, the design of a paired comparison experiment may be written as a collection of variables

$$\begin{matrix} (u_1,v_1) , & (u_2,v_2) , & \ldots , & (u_m,v_m) , & \\ n_1 , & n_2 & \ldots , & n_m & , N , \end{matrix} \tag{2.3.2}$$

where

$$\sum_{i=1}^{m} n_i = N \text{ , and } u_i \ , v_i \in X \ .$$

The design should be interpreted as follows. In a pair (u_i, v_i) n_i comparisons are made. Now a design may be constructed by choosing both the (u_i, v_i) and the n_i. This is a more general viewpoint. Mostly the objects have been specified and so the pairs (u_i, v_i) are fixed. In that case only the n_i can be chosen. This was the situation in the previous section, where results in the literature were discussed. In the construction of a design as defined in (2.3.2) both the pairs -and therefore the objects- and the n_i have to be chosen. In the notation of Fedorov (1972) the design (2.3.2) is denoted by $\epsilon(N)$ or just ϵ. In the standard experimental situation several criteria have been formulated for constructing optimal designs and many results have been obtained. A main result is a theorem about the equivalence of some criteria. Since the same criteria are applicable in paired comparison experiments, we like to formulate analogous theorems in this case. Therefore we give some well-known results for the standard experimental situation. Three criteria are mentioned in section 2.2.3 : A-, D- and E-optimality. Another important criterion is G-optimality. A G-optimal design minimizes the maximum variance (over X) of the estimated response function. All four criteria depend on the covariance matrix, or on its inverse, called the *information matrix*. In the standard experimental situation the collection of variables

$$\begin{array}{l} u_1, u_2, \ldots, u_m \\ n_1, n_2, \ldots, n_m \ , N , \end{array} \tag{2.3.3}$$

where

$$\sum_{i=1}^{m} n_i = N \ ,$$

is called the design of an experiment $\epsilon(N)$. If we assume model (2.3.1) and an ordinary least squares method, then the information matrix $M(\epsilon)$ may be written as

$$M(\epsilon) = \sum_{i=1}^{m} n_i \ f\,(u_i)(f\,(u_i))' \ , \tag{2.3.4}$$

where

$$f\,(u_i) = (f_1(u_i), f_2(u_i), \ldots, f_k(u_i))' \ . \tag{2.3.5}$$

Fedorov (1972) discusses the concept of a loss function $\lambda(x), x \in X$. This function can, for example, take into account the losses in time, money or material that come about and it will be used later on. Assuming this loss function $\lambda(x)$, we may generalize the information matrix as follows

$$M(\epsilon) = \sum_{i=1}^{m} n_i \ \lambda(u_i) \ f\,(u_i) \ (f\,(u_i))' \ . \tag{2.3.6}$$

The information matrix in (2.3.6) coincides with that in (2.3.4) when $\lambda(x) = 1$ for all $x \in X$. A normalized design $\epsilon(N)$ is a collection of variables

$$\begin{array}{l} u_1, u_2, \ldots, u_m, \\ p_1, p_2, \ldots, p_m, \end{array} \tag{2.3.7}$$

where

$$p_i = n_i / N \ ,$$

and

$$\sum_{i=1}^{m} p_i = 1 \ . \tag{2.3.8}$$

The design (2.3.7) is called an exact normalized design as distinct from a discrete normalized design, in which the p_i can take on any nonnegative value, satisfying (2.3.8). In a more general case a continuous normalized design will be characterized by a probability measure ξ on the region X. Continuous designs have no practical interest, but they are very useful in proving theorems concerning the optimality of designs. The information matrix of a continuous normalized design can be expressed by

$$M(\epsilon) = \int_X \lambda(x)\, f(x)\, (f(x))'\, d\,\xi(x) \ , \tag{2.3.9}$$

or in the case of an absolutely continuous measure

$$M(\epsilon) = \int_X \lambda(x)\, p(x)\, f(x)\, (f(x))'\, dx \ , \tag{2.3.10}$$

where

$$\int_X p(x)\, dx = 1 \ . \tag{2.3.11}$$

Remark

In Fedorov (1972) exact designs are called discrete and both discrete and continuous designs are called continuous. In Kiefer (1961) both exact and discrete designs are called discrete (or exact). □

Now, it is possible to formulate some theorems about D- and G-optimality. A design $\dot{\epsilon}$ is called D-optimal when

$$\det(M(\dot{\epsilon})) = \max_{\epsilon} \det(M(\epsilon)) \ . \tag{2.3.12}$$

A design $\dot{\epsilon}$ is called G-optimal when

$$\max_{x \in X} d(x, \dot{\epsilon}) = \min_{\epsilon} \max_{x \in X} d(x, \epsilon) \ , \tag{2.3.13}$$

where

$$d(x, \epsilon) = (f(x))'\, M^{-1}(\epsilon)\, f(x) \ , \tag{2.3.14}$$

the variance of the estimated response at a point $x \in X$.
The main theorem is

Theorem 2.3.1

a) The following assertions are equivalent:

(1) the design $\overset{*}{\epsilon}$ *maximizes* $\det(M(\epsilon))$,

(2) the design $\overset{*}{\epsilon}$ *minimizes* $\max\limits_{x \in X} \lambda(x)\, d(x,\epsilon)$,

(3) $\max\limits_{x \in X} \lambda(x)\, d(x,\overset{*}{\epsilon}) = k$, (2.3.15)

where k is the number of parameters.

b) The information matrices of all designs satisfying (1)-(3) coincide.

c) A linear combination of designs that satisfy (1)-(3) satisfies (1)-(3).

This theorem plays an important role in constructing D-optimal designs. In particular it follows that if $\lambda(x) = 1$ for all x, the continuous G-optimal designs are equivalent to continuous D-optimal designs. In the situation of paired comparisons theorem 2.3.1 does not apply. In general a D-optimal design is not G-optimal. Example 4.2.12 in chapter 4 will show this. But also statement (2.3.15) of theorem 2.3.1 does not apply. This can easily be seen as follows. Consider the situation where the model is defined by

$$y = \beta_1 x_1 \;, -1 \leqslant x_1 \leqslant 1 .$$

The design ϵ that is concentrated at the pair ((1),(−1)) is D-optimal. Now $M(\epsilon) = 4$ if $\lambda(x) = 1$ for $-1 \leqslant x \leqslant 1$.
But

$$\max_x \lambda(x)\, d(x,\epsilon) = \max_x \tfrac{1}{4}x^2 = \tfrac{1}{4} < 1$$

Moreover, one can question the usefulness of the G-criterion, because in paired comparison experiments one is interested in differences between objects. Therefore we define

$$d(x,y,\epsilon) = (f(x) - f(y))'\, M^{-1}(\epsilon)\, (f(x) - f(y)) \;, \qquad (2.3.16)$$

the variance of an estimated response difference between the points x and y. Now, a design $\overset{*}{\epsilon}$ is called $\overset{*}{G}$-optimal if

$$\max_{x,y \in X} d(x,y,\overset{*}{\epsilon}) = \min_{\epsilon} \max_{x,y \in X} d(x,y,\epsilon) . \qquad (2.3.17)$$

If the concept of a loss function is also introduced in the case of paired comparisons, then the information matrix can be generalized as follows

$$M(\epsilon) = \sum_{i=1}^{m} \lambda(u_i,v_i)\, n_i\, (f(u_i) - f(v_i))\,(f(u_i) - f(v_i))' \;, \qquad (2.3.18)$$

where $\lambda(u_i, v_i)$ is the loss function. Note that if we take

$$\lambda(u, v) = \frac{\pi_u \pi_v}{(\pi_u + \pi_v)^2} , \tag{2.3.19}$$

where

$$\log \pi_u = f_1(u)\beta_1 + \cdots + f_k(u)\beta_k , \tag{2.3.20}$$

then the information matrix of (2.3.18) coincides with the inverse of the covariance matrix in (1.6.4). This can easily be seen by using the expression of (1.5.4). A discrete normalized paired comparison design can be introduced by defining the p_i analogous to (2.3.8). A continuous normalized design will be characterized by a measure, or in the case of an absolutely continuous measure by a density function. In the latter case the information matrix takes the form

$$M(\epsilon) = \int_X \int_X p(x, y) \lambda(x, y) (f(x) - f(y)) (f(x) - f(y))' \, dxdy , \tag{2.3.21}$$

where

$$\int_X \int_X p(x, y) \, dxdy = 1 .$$

Now many theorems, analogous to theorems in the standard experimental situation, apply. We mention a few of them.

Theorem 2.3.2
For any design ϵ the matrix $M(\epsilon)$ can be represented in the form

$$M(\epsilon) = \sum_{i=1}^{m} p_i \lambda(u_i, v_i) (f(u_i) - f(v_i)) (f(u_i) - f(v_i))' , \tag{2.3.22}$$

where

$$m \leqslant \tfrac{1}{2}k(k+1) + 1 ,$$

$$0 \leqslant p_i \leqslant 1 , \sum_{i=1}^{m} p_i = 1 .$$

Theorem 2.3.3

The weighted sum of the variance of the estimated response differences, taken over all pairs of the design ϵ *is equal to the number of unknown parameters* k :

$$\sum_{i=1}^{m} p_i \, \lambda(u_i, v_i) \, d(u_i, v_i, \epsilon) = k \quad , \tag{2.3.23}$$

or in the case of a continuous normalized design with an absolutely continuous measure

$$\int_X \int_X p(x, y) \, \lambda(x, y) \, d(x, y, \epsilon) \, dx dy = k \; .$$

Theorem 2.3.4

The minimal value of $\max\limits_{x,y} \lambda(x, y) \, d(x, y, \epsilon)$ *is at least* k .

$$\max_{x,y} \lambda(x, y) \, d(x, y, \epsilon) \geqslant k \; . \tag{2.3.24}$$

Theorem 2.3.5

a) *The following assertions are equivalent:*

(1) *the design* $\overset{*}{\epsilon}$ *maximizes* det $(M(\epsilon))$,

(2) *the design* $\overset{*}{\epsilon}$ *minimizes* $\max\limits_{x,y \in X} \lambda(x, y) \, d(x, y, \epsilon)$,

(3) $$\max_{x,y \in X} \lambda(x, y) \, d(x, y, \overset{*}{\epsilon}) = k \, , \tag{2.3.25}$$

where k *is the number of parameters.*

b) *The information matrices of all designs satisfying (1)-(3) coincide.*

c) *A linear combination of designs that satisfy (1)-(3) satisfies (1)-(3).*

Theorem 2.3.6

If X *is compact and the functions* $\lambda(x, y)$ *and* $f(x)$ *are continuous, then a discrete D-optimal design exists with a number of pairs* $m \leqslant \frac{1}{2} k(k + 1)$.

Theorem 2.3.7

At the pairs of a discrete D-optimal design $\overset{*}{\epsilon}$ *the function* $\lambda(x, y) \, d(x, y, \overset{*}{\epsilon})$ *attains its maximal value* k .

The proofs of these theorems are analogous to the proofs of Fedorov (1972). We only give the proof of theorem 2.3.4 for a continuous normalized design with an absolutely continuous measure.

Proof of theorem 2.3.4

$$\max_{u,v} \lambda(u,v)\, d(u,v,\epsilon) = \max_{u,v} \lambda(u,v)\, d(u,v,\epsilon) \int_X \int_X p(x,y)\, dx dy$$

$$\geqslant \int_X \int_X \lambda(x,y)\, p(x,y)\, d(x,y,\epsilon)\, dx dy$$

$$= \int_X \int_X \lambda(x,y)\, p(x,y)\, (f(x) - f(y))' M^{-1}(\epsilon)\, (f(x) - f(y))\, dx dy$$

$$= tr \left(M^{-1}(\epsilon) \int_X \int_X \lambda(x,y) p(x,y) (f(x) - f(y))\, (f(x) - f(y))'\, dx dy \right)$$

$$= tr \left(M^{-1}(\epsilon)\, M(\epsilon) \right) = tr\ I = k\ . \qquad \Box$$

The theorems 2.3.2 - 2.3.7 can be used to find procedures to construct D-optimal designs. It is possible to show that the following iterative procedure converges and that its limit design is D-optimal. The steps of the procedure are as follows.

Iterative procedure 2.3.8

(1) *Let ϵ_0 be nondegenerate and not D-optimal. We compute its information matrix*

$$M(\epsilon_0) = \sum_{i=1}^{m} p_i\, \lambda(u_i, v_i)\, (f(u_i) - f(v_i))\, (f(u_i) - f(v_i))'\ .$$

(2) *A pair (u_0, v_0) is found at which $\lambda(x,y)\, d(x,y,\epsilon_0)$ is maximal. The design consisting of the pair (u_0, v_0) is called $\epsilon((u_0, v_0))$.*

(3) *The design $\epsilon_1 = (1 - \alpha_0)\, \epsilon_0 + \alpha_0\, \epsilon((u_0, v_0))$ is constructed for some value α_0, $0 < \alpha_0 < 1$. The value of α_0 can be chosen such that*

$$\det(M(\epsilon_1)) > \det(M(\epsilon_0))\ .$$

The increase in the determinant of the information matrix is maximal if

$$\alpha_0 = \delta_0 / [\delta_0 + (m - 1)]\, m \quad , \textit{ where}$$

$$\delta_0 = \lambda(u_0, v_0)\, d(u_0, v_0, \epsilon_0) - m\ .$$

(4) *The information matrix $M(\epsilon_1)$ of the design ϵ_1 is constructed.*

Now operations (2)-(4) are repeated with ϵ_0 replaced by ϵ_1, and ϵ_1 replaced by ϵ_2, etc.

Theorem 2.3.7 is very useful in checking the D-optimality of a design. An advantage of the criteria and the method discussed above is that it is possible to define the D-efficiency and $\overset{*}{G}$-efficiency of any design ϵ :

$$D-\text{efficiency} = \left\{ \det\,(M(\epsilon))/\det\,(M(\overset{*}{\epsilon})) \right\}^{1/k} , \tag{2.3.26}$$

where $\overset{*}{\epsilon}$ is a D-optimal design;

$$\overset{*}{G}-\text{efficiency} = k\,/(\max_{x,y} \lambda(x,y)\, d(x,y,\epsilon)\,) . \tag{2.3.27}$$

These efficiencies do not have the disadvantages of a relative efficiency, as is the case with the efficiency defined in section 2.2.1. These efficiencies are absolute. If the efficiency equals one, then the design is D-optimal. The method discussed above will be used in the next chapters to construct D-optimal designs. Sometimes the computation of $\max_{\epsilon} \det\,(M(\epsilon))$ is cumbersome. Then it is not easy to compute the D-efficiency. However, the $\overset{*}{G}$-efficiency can be used to obtain a lower bound for the D-efficiency.

Theorem 2.3.9
For any design ϵ

$$D-\text{eff}(\epsilon) \geqslant \exp\left(1 - \frac{1}{\overset{*}{G}-\text{eff}(\epsilon)}\right) . \tag{2.3.28}$$

This theorem can be proved in the same way as the analogous theorem in the standard experimental situation.

3. D-optimal designs in the case of a factorial model with main effects and first-order interactions

3.1. The model

In this chapter D-optimal designs will be constructed for factorial models with n factors. Some of the designs constructed in this chapter have been found by Quenouille and John (1971) and by El-Helbawy and Bradley (1978) (see also section 2.2). We will compare their results with the results of this chapter at the end of section 3.2. The model considered is model (2.3.1) where

$$f(x) = (x_1, \ldots, x_n, x_1x_2, \ldots, x_1x_n, x_2x_3, \ldots, x_{n-1}x_n)' \ , \qquad (3.1.1)$$

where

$x \in X$, the experimental region , $X \subset \mathbb{R}^n$,

so

$$\log \pi = \beta_1 x_1 + \cdots + \beta_n x_n + \beta_{12} x_1 x_2 + \cdots + \beta_{n-1\,n} x_{n-1} x_n \ . \qquad (3.1.2)$$

When constructing optimal designs, we make the assumption (1.8.6), or -equivalently- when dealing with a loss function

$$\lambda(x,y) = 1 \ \text{ for all } x,y \in X \ . \qquad (3.1.3)$$

In section 3.2 the experimental region X is chosen to be a hypercube, in section 3.3 X is a hypersphere.

The number of parameters k equals $n + \binom{n}{2}$, so $k = \frac{1}{2}n(n+1)$ and according to theorem 2.3.6 the following holds.

A discrete, D-optimal design exists with m pairs, where

$$m \leqslant \tfrac{1}{8} n\,(n+1)\,(n^2+n+2) \ . \qquad (3.1.4)$$

For reasons of symmetry and in analogy to the standard experimental situation one may expect that the information matrix of a D-optimal design $\overset{*}{\epsilon}$ has the following structure

$$M(\overset{*}{\epsilon}) = \left[\begin{array}{c|c} pI & \\ \hline & zI \end{array}\right] , \qquad (3.1.5)$$

where pI is related to the main effects and has dimension $n \times n$,

and zI is related to the first-order interactions and has dimension $\binom{n}{2} \times \binom{n}{2}$.

The covariance matrix $M^{-1}(\overset{*}{\epsilon})$ is denoted by

$$M^{-1}(\overset{*}{\epsilon}) = \left[\begin{array}{c|c} \gamma I & \\ \hline & \delta I \end{array}\right] . \qquad (3.1.6)$$

The function $d(x,y,\epsilon)$ given in (2.3.16) plays an important role in the

construction of D-optimal designs and will be used many times. The function $d(x,y,\epsilon)$ is an expression for the variance of an estimated response difference between the points x and y. It will be called variance function. The variance function depends on the covariance matrix. The definition of the variance function implies the following statement.

If a design ϵ has a covariance matrix of type (3.1.6),then

$$d(x,y,\epsilon) = \gamma \sum_{i=1}^{n} (x_i - y_i)^2 + \delta \sum\sum_{i<j} (x_i x_j - y_i y_j)^2 \ , \tag{3.1.7}$$

and consequently,

$$\begin{aligned} &d((x_1,\ldots,x_i,\ldots,x_n),(y_1,\ldots,y_i,\ldots,y_n),\epsilon) \\ &= d((x_1,\ldots,-x_i,\ldots,x_n),(y_1,\ldots,-y_i,\ldots,y_n),\epsilon) \ , \end{aligned} \tag{3.1.8}$$

and (3.1.9)

$$\begin{aligned} &d((x_1,\ldots,x_i,\ldots,x_j,\ldots,x_n),(y_1,\ldots,y_i,\ldots,y_j,\ldots,y_n),\epsilon) \\ &= d((x_1,\ldots,x_j,\ldots,x_i,\ldots,x_n),(y_1,\ldots,y_j,\ldots,y_i,\ldots,y_n),\epsilon) \ , \end{aligned}$$

where $1 \leqslant i \leqslant n$, $1 \leqslant j \leqslant n$.

In order to construct D-optimal designs we must find pairs $(\overset{*}{x},\overset{*}{y}) \in X^2$, such that $d(\overset{*}{x},\overset{*}{y},\epsilon)$ is maximal.

3.2. A hypercube as experimental region

The experimental region is defined by

$$x \in X \text{ if and only if } -1 \leqslant x_i \leqslant 1 \text{ for all } 1 \leqslant i \leqslant n \ , \tag{3.2.1}$$

where

$$x = (x_1,\ldots,x_n)' \ .$$

The following lemma is useful in finding pairs where the variance function attains its maximum .

Lemma 3.2.1

Let ϵ be a design with covariance matrix of type (3.1.6), and let X be as in (3.2.1). For a pair $(u,v) \in X^2$, where the variance function $d(\cdot,\cdot,\epsilon)$ attains its maximum , one has

$$|u_i| = |v_i| = 1 \textit{ for all } 1 \leqslant i \leqslant n \ . \tag{3.2.2}$$

Proof

Suppose that for some i we have $|u_i| < 1$ or $|v_i| < 1$.
Without loss of generality we may assume $|u_1| < 1$ (see (3.1.9)).
Define $d_1 = d((1,u_2,\ldots,u_n),(v_1,\ldots,v_n),\epsilon)$,

$d_2 = d((-1,u_2,\ldots,u_n),(v_1,\ldots,v_n),\epsilon)$.

Since $d(x,y,\epsilon)$ is maximal at the pair (u,v), we have

$d_1 - d(u,v,\epsilon) \leqslant 0$,

$d_2 - d(u,v,\epsilon) \leqslant 0$.

So,

$$d_1 - d(u,v,\epsilon) =$$

$$= \gamma\,[(1-v_1)^2 - (u_1 - v_1)^2] + \delta \sum_{j=2}^{n} [(u_j - v_1 v_j)^2 - (u_1 u_j - v_1 v_j)^2]$$

$$= \gamma\,(1 - u_1^2 - 2v_1(1-u_1)) + \delta \sum_{j=2}^{n} [\,u_j^2(1-u_1^2) - 2v_1 v_j u_j (1-u_1)]$$

$$= (1-u_1)\left|\,\gamma\,(1+u_1-2v_1) + \delta \sum_{j=2}^{n} [(1+u_1)u_j^2 - 2v_1 u_j v_j]\right| \leqslant 0. \qquad \text{(i)}$$

and similarly

$$d_2 - d(u,v,\epsilon) =$$

$$= (1+u_1)\left|\,\gamma\,(1-u_1+2v_1) + \delta \sum_{j=2}^{n} [(1-u_1)u_j^2 + 2v_1 u_j v_j]\right| \leqslant 0. \qquad \text{(ii)}$$

From (i) and (ii) it follows that

$$\gamma\,(1+u_1-2v_1) + \delta \sum_{j=2}^{n} [(1+u_1)u_j^2 - 2v_1 u_j v_j] \leqslant 0 \;,$$

$$\gamma\,(1-u_1+2v_1) + \delta \sum_{j=2}^{n} [(1-u_1)u_j^2 + 2v_1 u_j v_j] \leqslant 0 \;.$$

Hence

$$2\gamma + \delta \sum_{j=2}^{n} u_j^2 \leqslant 0. \qquad \text{(iii)}$$

Note that $\gamma \geqslant 0$ and $\delta \geqslant 0$ since $M^{-1}(\epsilon)$ is a covariance matrix of a nondegenerate design. So (iii) yields a contradiction and the proof is completed. ▯

From lemma 3.2.1 it follows that the elements of all pairs of a D-optimal design are vertices of the hypercube X. So the objects of the pairs of a D-optimal design are objects in a 2^n-factorial.
It is useful to define the following sets

Definition 3.2.2
$S(k_1,k_2)$ is the set of all pairs with k_1 factors at the same level, $k_1 + k_2 = n$.

It can easily be seen that each object is compared with $\binom{n}{k_1}$ other objects. A set $S(k_1,k_2)$ can be broken up into $\binom{n}{k_1}$ blocks of 2^{n-1} pairs, in which all 2^n objects occur. So the set $S(k_1,k_2)$ contains $\binom{n}{k_1}2^{n-1}$ pairs.
The set $S(0,3)$, for example, contains the pairs

$$\begin{array}{l}((\ 1,\ 1,\ 1),(-1,-1,-1)),\\ ((-1,\ 1,\ 1),(\ 1,-1,-1)),\\ ((\ 1,-1,\ 1),(-1,\ 1,-1)),\\ ((\ 1,\ 1,-1),(-1,-1,\ 1)).\end{array}$$

The set $S(k_1,k_2)$ can be seen as a design with, in the notation of (2.3.2), $n_i = 1$, $1 \leqslant i \leqslant m$, and $m = N = \binom{n}{k_1}2^{n-1}$.
The information matrix of this design is denoted by $M(k_1,k_2)$.

Lemma 3.2.3

$$M(k_1,k_2) = \left|\begin{array}{c|c} pI & \\ \hline & zI \end{array}\right| , \tag{3.2.3}$$

where

$$p = \binom{n-1}{k_1} 2^{n+1} , \tag{3.2.4}$$

$$z = \binom{n-2}{k_1-1} 2^{n+2} .$$

Outline of the proof
This lemma can be proved by using the expression (4.2.20). Some of the arguments are given here. The set $S(k_1,k_2)$ can be broken up into $\binom{n}{k_1}$ blocks of 2^{n-1} pairs. One set of 2^{n-1} pairs measures k_2 main effects and k_1k_2 first-order interactions. The information matrix of one set of 2^{n-1} pairs is a diagonal matrix with diagonal elements $4\ 2^{n-1}$ or zero. A diagonal element is $4\ 2^{n-1}$ if the particular main effect or first-order interaction, to which it relates , is measured by that particular block of 2^{n-1} pairs. There are $\binom{n}{k_1}$ of these blocks. For reasons of symmetry we have

$$p = \frac{1}{n}\binom{n}{k_1} 4k_2\, 2^{n-1} = \binom{n-1}{k_1} 2^{n+1} ,$$

$$z = \frac{1}{\binom{n}{2}}\binom{n}{k_1} 4k_1k_2\, 2^{n-1} = \binom{n-2}{k_1-1} 2^{n+2} .$$

□

The normalized design $SN(k_1,k_2)$ is a design with the same pairs but with weights $1/N$, where $N = \binom{n}{k_1} 2^{n-1}$. The information matrix of this normalized design is denoted by $MN(k_1,k_2)$. In view of (3.2.3) the information matrix of this normalized design can be expressed by

$$MN(k_1,k_2) = \left[\begin{array}{c|c} pI & \\ \hline & zI \end{array}\right], \tag{3.2.5}$$

where

$$p = 4\frac{k_2}{n}, \tag{3.2.6}$$

$$z = \frac{8k_1k_2}{n(n-1)}.$$

The value of the variance function is the same for all pairs of the set $S(k_1,k_2)$. This can be seen by using (3.1.8) and (3.1.9). Therefore, we may describe this value as follows:

> $d(k_1,k_2,\epsilon)$ is the value of $d(x,y,\epsilon)$ where ϵ is a design with information matrix of type (3.1.6) and (x,y) is a pair of the set $S(k_1,k_2)$. (3.2.7)

From (3.1.7) it follows that

$$d(k_1,k_2,\epsilon) = 4k_2\gamma + 4k_1k_2\delta. \tag{3.2.8}$$

A D-optimal design is composed of pairs where the function $d(x,y,\epsilon)$ is maximal. According to lemma 3.2.1 and the fact that the variance function has the same value for all pairs of a set $S(k_1,k_2)$ a D-optimal design exists which is the union of some $S(k_1,k_2)$. To give such D-optimal designs we have to distinguish between two cases: n is even and n is odd. The D-optimal designs are given in the following theorem.

Theorem 3.2.4

a) The following design ϵ is D-optimal

i) Let n be odd.

Choose

- *the pairs of $S(\frac{1}{2}(n-1),\frac{1}{2}(n+1))$,*
- *the same weights for all pairs: $1/N$,*
  where N is the number of pairs;

$$N = \binom{n}{\frac{1}{2}(n-1)} 2^{n-1}.$$

So ,

$$MN(\tfrac{1}{2}(n-1),\tfrac{1}{2}(n+1)) = \left|\begin{array}{c|c} pI & \\ \hline & zI \end{array}\right|, \tag{3.2.9}$$

where $p = z = 2\dfrac{n+1}{n}$,

and in the notation of (3.1.6) $\gamma = \delta = \frac{1}{2}\dfrac{n}{n+1}$.

ii) Let n be even.

Choose

- *the pairs of* $S(\frac{1}{2}n-1,\frac{1}{2}n+1)$ *and the pairs of* $S(\frac{1}{2}n,\frac{1}{2}n)$,
- *the same weight for all pairs:* $1/N$,

where N is the number of pairs;

$$N = \binom{n+1}{\frac{1}{2}n} 2^{n-1}.$$

So,

$$M(\epsilon) = \nu\, MN(\tfrac{1}{2}n,\tfrac{1}{2}n) + (1-\nu)\, MN(\tfrac{1}{2}n-1,\tfrac{1}{2}n+1), \tag{3.2.10}$$

where $\nu = \dfrac{n+2}{2(n+1)}$.

So,

$$M(\epsilon) = \left|\begin{array}{c|c} pI & \\ \hline & zI \end{array}\right|,$$

with $p = z = 2\dfrac{n+2}{n+1}$,

and in the notation of (3.1.6) $\gamma = \delta = \frac{1}{2}\dfrac{n+1}{n+2}$.

b) The set of pairs of any D-optimal design is contained in the set of pairs of the design ϵ.

Proof

a) The expression for $M(\epsilon)$ can be found by using (3.2.3) and (3.2.5). According to theorem 2.3.5 the proof of the D-optimality of ϵ is complete if it is shown that $d(x,y,\epsilon) \leqslant \frac{1}{2}n(n+1)$ for all $x,y \in X$. So we have to find the maximal value of $d(x,y,\epsilon)$. From lemma 3.2.1 and (3.2.7) it follows that the maximal value is obtained by maximizing $d(k_1,k_2,\epsilon)$ over k_1, $0 \leqslant k_1 \leqslant n-1$; $k_2 = n-k_1$. So, according to (3.2.8), we have to maximize $[4(n-k_1) + 4k_1(n-k_1)]\,\gamma$. If k_1 can take all values in $\{0,1,\ldots,n-1\}$, then this function is maximal for $k = \frac{1}{2}(n-1)$.

i) n is odd.
Now $\frac{1}{2}(n-1)$ is an integer, so the maximal value of $d(x,y,\epsilon)$ equals $d(\frac{1}{2}(n-1),\frac{1}{2}(n+1),\epsilon) = \frac{1}{2}n(n+1)$.

ii) n is even.

Now $\frac{1}{2}(n-1)$ is not an integer, so the maximal value of $d(x,y,\epsilon)$ is one of the values $d(\frac{1}{2}n,\frac{1}{2}n,\epsilon)$ and $d(\frac{1}{2}n-1,\frac{1}{2}n+1,\epsilon)$. Using (3.2.8) and the expression for $M(\epsilon)$ we find

$d(\frac{1}{2}n,\frac{1}{2}n,\epsilon) = d(\frac{1}{2}n-1,\frac{1}{2}n+1,\epsilon) = \frac{1}{2}n(n+1)$.

and the proof of the D-optimality of the design ϵ is complete.

b) The information matrix of any D-optimal design coincides with the matrix of the design mentioned in a). Therefore, the set of pairs where the variance function is maximal coincides with the set of pairs of the design ϵ. □

The D-efficiency and $\mathring{G}$-efficiency ,as defined in (2.3.26) and (2.3.27), of the round robin design are given in the following theorem.

Theorem 3.2.5

The D-efficiency and the $\mathring{G}$-efficiency of the round robin design have the same value:

$$D-eff = \mathring{G}-eff = \begin{cases} \dfrac{n+1}{n+2}\,\dfrac{2^n}{2^n-1} & ,\textit{if } n \textit{ even} ,\\[2ex] \dfrac{n}{n+1}\,\dfrac{2^n}{2^n-1} & ,\textit{if } n \textit{ odd}. \end{cases} \tag{3.2.11}$$

The information matrix M of a round robin design can be expressed by

$$M = \left[\begin{array}{c|c} pI & \\ \hline & zI \end{array}\right], \tag{3.2.12}$$

where $p = z = \dfrac{2^{n+1}}{2^n-1}$.

Proof

The number of pairs N of the round robin design is $N = \frac{1}{2}2^n(2^n-1)$.

So, according to lemma 3.2.3 we find

$$p = \sum_{k_1=0}^{n-1} \frac{1}{\frac{1}{2}2^n(2^n-1)} \binom{n-1}{k_1} 2^{n+1} = \frac{2^{n+1}}{2^n-1},$$

and

$$z = \sum_{k_1=1}^{n-1} \frac{1}{\frac{1}{2}2^n(2^n-1)} \binom{n-2}{k_1-1} 2^{n+2} = \frac{2^{n+2}}{2^n-1}.$$

Now the expression for the D-efficiency can be computed (see definition (2.3.26)). In order to compute the $\mathring{G}$-efficiency, we need the maximal value of the

variance function. From the expression (3.2.12) it follows that the variance function of the round robin design ϵ_1 has the value $d(\frac{1}{2}(n-1),\frac{1}{2}(n+1),\epsilon_1)$ if n is odd and the value $d(\frac{1}{2}n,\frac{1}{2}n,\epsilon_1)$ if n is even. Using (3.2.8) we find

$$d(\tfrac{1}{2}(n-1),\tfrac{1}{2}(n+1),\epsilon_1) = (n+1)^2 \frac{2^n-1}{2^{n+1}} ,$$

and

$$d(\tfrac{1}{2}n,\tfrac{1}{2}n,\epsilon_1) = n(n+2)\frac{2^n-1}{2^{n+1}} .$$

Substitution into (2.3.27) completes the proof. □

In table 3.2.6 some results of theorems 3.2.4 and 3.2.5 are given for $2 \leqslant n \leqslant 7$. In this table a value m is listed defined by $m = \frac{1}{8}n(n+1)(n^2+n+2)$. This value is important because according to (3.1.4) a discrete D-optimal design can be found with a number of pairs N_1, where $N_1 \leqslant m$. In section 5.4 a method will be given to reduce the number of pairs of designs. Some of the results will be used in this section. These results are given between brackets in table 3.2.6.

Table 3.2.6
Values of quantities related to D-optimal designs

n	2	3	4	5	6	7
Number of pairs of						
$-S(\frac{1}{2}n-1,\frac{1}{2}n+1)$	2		32		480 (240)	
$-S(\frac{1}{2}n,\frac{1}{2}n)$	4		48 (24)		640 (320)	
$-S(\frac{1}{2}(n-1),\frac{1}{2}(n+1))$		12		160 (80)		2240 (560)
−the D-optimal design given in theorem 3.2.4.	6	12	80 (56)	160 (80)	1120 (560)	2240 (560)
$m = \frac{1}{8}n(n+1)(n^2+n+2)$	6	21	55	120	231	406
γ, δ	3/8	3/8	5/12	5/12	7/16	7/16
Round robin:						
−number of pairs	6	28	120	496	2016	8128
−D−efficiency	1	0.86	0.89	0.86	0.89	0.88

It is also possible to construct designs having a considerably smaller number of pairs than the D-optimal designs given in theorem 3.2.4 and with a relative high D-efficiency. Such designs may be attractive for practical applications. In table 3.2.8 the D-efficiency and $\overset{*}{G}$-efficiency are given of some designs $SN(k_1,k_2)$. The values given in the table can be computed by use of the following lemma .

Lemma 3.2.7

Let ϵ be the design constructed by choosing
-the pairs of $S(k_1,k_2)$
-equal weights for all pairs .
Then the following holds:

$$D-eff = 4\frac{k_2}{n}\left(\frac{2k_1}{n-1}\right)^{\frac{n-1}{n+1}}\gamma \ , \tag{3.2.13}$$

where

$$\gamma = \begin{cases} \frac{1}{2}\frac{n}{n+1} & ,if \;\; n \;\; odd \;\; , \\ \\ \frac{1}{2}\frac{n+1}{n+2} & ,if \;\; n \;\; even \;\; . \end{cases}$$

The $\mathring{G}$-efficiency of ϵ can be found by minimizing

$$\frac{\frac{1}{2}n\,(n+1)}{d\,(l_1,l_2,\epsilon)} = \frac{k_1k_2(n+1)}{l_1l_2(2\frac{k_1}{l_1} + (n-1))} \tag{3.2.14}$$

over l_2 ,$1 \leqslant l_2 \leqslant n$, l_2 is integer-valued.
If the restriction that l_2 is an integer is dropped, then the variance function $d\,(l_1,l_2,\epsilon)$ is maximal for $l_2 = \frac{1}{2}n + \frac{k_1}{n-1}$.

Proof
From the definition of the D-efficiency and (3.2.5) we have

$$D-\text{eff} = \left| \left(\frac{4k_2}{n}\right)^n \left(\frac{8k_1k_2}{n\,(n-1)}\right)^{\frac{1}{2}n\,(n-1)} / \left(p^n z^{\frac{1}{2}n\,(n-1)}\right) \right|^{2/n\,(n+1)} ,$$

where p and z have the value given in theorem 3.2.4.
So,

$$D-\text{eff} = \frac{1}{p}\,\frac{4k_2}{n} \left(\frac{2k_1}{n-1} \right)^{\frac{n-1}{n+1}} .$$

The statement concerning the $\mathring{G}$-efficiency is proven by lemma 3.2.1 and the fact that

$$d\,(l_1,l_2,\epsilon) = 4l_2\,\frac{n}{4k_2} + 4l_1l_2\frac{n\,(n-1)}{8k_1k_2} . \qquad \square$$

In table 3.2.8 the numbers between brackets can be found by using results of chapter 5 concerning the reduction of the numbers of pairs of a design.

Table 3.2.8
Exact designs and values of quantities related to these designs

n	Design	Number of pairs	γ	δ	D-eff	G-eff
2	$SN(1,1)$	4	1/2	1/4	0.94	0.75
4	$SN(2,2)$	48 (24)	1/2	3/8	0.99	0.95
	$SN(1,3)$	32	1/3	1/2	0.98	0.94
5	$SN(1,4)$	80 (40)	5/16	5/8	0.84	0.80
6	$SN(3,3)$	640 (320)	1/2	5/12	0.997	0.98
	$SN(2,4)$	480 (240)	3/8	15/32	0.995	0.98
	$SN(1,5)$	192 (96)	3/10	3/4	0.76	0.69
7	$SN(2,5)$	1344 (336)	7/20	21/40	0.92	0.91
	$SN(1,6)$	448 (124)	7/24	7/8	0.66	0.60

Some of the designs mentioned in tables 3.2.6 and 3.2.8 are known in the literature. As we have seen in section 2.2.1 Quenouille and John (1971) present 2^n-factorial paired comparison designs. They give a table of designs and their efficiencies for $2 \leqslant n \leqslant 8$. Among these designs are the D-optimal designs of theorem 3.2.3 for $2 \leqslant n \leqslant 5$. The designs of table 3.2.7 can be found in the table of Quenouille and John but the efficiency they give is the efficiency of the design compared with the round robin design for each effect to be estimated.

3.3. A hypersphere as experimental region

The experimental region X is defined by

$$X = \{ x \in \mathbf{R}^n \mid \sum_{i=1}^{n} x_i^2 \leqslant 1 \} . \tag{3.3.1}$$

The following lemma is useful for finding pairs at which the variance function attains its maximum .

Lemma 3.3.1

Let ϵ be a design with covariance matrix of type (3.1.6). For a pair $(u,v) \in X^2$ where the variance function $d(\,.\,,\,.\,,\epsilon)$ is maximal the following holds :

$$\sum_{i=1}^{n} u_i^2 = \sum_{i=1}^{n} v_i^2 = 1 \,. \tag{3.3.2}$$

Proof

The proof is analogous to the proof of lemma 3.2.1. Suppose that statement (3.3.2) is not true and assume without loss of generality that $\sum_{i=1}^{n} u_i^2 < 1$.

Consider $d_1 = d(\overset{*}{u}, v, \epsilon)$, where $\overset{*}{u} = (\overset{*}{u}_1, u_2, \ldots, u_n)$, with
$\overset{*}{u}_1 = \sqrt{1-(u_2^2 + \cdots + u_n^2)}$, so $\overset{*}{u}_1 > u_1$,
and $\quad d_2 = d(\overline{u}, v, \epsilon)$, where $\overline{u} = (-\overset{*}{u}_1, u_2, \ldots, u_n)$.
Since $d(x,y,\epsilon)$ is maximal at (u,v) we have

$$d_1 - d(u,v,\epsilon) \leqslant 0 \,,$$
$$d_2 - d(u,v,\epsilon) \leqslant 0 \,.$$

These expressions yield a contradiction similar to the one found in the proof of lemma 3.2.1, and this completes the proof. □

Lemma 3.3.2

Let ϵ be a design with covariance matrix of type (3.1.6). For a pair (x,y) with $\sum_{i=1}^{n} x_i^2 = \sum_{i=1}^{n} y_i^2 = 1$ the variance function takes the form

$$d(x,y,\epsilon) = 2\gamma\,(1 - \sum_{i=1}^{n} x_i y_i) + \delta\,(1 - (\sum_{i=1}^{n} x_i y_i)^2) \tag{3.3.3}$$
$$- \tfrac{1}{2}\delta \sum_{i=1}^{n} (x_i^2 - y_i^2)^2 \,.$$

An upperbound for $d(x,y,\epsilon)$ is given by $d(u,v,\epsilon)$ where (u,v) is a pair, such that

$$\sum_{i=1}^{n} u_i^2 = \sum_{i=1}^{n} v_i^2 = 1 \text{ , and } \sum_{i=1}^{n} u_i v_i = -\frac{\gamma}{\delta} \,. \tag{3.3.4}$$

Proof

The expression (3.3.3) can be found by using (3.1.7):

$$d(x,y,\epsilon) = \gamma \sum_{i=1}^{n} (x_i - y_i)^2 + \delta \sum_{i<j}\sum (x_i x_j - y_i y_j)^2$$
$$= 2\gamma - 2\gamma \sum_{i=1}^{n} x_i y_i + \delta \sum_{i<j}\sum (x_i^2 x_j^2 + y_i^2 y_j^2 - 2 x_i x_j y_i y_j)$$
$$= 2\gamma\,(1 - \sum_{i=1}^{n} x_i y_i) + \tfrac{1}{2}\delta\,[\,(\sum_{i=1}^{n} x_i^2)^2 + (\sum_{i=1}^{n} y_i^2)^2\,]$$

$$- \tfrac{1}{2}\delta \left(\sum_{i=1}^{n} x_i^4 + \sum_{i=1}^{n} y_i^4\right) - \delta \left(\sum_{i=1}^{n} x_i y_i\right)^2 + \delta \sum_{i=1}^{n} x_i^2 y_i^2$$

$$= 2\gamma \left(1 - \sum_{i=1}^{n} x_i y_i\right) + \delta \left[1 - \left(\sum_{i=1}^{n} x_i y_i\right)^2\right] - \tfrac{1}{2}\delta \sum_{i=1}^{n} (x_i^2 - y_i^2)^2 .$$

The statement concerning the maximal value of the variance function can be proved by using the fact that

$$d(x,y,\epsilon) \leqslant 2\gamma \left(1 - \sum_{i=1}^{n} x_i y_i\right) + \delta \left(1 - \left(\sum_{i=1}^{n} x_i y_i\right)^2\right) ,$$

and the fact that the right-hand side of this inequality attains is maximum for

$$\sum_{i=1}^{n} x_i y_i = -\frac{\gamma}{\delta} .$$

Many D-optimal designs can be found by use of (3.3.4). We just give one of the D-optimal designs for which the number of pairs is small.
Consider the pairs

$$\begin{aligned}
(u_1,v_1) &= ((\ \sin\phi,\ \cos\phi,0,\ldots,0),(\ \sin\phi,-\cos\phi,0,\ldots,0)) ,\\
(u_2,v_2) &= ((-\sin\phi,\ \cos\phi,0,\ldots,0),(-\sin\phi,-\cos\phi,0,\ldots,0)) ,\\
(u_3,v_3) &= ((\ \cos\phi,\ \sin\phi,0,\ldots,0),(-\cos\phi,\ \sin\phi,0,\ldots,0)) ,\\
(u_4,v_4) &= ((\ \cos\phi,-\sin\phi,0,\ldots,0),(-\cos\phi,-\sin\phi,0,\ldots,0)) .
\end{aligned}$$

where $\sin\phi = \frac{1}{2}\sqrt{2}[\frac{n-1}{n}]^{\frac{1}{2}}$, $\cos\phi = \frac{1}{2}\sqrt{2}[\frac{n+1}{n}]^{\frac{1}{2}}$ and $(u_i,v_i) \in X^2$.
Let S be the set defined by

$$S = \left\{(\bar{p}(u_i),\bar{p}(v_i)) \mid 1 \leqslant i \leqslant 4, \bar{p} \text{ is a permutation of order } n\right\} . \quad (3.3.5)$$

The set S contains $4\binom{n}{2}$ pairs.

Theorem 3.3.3

The design ϵ constructed by choosing
-the pairs of the set S which is defined in (3.3.5)
-equal weights for all pairs: $1/N$, where N is the number of pairs
is D-optimal.

$$M(\epsilon) = \left|\begin{array}{c|c} pI & \\ \hline & zI \end{array}\right| \qquad (3.3.6)$$

where $p = 2\frac{n+1}{n^2}$, $z = 2\frac{n+1}{n^3}$.

Proof

The expression (3.3.6) can be found as follows.

The set S can be broken up into $\binom{n}{2}$ blocks of 4 pairs. Consider the block ϵ_1 consisting of the pairs (u_i, v_i) , $1 \leqslant i \leqslant n$. Then

$$M(\epsilon_1) = diag(2\cos^2\phi, 2\cos^2\phi, 0, \ldots, 0, 4\sin^2\phi\cos^2\phi, 0, \ldots, 0).$$

The information matrices of the other blocks are diagonal matrices, where the diagonal elements have been permuted. For reasons of symmetry we find

$$p = \frac{2(n-1)\cos^2\phi}{\binom{n}{2}} = 2\frac{n+1}{n^2} ,$$

and

$$z = \frac{4\sin^2\phi\cos^2\phi}{\binom{n}{2}} = 2\frac{n+1}{n^3} .$$

The D-optimality can be proved by computing the maximal value of $d(x, y, \epsilon)$. The pairs (u, v) of the design ϵ satisfy the conditions mentioned in (3.3.4) in theorem 3.3.2. So, an upperbound for the variance function is the value $d(u_1, v_1, \epsilon)$ and this is the maximal value of $d(x, y, \epsilon)$.
The fact that $d(u_1, v_1, \epsilon) = \frac{1}{2}n(n+1)$ completes the proof. ▯

In table 3.3.4 some results are shown.

Table 3.3.4
Values of quantities related to D-optimal designs

n	2	3	4	5	6	7
Number of pairs of the D-optimal design of theorem 3.3.3	4	12 (6)	24	40 (20)	60	84 (42)
$\frac{1}{8}n(n+1)(n^2+n+2)$	6	21	55	120	231	406
γ	2/3	9/8	8/5	25/12	18/7	49/16
δ	4/3	27/8	32/5	125/12	128/7	343/16

Between brackets a reduction of the number of pairs is given. This is a result of section 4.3.

4. D-optimal designs in the case of a quadratic model with a hypersphere as experimental region

4.1. The model

In this chapter the design for quadratic models will be discussed. The model (2.3.1) will be considered, where

$$f(x) = (x_1, \ldots, x_n, x_1^2, \ldots, x_n^2, x_1x_2, \ldots, x_{n-1}x_n)' \ , \tag{4.1.1}$$

where X is defined by

$$X = \{ x \in \mathbf{R}^n : \sum_{i=1}^{n} x_i^2 \leqslant 1 \} . \tag{4.1.2}$$

So

$$\begin{aligned} \log \pi = {} & \beta_1 x_1 + \cdots + \beta_n x_n + \beta_{11} x_1^2 + \cdots + \beta_{nn} x_n^2 \\ & + \beta_{12} x_1 x_2 + \cdots + \beta_{n-1\,n} x_{n-1} x_n . \end{aligned} \tag{4.1.3}$$

When constructing optimal designs we make the assumption $\pi = (1, \ldots, 1)'$ (1.8.6). In section 4.2 we will give the necessary conditions for a design to be D-optimal and we compute the information matrix of such a design. In section 4.3 discrete D-optimal designs are given having a relatively small number of pairs. In section 4.4 exact designs are constructed. In section 4.5 the efficiency of the designs is discussed when the assumption (1.8.6) does not hold. The number of parameters equals $2n + \binom{n}{2}$, i.e. $k = \frac{1}{2}n(n+3)$ and according to theorem 2.3.6 the following holds:
A discrete D-optimal design exists with m pairs, where

$$m \leqslant \tfrac{1}{8} n(n+1)(n+2)(n+3) . \tag{4.1.4}$$

For reasons of symmetry and in analogy to the standard experimental situation one may expect that the information matrix of a D-optimal design ϵ has the following structure:

$$M(\epsilon) = \left[\begin{array}{c|c|c} pI & & \\ \hline & sI + tJ & \\ \hline & & zI \end{array} \right] , \tag{4.1.5}$$

where pI is related to the main effects,
$sI + tJ$ is related to the quadratic effects,
zI is related to the interactions;
J is a matrix with $J_{ij} = 1$ for all i, j .

The covariance matrix $M^{-1}(\epsilon)$ is denoted by

$$M^{-1}(\epsilon) = \left[\begin{array}{c|c|c} \gamma I & & \\ \hline & \alpha I + \xi J & \\ \hline & & \delta I \end{array} \right] , \tag{4.1.6}$$

The parameters in (4.1.5) and (4.1.6) are related by

$$p = \frac{1}{\gamma}\, , s = \frac{1}{\alpha}\, , s + nt = \frac{1}{\alpha + n\xi}\, , z = \frac{1}{\delta}\ . \tag{4.1.7}$$

Again the variance function plays an important role in the construction of D-optimal designs. It can be expressed as follows.
If ϵ is a design with covariance matrix of type (4.1.6), then

$$d(x, y, \epsilon) = \gamma \sum_{i=1}^{n} (x_i - y_i)^2 + \alpha \sum_{i=1}^{n} (x_i^2 - y_i^2)^2 \tag{4.1.8}$$

$$+ \xi \left(\sum_{i=1}^{n} (x_i^2 - y_i^2)\right)^2 + \delta \sum_{i<j}\sum (x_i x_j - y_i y_j)^2 \ .$$

4.2. Conditions to be satisfied by D-optimal designs

We shall investigate the variance function. If the variance function can be expressed by (4.1.8), then (3.1.8) and (3.1.9) hold. Due to the fact that the experimental region is a hypersphere and in analogy to the standard experimental situation one might expect that a D-optimal design is rotatable in the sense that the variance function $d(x, y, \epsilon)$ only depends on
$r_1^2 = \sum_{i=1}^{n} x_i^2\ , r_2^2 = \sum_{i=1}^{n} y_i^2$ and on the angle between the position vectors of x and y.
We formulate this property as follows.

Definition 4.2.1
A design ϵ is called strongly rotatable if the variance function $d(x, y, \epsilon)$ only depends on r_1, r_2 and θ, where

$$r_1^2 = \sum_{i=1}^{n} x_i^2\ , r_2^2 = \sum_{i=1}^{n} y_i^2$$

and (4.2.1)

$$\theta \textit{ is such that } r_1 r_2 \cos\theta = \sum_{i=1}^{n} x_i y_i \ .$$

This property is called *strong* rotatibility as distinct from rotatability which is defined as follows.

A design ϵ is called rotatable if the function $d(x,\epsilon)$ only depends on r_1, with $d(x,\epsilon)$ as defined in (2.3.14). (4.2.2)

Strong rotatability implies rotatability. In the following lemma a relation is given between strong rotatibility and the structure of the information matrix.

Lemma 4.2.2

Let ϵ be a design with covariance matrix of type (4.1.6). Then the following holds. The design ϵ is strongly rotatable if and only if

$$2\alpha = \delta \tag{4.2.3}$$

Proof

According to (4.1.8) we have

$$\begin{aligned} d(x,y,\epsilon) = {} & \gamma r_1^2 + \gamma r_2^2 - 2\gamma \sum_{i=1}^{n} x_i y_i + \alpha \sum_{i=1}^{n} x_i^4 + \alpha \sum_{i=1}^{n} y_i^4 \\ & -2\alpha \sum_{i=1}^{n} x_i^2 y_i^2 + \xi (r_1^2 - r_2^2)^2 + (\delta - 2\alpha) \sum_{i<j}\sum (x_i x_j - y_i y_j)^2 \\ & + 2\alpha \sum_{i<j}\sum x_i^2 x_j^2 + 2\alpha \sum_{i<j}\sum y_i^2 y_j^2 - 2\alpha \sum_{i}\sum_{j} x_i x_j y_i y_j \\ = {} & \gamma (r_1^2 + r_2^2) - 2\gamma \sum_{i=1}^{n} x_i y_i + \alpha (\sum_{i=1}^{n} y_i^2)^2 + \alpha (\sum_{i=1}^{n} x_i^2)^2 \\ & -2\alpha (\sum_{i=1}^{n} x_i y_i)^2 + \xi (r_1^2 - r_2^2)^2 + (\delta - 2\alpha) \sum_{i<j}\sum (x_i x_j - y_i y_j)^2 . \end{aligned}$$

Now it is obvious that if $2\alpha = \delta$ then the function $d(x,y,\epsilon)$ only depends on r_1, r_2 and $\sum_{i=1}^{n} x_i y_i$.

Let the design ϵ be strongly rotatable. Then $d(w_1,w_2,\epsilon) = d(w_3,w_4,\epsilon)$, where

$w_1 = (1,0,0,\ldots,0)$,

$w_2 = (\frac{1}{2}\sqrt{3},\frac{1}{2},0,\ldots,0)$,

$w_3 = (\frac{1}{2}\sqrt{3},\frac{1}{2},0,\ldots,0)$,

$w_4 = (\frac{1}{2},\frac{1}{2}\sqrt{3},0,\ldots,0)$.

A simple computation yields $2\alpha = \delta$. □

It will be proved in theorem 4.2.11 that a D-optimal design is strongly rotatable. Therefore, assumption (4.2.3) will be made very often in this chapter. If ϵ is a design with covariance matrix of type (4.1.6) for which the assumption (4.2.3) holds, then the variance function can be expressed by

$$\begin{aligned} d(x,y,\epsilon) = {} & \gamma r_1^2 + \gamma r_2^2 - 2\gamma r_1 r_2 \cos\theta + \alpha r_1^4 + \alpha r_2^4 \\ & + 2\alpha r_1^2 r_2^2 \cos^2\theta + \xi (r_1^2 - r_2^2)^2 , \end{aligned} \tag{4.2.4}$$

where

$$r_1^2 = \sum_{i=1}^{n} x_i^2 \ , \ r_2^2 = \sum_{i=1}^{n} y_i^2$$

and θ is such that

$$r_1 r_2 \cos\theta = \sum_{i=1}^{n} x_i y_i \ .$$

This is easily seen by using the expression given in the proof of lemma 4.2.2. The following lemma is useful in finding the maximal value of the variance function.

Lemma 4.2.3

Let ϵ be a design for which the variance function can be expressed by (4.2.4). If the variance function is maximal at (u,v), then

$$r_1 = \sum_{i=1}^{n} u_i^2 = 1 \ , \ \text{or} \ \ r_2 = \sum_{i=1}^{n} v_i^2 = 1 \ .$$

Proof

Suppose that $r_1 < 1$ and $r_2 < 1$.

Consider $d_1 = d(\bar{u},v,\epsilon)$, where $\bar{u} = \dfrac{1}{r_1} u$, so $\sum_{i=1}^{n} \bar{u}_1^2 = 1$;

$d_2 = d(\overset{*}{u},v,\epsilon)$, where $\overset{*}{u} = -\dfrac{1}{r_1} u$,

$d_3 = d(u,\bar{v},\epsilon)$, where $\bar{v} = \dfrac{1}{r_2} v$,

and $d_4 = d(u,\overset{*}{v},\epsilon)$, where $\overset{*}{v} = -\dfrac{1}{r_2} v$.

Since the variance function is maximal at (u,v) we have $d_i - d(u,v,\epsilon) \leqslant 0$.
So

$$\begin{aligned}
&d_1 - d(u,v,\epsilon) = \\
&= \gamma(1-r_1^2) - 2\gamma\, r_2 \cos\theta(1-r_1) + \alpha\,(1-r_1^4) \\
&\quad -2\alpha\, r_2^2 \cos^2\theta\,(1-r_1^2) + \xi\,(1-r_1^4) - 2\xi\,(1-r_1^2) r_2^2 \\
&= (1-r_1)\,[\gamma\,(1+r_1) - 2\gamma\, r_2 \cos\theta + (\alpha+\xi)(1+r_1+r_1^2+r_1^3) \\
&\quad -2\alpha\,(1+r_1)\, r_2^2 \cos^2\theta - 2\xi\, r_2^2\,(1+r_1)] \leqslant 0 \ ,
\end{aligned} \tag{i}$$

and similarly

$$\begin{aligned}
&d_2 - d(u,v,\epsilon) = \\
&= (1+r_1)\,[\gamma\,(1-r_1) + 2\gamma\, r_2 \cos\theta + (\alpha+\xi)(1-r_1+r_1^2-r_1^3) \\
&\quad -2\alpha\, r_2^2 \cos^2\theta\,(1-r_1) - 2\xi\,(1-r_1)\, r_2^2\ ] \leqslant 0 \ .
\end{aligned} \tag{ii}$$

From (i) and (ii) it follows that

$$2\gamma + 2(\alpha+\xi)(1+r_1^2) - 4\alpha\, r_2^2 \cos^2\theta - 4\xi\, r_2^2 \leqslant 0\,. \tag{iii}$$

Using $d_3 - d(u,v,\epsilon) \leqslant 0$ and $d_4 - d(u,v,\epsilon) \leqslant 0$ it can be seen that

$$2\gamma + 2(\alpha+\xi)(1+r_2^2) - 4\alpha\, r_1^2 \cos^2\theta - 4\xi\, r_1^2 \leqslant 0\,. \tag{iv}$$

So with (iii) and (iv) we have

$$4\gamma + 2(\alpha+\xi)(2+r_1^2+r_2^2) - 4\alpha\,(r_1^2+r_2^2)\cos^2\theta - 4\xi\,(r_1^2+r_2^2) \leqslant 0\,.$$

However,

$$\begin{aligned} & 4\gamma + 2(\alpha+\xi)(2+r_1^2+r_2^2) - 4\alpha\,(r_1^2+r_2^2)\cos^2\theta - 4\xi\,(r_1^2+r_2^2) \\ \geqslant\; & 4\gamma + 2(\alpha+\xi)(2+r_1^2+r_2^2) - 4\alpha\,(r_1^2+r_2^2) - 4\xi\,(r_1^2+r_2^2) \\ =\; & 4\gamma + 2(\alpha+\xi)(2-r_1^2-r_2^2) > 0\,. \end{aligned}$$

This is a contradiction and completes the proof. $\square$

Corollary 4.2.4

If the variance function of a design ϵ can be expressed by (4.2.4), then the maximal value of the variance function is equal to the maximum of

$$d = \gamma + \gamma\, r^2 - 2\gamma\, r\cos\theta + \alpha + \alpha\, r^4 - 2\alpha\, r^2\cos^2\theta + \xi\,(1-r^2)^2\,, \tag{4.2.6}$$

where

$$0 \leqslant \theta \leqslant 2\pi\,,\quad 0 \leqslant r \leqslant 1\,.$$

Lemma 4.2.5

Let ϵ be a design for which the variance function can be expressed by (4.2.4). Let (u,v) be a pair where the variance function is maximal and such that

$$\sum_{i=1}^{n} u_i^2 = r_1^2\,,\quad \sum_{i=1}^{n} v_i^2 = r_2^2\,,$$

and

$$\theta \text{ is such that } r_1 r_2 \cos\theta = \sum_{i=1}^{n} u_i v_i\,.$$

Then the following holds

$$\theta = \pi \quad \text{and} \quad r_1, r_2 \text{ have the values } 1 \text{ and } \tfrac{1}{2} - \tfrac{1}{2}\,[1-\frac{2\gamma}{\alpha+\xi}]^{\frac{1}{2}}\,, \tag{4.2.7}$$

or

$$\theta = \arccos\,(-\frac{\gamma}{2\alpha}) \quad \text{and} \quad r_1 = r_2 = 1\,. \tag{4.2.8}$$

Proof

Assume without loss of generality $r_1 = 1$. According to corollary 4.2.4 we have to maximize

$$f(r,\theta) = \gamma + \gamma r^2 - 2\gamma r\cos\theta + \alpha + \alpha r^4 - 2\alpha r^2\cos^2\theta + \xi(1-r^2)^2,$$

where $0 \leqslant \theta \leqslant 2\pi$, $0 \leqslant r \leqslant 1$. We have

$$\frac{\partial f(r,\theta)}{\partial\theta} = 2\gamma r\sin\theta + 4\alpha r^2\cos\theta\sin\theta$$

$$= 4\alpha r^2\sin\theta\,(\cos\theta + \frac{\gamma}{2\alpha r}). \qquad \text{(i)}$$

Consider the region defined by $0 \leqslant r < \frac{\gamma}{2\alpha}$ and $0 \leqslant \theta \leqslant 2\pi$. Using (i) we find that the function $f(r,\theta)$ is maximal when $\theta = \pi$. Substituting this in $f(r,\theta)$ we find $r = \frac{1}{2} - \frac{1}{2}[1-\frac{2\gamma}{\alpha+\xi}]^{\frac{1}{2}}$.

Consider the region defined by $\frac{\gamma}{2\alpha} \leqslant r \leqslant 1$, and $0 \leqslant \theta \leqslant 2\pi$.

For fixed r the function $f(r,\theta)$ is maximal when

$$\theta = \arccos -\frac{\gamma}{2\alpha r}.$$

Substituting this we find

$$f(r,\theta) = \gamma + \alpha + \frac{\gamma^2}{2\alpha} + \gamma r^2 + \alpha r^4 + \xi(1-r^2)^2.$$

This function is maximal when $r = 1$. This completes the proof. □

Corollary 4.2.6

The maximal value of a variance function of type (4.2.4) equals one of the values

$$2\gamma + 2\alpha + \frac{\gamma^2}{2\alpha}, \qquad (4.2.9)$$

$$\tfrac{5}{2}\gamma + \tfrac{1}{2}(\alpha+\xi) - \frac{\gamma^2}{4(\alpha+\xi)} + [\tfrac{1}{2}(\alpha+\xi) - \gamma][1-\frac{2\gamma}{\alpha+\xi}]^{\frac{1}{2}}. \qquad (4.2.10)$$

If one assumes that a D-optimal design has a covariance matrix that satisfies (4.1.6), and (4.2.3), which means that it is strongly rotatable, then a D-optimal design consists of pairs of the type mentioned in lemma 4.2.5. Therefore, it is useful to consider pairs (x,y) and $(w,-rw)$ for which

$$\sum_{i=1}^{n} x_i^2 = \sum_{i=1}^{n} y_i^2 = \sum_{i=1}^{n} w_i^2 = 1. \qquad (4.2.11)$$

We define the following sets of pairs.

Definition 4.2.7

$S((u,v))$ is the set containing all 2^n pairs that can be found by multiplying pairs of coordinates (u_i, v_i) of (u,v) by -1 or $+1$.

$SP((u,v))$ is the union over all permutations p of the sets $S((p(u), p(v)))$, where p is a permutation of order n. In general the set $SP((u,v))$ contains $2^n\ n!$ pairs. The information matrix of $SP((u,v))$ is denoted by $MP((u,v))$.

The design matrix in the case of a 2^n-factorial can be used to compute the information matrices $M((u,v))$ and $MP((u,v))$. This design matrix contains only $+1$'s and -1 's.
Define

$$X_1(n) = (\ X_{11}(n) \mid K \mid X_{13}(n)\ ), \tag{4.2.12}$$

where

$$X_{11}(n) = \begin{bmatrix} X_{11}(n-1) & -u \\ & \\ X_{11}(n-1) & u \end{bmatrix}, \quad X_{11}(1) = \begin{bmatrix} -1 \\ 1 \end{bmatrix}, \tag{4.2.13}$$

$u = (1, \ldots, 1)'$,

K is a matrix with $K_{ij} = 1$ for all i and j ,

$$X_{13}(n) = \begin{bmatrix} X_{13}(n-1) & -X_{11}(n-1) \\ & \\ X_{13}(n-1) & X_{11}(n-1) \end{bmatrix}, \quad X_{13}(1) = \emptyset . \tag{4.2.14}$$

$X_{11}(n)$ is the notation for the main effects of a 2^n-factorial,
K is related to the quadratic effects,
$X_{13}(n)$ is related to the first-order interactions.

It is easy to prove that

$$(X_1(n))'X_1(n) = 2^n \left[\begin{array}{c|c|c} I & & \\ \hline & J & \\ \hline & & I \end{array} \right], \tag{4.2.15}$$

Now the design matrix D of $S((u,v))$ can be expressed by

$$D = X_1(n)\,(U - V), \tag{4.2.16}$$

where

$$\begin{aligned} U &= diag\ (u_1, \ldots, u_n \mid u_1^2, \ldots, u_n^2 \mid u_1u_2, \ldots, u_{n-1}u_n), \\ V &= diag\ (v_1, \ldots, v_n \mid v_1^2, \ldots, v_n^2 \mid v_1v_2, \ldots, v_{n-1}v_n). \end{aligned} \tag{4.2.17}$$

So, the information matrix $M((u,v))$ is

$$M((u,v)) = 2^n\ (U-V) \left[\begin{array}{c|c|c} I & & \\ \hline & J & \\ \hline & & J \end{array}\right] (U-V)\ . \qquad (4.2.18)$$

If $M((u,v))$ is denoted by

$$M((u,v)) = \left[\begin{array}{c|c|c} M_{11} & & \\ \hline & M_{22} & \\ \hline & & M_{33} \end{array}\right] ,$$

(4.2.19)

$$\begin{aligned} M_{11} &= 2^n\ diag\ ((u_1-v_1)^2, \ldots, (u_n-v_n)^2)\ , \\ (M_{22})_{ij} &= 2^n\ (u_i^2-v_i^2)\,(u_j^2-v_j^2)\ , \\ M_{33} &= 2^n\ diag\ ((u_1u_2-v_1v_2)^2, \ldots, (u_{n-1}u_n-v_{n-1}v_n)^2)\ . \end{aligned}$$

The information matrices $MP((u,v))$ can be written as

$$MP((u,v)) = \left[\begin{array}{c|c|c} p_0 I & & \\ \hline & s_0 I + t_0 J & \\ \hline & & z_0 I \end{array}\right] , \qquad (4.2.20)$$

where

$$\begin{aligned} p_0 &= 2^n\ (n-1)!\ \sum_{i=1}^{n} (u_i - v_i)^2\ , \\ s_0 + t_0 &= 2^n\ (n-1)!\ \sum_{i=1}^{n} (u_i^2 - v_i^2)^2\ , \\ t_0 &= 2^{n+1}\,(n-2)!\ \sum\sum_{i<j} (u_i^2 - v_i^2)(u_j^2 - v_j^2)\ , \\ z_0 &= 2^{n+1}\,(n-2)!\ \sum\sum_{i<j} (u_iu_j - v_iv_j)^2\ . \end{aligned}$$

As will be seen in theorem 4.2.11 a D-optimal design ϵ can be constructed by choosing the pairs of $SP((x,y))$ and $SP((w,-rw))$,$0 \leqslant r < 1$, with suitable weights ν_1 and ν_2 and suitable x , y and w that satisfy (4.2.11).
The weights must satisfy

$$2^n\ n!\,(\nu_1 + \nu_2) = 1\ . \qquad (4.2.21)$$

The information matrix $M(\epsilon)$ of such a design ϵ can be computed by using (4.2.20).

$$M(\epsilon) = M_1 + M_2 , \tag{4.2.22}$$

with

$$M_i = \left[\begin{array}{c|c|c} p_i I & & \\ \hline & s_i I + t_i J & \\ \hline & & z_i I \end{array}\right] \qquad (i = 1, 2),$$

where

$$\begin{aligned}
p_1 &= \nu_1 2^n (n-1)!\, 2(1-\sum_{i=1}^{n} x_i y_i) , \\
s_1 + t_1 &= \nu_1 2^n (n-1)! \sum_{i=1}^{n} (x_i^2 - y_i^2)^2 , \\
t_1 &= \nu_1 2^{n+1} (n-2)! \sum\sum_{i<j} (x_i^2 - y_i^2)(x_j^2 - y_j^2) , \\
z_1 &= \nu_1 2^{n+1} (n-2)! \sum\sum_{i<j} (x_i x_j - y_i y_j)^2 ,
\end{aligned}$$

$$\tag{4.2.23}$$

$$\begin{aligned}
p_2 &= \nu_2 2^n (n-1)!\, (1+r)^2 , \\
s_2 + t_2 &= \nu_2 2^n (n-1)!\, (1-r^2)^2 \sum_{i=1}^{n} w_i^4 , \\
t_2 &= \nu_2 2^{n+1} (n-2)!\, (1-r^2)^2 \sum\sum_{i<j} w_i^2 w_j^2 , \\
z_2 &= \nu_2 2^{n+1} (n-2)!\, (1-r^2)^2 \sum\sum_{i<j} w_i^2 w_j^2 .
\end{aligned}$$

With the notation of (4.1.6) we find

$$\tag{4.2.24}$$

$$\begin{aligned}
\gamma &= \frac{1}{p_1 + p_2} , \\
\alpha &= \frac{1}{s_1 + s_2} , \\
\alpha + n\xi &= \frac{1}{(s_1 + nt_1) + (s_2 + nt_2)} , \\
\delta &= \frac{1}{z_1 + z_2} .
\end{aligned}$$

From lemma 4.2.5 and theorem 2.3.7 it follows that, if $2\alpha = \delta$ then x , y and r must satisfy the conditions

$$\sum_{i=1}^{n} x_i y_i = -\frac{\gamma}{2\alpha} =: \cos\theta_0 \,, \tag{4.2.25}$$

$$r = \tfrac{1}{2} - \tfrac{1}{2}\,[1-\frac{2\gamma}{\alpha+\xi}]^{\frac{1}{2}} =: r_0 \,. \tag{4.2.26}$$

A condition equivalent to $2\alpha = \delta$ is given in the following lemma.

Lemma 4.2.8

Let x, y and w satisfy (4.2.11).
Let ϵ be a normalized design consisting of the pairs of $SP((x,y))$ with weights ν_1 and of the pairs of $SP((w,-rw))$ with weights ν_2. The condition $2\alpha = \delta$ is equivalent to

$$2\nu_1 (n+2) \sum\sum_{i<j} (x_i x_j - y_i y_j)^2 + 2\nu_2 (n+2)(1-r^2)^2 \sum\sum_{i<j} w_i^2 w_j^2$$
$$= 2n\ \nu_1 \sin^2\theta + \nu_2 (n-1)\,(1-r^2)^2 \,, \tag{4.2.27}$$

where

$$\cos\theta = \sum_{i=1}^{n} x_i y_i \,.$$

If (4.2.27) holds, then

$$z = \frac{1}{n+2}\, 2^{n+1}\, n\ \nu_1 (n-2)!\,\sin^2\theta + \frac{1}{n+2}\, 2^n\ \nu_2 (n-1)!\,(1-r^2)^2 \,,$$
$$p = 2\nu_1\, 2^n\ (n-1)!\,(1-\cos\theta) + \nu_2 (n-1)!\,(1+r)^2 \,, \tag{4.2.28}$$
$$s + nt = 2^n\ \nu_2 (n-1)!\,(1-r^2)^2 \,,$$

where

$$z = z_1 + z_2 \,,\ p = p_1 + p_2 \,,\ s = s_1 + s_2 \text{ and } t = t_1 + t_2 \,.$$

Proof

The condition $2\alpha = \delta$ is equivalent to $s_1 - 2z_1 = -(s_2 - 2z_2)$.
From (4.2.23) we have

$$s_1 - 2z_1 =$$
$$= 2^n \nu_1 (n-2)!\,[(n-1)\sum_{i=1}^{n} (x_i^4 + y_i^4 - 2x_i^2 y_i^2) - 4\sum\sum_{i<j} (x_i x_j - y_i y_j)^2$$
$$-2\sum\sum_{i<j} (x_i^2 x_j^2 + y_i^2 y_j^2 - x_i^2 y_j^2 - x_j^2 y_i^2)]$$
$$= 2^n \nu_1 (n-2)!\,[2(n-1) - 2(n-1)\sum\sum_{i<j} x_i^2 x_j^2 - 2(n-1)\sum\sum_{i<j} y_i^2 y_j^2$$
$$-2(n-1)\sum_{i=1}^{n} x_i^2 y_i^2\ -4\sum\sum_{i<j} (x_i x_j - y_i y_j)^2$$

$$-2\sum_{i<j}\sum x_i^2x_j^2 - 2\sum_{i<j}\sum y_i^2y_j^2 + 2 - 2\sum_{i=1}^{n} x_i^2y_i^2\,]$$

$$= 2^n\ \nu_1\,(n-2)!\,[2n - 2(n+2)\sum_{i<j}\sum (x_ix_j - y_iy_j)^2 - 2n\,(\sum_{i=1}^{n} x_iy_i)^2\,]\,.$$

$$s_2 - 2z_2 =$$

$$= 2^n\ \nu_2\,(n-2)!\,(1-r^2)^2\,[(n-1)\sum_{i=1}^{n} w_i^4 - 6\sum_{i<j}\sum w_i^2w_j^2\,]$$

$$= 2^n\ \nu_2\,(n-2)!\,(1-r^2)^2\,[(n-1) - 2(n-1)\sum_{i<j}\sum w_i^2w_j^2 - 6\sum_{i<j}\sum w_i^2w_j^2\,]$$

$$= 2^n\ \nu_2\,(n-2)!\,(1-r^2)^2\,[(n-1) - 2(n+2)\sum_{i<j}\sum w_i^2w_j^2\,]\,.$$

Substituting these expressions in $s_1 - 2z_1 = -(s_2 - 2z_2)$ completes the first part of the proof. The correctness of expressions (4.2.28) can be verified by substituting (4.2.27) in (4.2.23). □

The weights ν_1 and ν_2 may be found by use of the following lemma.

Lemma 4.2.9

Let ϵ be a design of the type defined in lemma 4.2.8 and let (4.2.27) be satisfied. The determinant of the information matrix $\det(M(\epsilon))$ *satisfies*

$$\det(M(\epsilon)) = C\ \nu_2\,(a\,\nu_2 + b\,)^n\ (c\,\nu_2 + d\,)^{\binom{n}{2}+(n-1)}\ , \qquad (4.2.29)$$

where

C *is a constant not depending on* ν_1 *and* ν_2 ,

$a = (1+r)^2 - 2(1-\cos\theta)\,,$

$b = 2(1-\cos\theta)\,\dfrac{1}{2^n\ n!}\,,$

$c = (n-1)\,(1-r^2)^2 - 2n\sin^2\theta\,,$

$d = \dfrac{2n\sin^2\theta}{2^n\ n!}\,.$

The value of ν_2 *at which* $\det(M(\epsilon))$ *is maximal is a solution of the equation:*

$$\nu_2^2\,\tfrac{1}{2}n\,(n+3)\,ac + \nu_2\,(n+1)(ad + \tfrac{1}{2}n\ bc\,) + bd = 0 \qquad (4.2.30)$$

Proof

From (4.2.28) we have

$$\det(M(\epsilon)) = C\,\nu_2\left[\nu_2(1+r)^2 + 2(1-\cos\theta)(\frac{1}{2^n n!} - \nu_2)\right]^n$$

$$\cdot\left[2n\sin^2\theta\,(\frac{1}{2^n n!} - \nu_2) + (n-1)\nu_2(1-r^2)^2\right]^{\binom{n}{2}+(n-1)}\,.$$

This gives the expression (4.2.29). Differentiation of this expression with respect to ν_2 gives the second part of the theorem. $\square$

It is possible to construct a D-optimal design ϵ of the type defined in lemma 4.2.8. Then x, y, w and r must satisfy the conditions (4.2.25), (4.2.26) and (4.2.27). Since the covariance matrices of D-optimal designs coincide, $\cos\theta_0$ and r_0 are fixed. By a procedure similar to procedure 2.3.8 the values of $\cos\theta_0$ and r_0 can be computed as follows. Choose $\theta_{0,0}$ and $r_{0,0}$, for example $\theta_{0,0} = \frac{1}{2}\pi$ and $r_{0,0} = 0$. Let ϵ_0 be a design of the type defined in lemma 4.2.8 with $\theta = \theta_{0,0}$, $r = r_{0,0}$, satisfying (4.2.27) and let ν_2 be as given in lemma 4.2.9. The information matrix $M(\epsilon_0)$ can be computed and the variance function can be expressed by (4.2.4). Use of lemma 4.2.5 yields pairs where the variance function attains its maximum. This gives new values $\theta_{0,1}$ and $r_{0,1}$. Now this procedure is repeated with ϵ_1, $\cos\theta_{0,1}$ and $r_{0,1}$, etc.
This process converges and the values of $\cos\theta_0$ and r_0 can be computed. A priori it is not obvious that this procedure converges. The condition $2\alpha = \delta$ is used, which will be proved to hold for D-optimal designs in theorem 4.2.11. This knowledge enables us to prove the convergence. Note that it is not necessary to give the designs ϵ_i explicitly. When computing the information matrix $M(\epsilon_i)$, one only needs the values of $\cos\theta_{0,i}$ and $r_{0,i}$. Some results are given in table 4.2.10; the condition $2\alpha = \delta$ is satisfied there. As can be seen from this table, r_0 and θ_0 are decreasing functions of n, and $\alpha, \delta, \gamma, \xi$ and $\det(M^{-1}(\epsilon))$ are all increasing with n. The design consists for 68% of pairs of $SP((x,y))$ when $n = 2$, and for 95% when $n = 7$.

Table 4.2.10
Values of constants determining the information matrix of a D-optimal design

n	2	3	4	5	6	7
α	1.4475	2.9972	5.0307	7.5558	10.576	14.092
δ	2.8950	5.9944	10.0613	15.1115	21.151	28.183
γ	0.9096	1.3507	1.8071	2.2733	2.7462	3.224
ξ	2.5241	4.5181	7.0152	10.0133	13.5119	17.5108
r_0	0.1319	0.0998	0.08168	0.06953	0.06069	0.05392
θ_0	108.3°	103.0°	100.3°	98.7°	97.5°	96.6°
$2^n\, n!\, \nu_1$	0.6811	0.8151	0.8775	0.9124	0.9340	0.9485
$\det(M^{-1}(\epsilon))$	22.5	7.89 10^4	4.66 10^{10}	7.08 10^{18}	3.95 10^{29}	0.914 10^{44}

Now the following theorem can be formulated.

Theorem 4.2.11

a) Let x, y, w and r be such that they satisfy the conditions

$$\sum_{i=1}^{n} x_i^2 = \sum_{i=1}^{n} y_i^2 = \sum_{i=1}^{n} w_i^2 = 1\ , \tag{4.2.11}$$

$$\sum_{i=1}^{n} x_i y_i = \cos\theta_0\ , \tag{4.2.25}$$

$$r = \tfrac{1}{2} - \tfrac{1}{2}\left[1 - \frac{2\gamma}{\alpha+\xi}\right]^{\frac{1}{2}} = r_0\ , \tag{4.2.26}$$

$$2\nu_1(n+2)\sum_{i<j}\sum (x_i x_j - y_i y_j)^2 + 2\nu_2(n+2)(1-r^2)^2\sum_{i<j}\sum w_i^2 w_j^2$$
$$= 2n\,\nu_1 \sin^2\theta + \nu_2(n-1)(1-r^2)^2\ , \tag{4.2.27}$$

where r_0 and θ_0 have the value given in table 4.2.10. The design ϵ consisting of the pairs of $SP((x,y))$ with weights ν_1, and of the pairs of $SP((w,-rw))$ with weights ν_2, that satisfy (4.2.21) and (4.2.30) is D-optimal. The design is strongly rotatable.

b) Let (u,v) be a pair of a D-optimal design, and let $\sum_{i=1}^{n} u_i^2 = 1$.

Now v satisfies

$$v = -r_0 u\ ,$$

or

$$\sum_{i=1}^{n} v_i^2 = 1 \text{ and } \sum_{i=1}^{n} u_i v_i = \cos\theta_0 .$$

Proof

From lemma 4.2.5 it follows that the variance function attains is maximum at the pairs of the design. According to corollary 4.2.6 this maximum is one of the values given in (4.2.9) and (4.2.10). Computation of these values completes the first part of the proof. Part b) of the theorem is proved by applying lemma 4.2.5 and theorem 2.3.7. □

When discussing theorem 2.3.1 in chapter 2, we mentioned that in the case of paired comparisons D-optimality and G-optimality are *not* equivalent. Now we can give an example that shows this.

Example 4.2.12

Let $n = 2$ and consider the information matrix of a D-optimal design ϵ. To consider the G-efficiency of such a design, one has to compute the maximum of the variance function $d(x,\epsilon)$. We have

$$\begin{aligned} d(x,\epsilon) &= \gamma\,(x_1^2 + x_2^2) + (\alpha+\xi)\,(x_1^4 + x_2^4) + (2\xi+\delta)\,x_1^2x_2^2 \\ &= \gamma\, r^2 + (\alpha+\xi)\, r^4 . \end{aligned}$$

So

$$\max_{x \in X} d(x,\epsilon) = \gamma + \alpha + \xi = 4.88$$

It is easy to show that a D-optimal design is not G-optimal by constructing a design ϵ_1 for which

$$\max_{x} d(x,\epsilon_1) < 4.88 .$$

Let ϵ_1 be the normalized design consisting of the pairs of $SP((w, -rw))$ with $w = (\cos\phi, \sin\phi)$, $\phi = 22.5°$ and $r_1 = \frac{1}{5}$.

Then

$$MP((w, -rw)) = \left|\begin{array}{c|c|c} p_1 I & & \\ \hline & s_1 I + t_1 J & \\ \hline & & z_1 I \end{array}\right| ,$$

with

$$p_1 = \tfrac{1}{2}(1+r_1)^2 ,$$

$$s_1 = \tfrac{1}{4}(1-r^2)^2 ,$$

$$t_1 = z_1 = \tfrac{1}{8}(1-r_1^2)^2 .$$

This yields

$$d(x,\epsilon_1) = \frac{2}{(1+r_1)^2} r^2 + \frac{3}{(1-r^2)^2} r^4 .$$

So,

$$\max_x d(x,\epsilon_1) = \frac{2}{(1+r_1)^2} + \frac{3}{(1-r_1^2)^2} = 4.64 ,$$

which shows that a D-optimal design is not G-optimal in this case. $\square$

4.3. Some discrete D-optimal designs

In general a design of the type given in theorem 4.2.11 consists of $2\ 2^n\ n!$ pairs. If we choose suitable x, y and w, a discrete D-optimal design can be constructed for which the number of pairs is considerably smaller than $2^{n+1} n!$. In this section $\cos\theta_0$, r_0, ν_1 and ν_2 are fixed and have the value given in table 4.2.10.

Choose

$$w = (1,0,\ldots,0)' , \tag{4.3.1}$$

$$x = (\cos\phi_1, \sin\phi_1, 0, \ldots, 0)' , \tag{4.3.2}$$

$$y = (\cos\phi_2, \sin\phi_2, 0, \ldots, 0)' ,$$

Now $SP((x,y))$ contains $4n(n-1)$ pairs and $SP((w,-r_0w))$ contains $2n$ pairs. The points x, y and w must satisfy the conditions (4.2.11), (4.2.25), (4.2.27). Using these conditions we find

$$\cos\phi_1\cos\phi_2 + \sin\phi_1\sin\phi_2 = \cos\theta_0 ,$$

$$\cos(\phi_1 - \phi_2) = \cos\theta_0 ,$$

$$\phi_1 - \phi_2 = \theta_0 , \tag{4.3.3}$$

and

$$2\nu_1(n+2)(\cos\phi_1\sin\phi_1 - \cos\phi_2\sin\phi_2)^2 = 2n\,\nu_1\sin^2\theta_0 + \nu_2(n-1)(1-r_0^2)^2 ,$$

$$2\nu_1(n+2)\sin^2(\phi_1 - \phi_2)\cos^2(\phi_1+\phi_2) = 2n\,\nu_1\sin^2\theta_0 + \nu_2(n-1)(1-r_0^2)^2 .$$

Using (4.3.3) we obtain

$$\cos^2\zeta = \frac{n}{n+2} + \frac{\nu_2}{\nu_1}\,\frac{n-1}{2(n+2)}\,\frac{(1-r_0^2)^2}{\sin^2\theta_0} , \tag{4.3.4}$$

where

$$\zeta = \phi_1 + \phi_2 .$$

According to (4.2.23) p_i, s_i, t_i and z_i $(i=1,2)$ have the following values, where p_i, s_i, t_i and z_i are such as in (4.2.22).

$$\begin{aligned} p_1 &= \nu_1\, 2^n\, (n-1)!\, (1-\cos\theta_0)\,, \\ s_1 + t_1 &= 2\nu_1\, 2^n\, (n-1)!\, \sin^2\theta_0 \sin^2\zeta\,, \\ t_1 &= -2\nu_1\, 2^n\, (n-2)!\, \sin^2\theta_0 \sin^2\zeta\,, \\ z_1 &= 2\nu_1\, 2^n\, (n-2)!\, \sin^2\theta_0 \sin^2\zeta\,, \end{aligned} \tag{4.3.5}$$

$$\begin{aligned} p_2 &= \nu_2\, 2^n\, (n-1)!\, (1+r_0)^2\,, \\ s_2 &= \nu_2\, 2^n\, (n-1)!\, (1-r_0^2)^2\,, \\ t_2 &= 0\,, \\ z_2 &= 0\,. \end{aligned} \tag{4.3.6}$$

When n is odd, the number of pairs of $SP((x,y))$ can be even more reduced. $SP((x,y))$ is the union of $n(n-1)$ sets of 4 pairs. In every set one interaction is measured. So, $\binom{n}{2}$ sets of 4 pairs are needed to measure all interactions with the same accuracy. In every set two main effects (and two quadratic effects) are measured, but not with the same accuracy. So, in general $2\binom{n}{2}$ sets are needed. When n is odd $\binom{n}{2}$ sets can be chosen such that the main effects (and quadratic effects) are measured with the same accuracy.
Example in the case $n = 3$.

Choose $S((\cos\phi_1,\sin\phi_1,\ 0\ ),(\cos\phi_2,\sin\phi_2\ ,\ 0\ ))$,
$S((\sin\phi_1,\ 0\ ,\cos\phi_1\ ),(\sin\phi_2,\ 0\ ,\cos\phi_2))$,
and $S((\ 0\ ,\cos\phi_1,\sin\phi_1),(\ 0\ ,\cos\phi_2\ ,\sin\phi_2))$.

When n is even, this reduction is not possible.
Now the number, say N, of pairs of the design is given by

$$N = \begin{cases} 2n\,(2n-1) & ,\text{if } n \text{ even}\,, \\ 2n^2 & ,\text{if } n \text{ odd}\,. \end{cases}$$

The following theorem is a special case of theorem 4.2.11.

Theorem 4.3.1

Let x, y and w be such as defined in (4.3.1) and (4.3.2), satisfying the conditions (4.3.3) and (4.3.4). The following design is D-optimal.
Choose

- *the pairs of $SP((w, -r_0 w))$ with weights ν_2^*, where $\nu_2^* = 2^{n-1}(n-1)!\,\nu_2$,*
- *the pairs of $SP((x, y))$ as described above; so all $4n(n-1)$ pairs if n is even, and $2n(n-1)$ pairs if n is odd; the pairs have weight ν_1^*, where*

$$\nu_1^* = \begin{cases} 2^{n-2}(n-1)!\,\nu_1 & ,\text{if } n \text{ even}, \\ 2^{n-1}(n-2)!\,\nu_1 & ,\text{if } n \text{ odd}. \end{cases}$$

Some results are given in table 4.3.2.

Table 4.3.2
Values of constants determining the design given in theorem 4.3.1

n	2	3	4	5	6	7
N	12	18	56	50	132	98
m	15	45	105	210	378	630
ϕ_1	74.85°	69.74°	66.71°	64.59°	62.98°	61.71°
ϕ_2	−33.46°	−33.28°	−33.64°	−34.07°	−34.48°	−34.86°

In this table $m = \frac{1}{8}n(n+1)(n+2)(n+3)$ (see (4.1.4)).

We give a few more D-optimal designs for the case $n = 2$.
Choose

$$x = (\cos\phi_1, \sin\phi_1), \tag{4.3.7}$$

$$y = (\cos\phi_2, \sin\phi_2),$$

$$w = (\cos\omega, \sin\omega). \tag{4.3.8}$$

The conditions (4.2.25) and (4,2,27) yield

$$\phi_1 - \phi_2 = \theta_0, \tag{4.3.9}$$

and

$$8\nu_1(\cos\phi_1\sin\phi_1 - \cos\phi_2\sin\phi_2)^2 + 8\nu_2(1-r_0^2)^2\cos^2\omega\,\sin^2\omega$$
$$= 4\nu_1\sin^2\theta_0 + \nu_2(1-r_0^2)^2,$$

This last equation can be rewritten as

$$8\nu_1 \sin^2\theta_0 \sin^2\zeta + 2\nu_2 (1-r_0^2)^2 \sin^2 2\omega = 4\nu_1 \sin^2\theta_0 + \nu_2 (1-r_0^2)^2 ,$$

or

$$\sin^2 2\omega = \tfrac{1}{2} - 2\frac{\nu_1}{\nu_2} \frac{\sin^2\theta_0}{(1-r_0^2)^2} \cos 2\zeta . \qquad (4.3.10)$$

From this we find

$$-0.1254 \leqslant \cos 2\zeta \leqslant 0.1254 . \qquad (4.3.11)$$

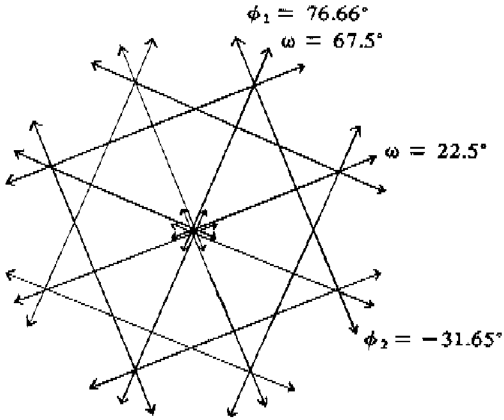
Some choices of ω and ζ are listed in table 4.3.3.

Table 4.3.3
Choices of ω and ϕ_1 in the D-optimal design defined by (4.3.7) and (4.3.8)

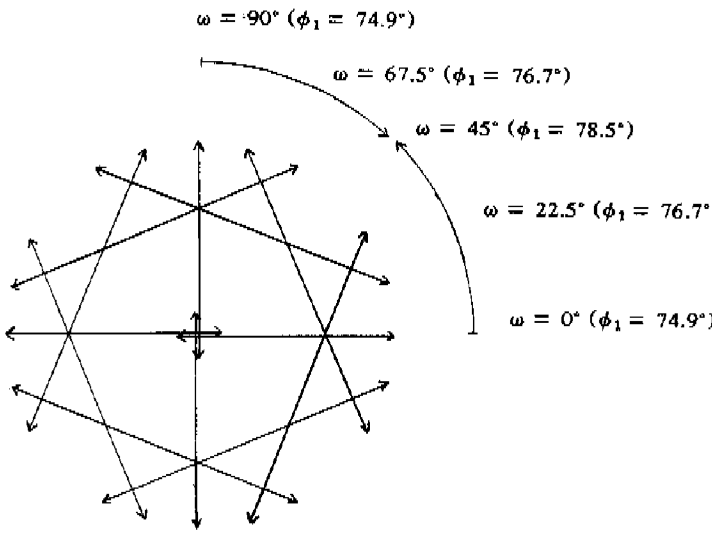
ω	$\cos 2\zeta$	ϕ_1
0°,90°	0.125	74.86°
5°,85°	0.117	74.96°
10°,80°	0.096	75.28°
15°,75°	0.063	75.76°
20°,70°	0.022	76.34°
22.5°,67.5°	0	76.66°
25°,65°	—0.022	76.97°
30°,60°	—0.063	77.55°
35°,55°	—0.096	78.03°
40°,50°	—0.117	78.35°
45°	—0.125	78.46°

As an illustration two choices are given in the pictures below. The arrows in the pictures indicate the pairs.

Picture 4.3.4
The pairs of some exact designs in the case $n = 2$
a) $\omega = 22.5°$



b) $\omega = 0°$



4.4. Exact designs

It is possible to construct exact designs with efficiency $1-\eta$ for any small positive value of η (see theorem 3.1.1 of Fedorov (1972)). For such a design, since the product of the weights and the number of pairs must be an integer, in general a large number of observations has to be chosen. Such designs are not very useful for practical applications. In this section exact designs are constructed for which the efficiency is high and the number of pairs is relatively small.

In section 4.4.1 designs are given that consist of pairs of $SP((w,-rw))$ for some r and w. In section 4.4.2 designs are given that consist of pairs of $SP((x,y))$ and of pairs of $SP((w,-rw))$ for some x, y, w and r, satisfying (4.2.11). Note that the covariance matrix of a design consisting only of pairs of $SP((x,y))$ is singular.

4.4.1. Exact designs consisting of pairs of SP((w, -rw))

We choose an exact normalized design consisting of the pairs of $SP((w,-rw))$ with weights $\nu = 2^{-n}/n!$, where

$$w = (w_1, \ldots, w_n)' \ ,$$

$$\sum_{i=1}^{n} w_i^2 = 1 \ .$$

From the second half of (4.2.23) it follows that

$$MP((w,-rw)) = \left[\begin{array}{c|c|c} pI & & \\ \hline & sI+tJ & \\ \hline & & zI \end{array}\right] , \qquad (4.4.1)$$

where

$$p = \frac{1}{n}(1+r)^2 \ , \qquad (4.4.2)$$

$$z = t = \frac{1}{n(n-1)}(1-r^2)^2 \left(1-\sum_{i=1}^{n} w_i^4\right) \ ,$$

$$s = \frac{1}{n(n-1)}(1-r^2)^2 \left(n\sum_{i=1}^{n} w_i^4 - 1\right) \ .$$

Now r and w have to be chosen. The D-criterion can be used in choosing r and w. This gives conditions for r and w which are given in the following lemma.

Lemma 4.4.1
The determinant of $MP((w, -rw))$ has a unique maximum at

$$r = \frac{1}{n+2} , \tag{4.4.3}$$

and

$$\sum_{i=1}^{n} w_i^4 = \frac{3}{n+2} . \tag{4.4.4}$$

Proof
For det $(MP((w, -rw)))$ we have

$$p^n s^{n-1} (s+nt) z^{\binom{n}{2}}$$

$$= C \ (1+r)^{2n} \ (1-r^2)^{2n} \ (nw_0-1)^{n-1} (1-r^2)^{n(n-1)} (1-w_0)^{\frac{1}{2}n(n-1)} ,$$

where C is a constant and

$$w_0 = \sum_{i=1}^{n} w_i^4 .$$

So, det $(MP((w, -rw)))$ equals

$$C \ (1+r)^{n(n+3)} (1-r)^{n(n+1)} (nw_0-1)^{n-1} (1-w_0)^{\frac{1}{2}n(n-1)} .$$

This function has a unique maximum at

$$(r, w_0) = (1/(n+2) , 3/(n+2)).$$

Corollary 4.4.2
Let ϵ be a design consisting of the pairs of $SP((w, -rw))$ with weights $\nu = \frac{1}{2^n n!}$, and let r and w satisfy the conditions (4.4.3) and (4.4.4). Then

$$\begin{aligned} p &= \frac{(n+3)^2}{n(n+2)^2} , \\ t = z &= \frac{(n+1)^2(n+3)^2}{n(n+2)^5} , \\ s &= 2z \\ s + nt &= \frac{(n+1)^2(n+3)^2}{n(n+2)^4} , \end{aligned} \tag{4.4.5}$$

$$\begin{aligned} \gamma &= p^{-1} , \\ \delta &= z^{-1} , \\ 2\alpha &= \delta , \end{aligned}$$

$$\xi = \frac{-n(n+2)^4}{2(n+1)^2(n+3)^2} .$$

From (4.4.5) the D-efficiency of a design $SP((w, -rw))$ can be computed. We wish to compute the $\mathring{G}$-efficiency as well. The function $d(x, y, \epsilon)$ attains its maximum at the pair (u, v) satisfying

$$\sum_{i=1}^{n} u_i^2 = \sum_{i=1}^{n} v_i^2 = 1 ,$$

and (4.4.6)

$$\sum_{i=1}^{n} u_i v_i = -\frac{\gamma}{\delta} .$$

The maximal value of $d(x, y, \epsilon)$ is given by

$$\max_{x,y} d(x, y, \epsilon) = 2\gamma + \delta + \frac{\gamma^2}{\delta} . \tag{4.4.7}$$

Now the $\mathring{G}$-efficiency can be computed:

$$\mathring{G}\text{-eff}(\epsilon) = \frac{(n+3)^3 (n+2) (n+1)^2}{4(n+2)^3 (n+1)^2 + 2(n+2)^6 + 2(n+1)^4} . \tag{4.4.8}$$

Some results are given in table 4.4.4. The D-efficiency is 68% when $n = 2$, and even less when $n > 2$. Therefore the results are not satisfactory, although the number of pairs is rather small.
Another criterion to choose r and w is the $\mathring{G}$-criterion. In order to use this criterion, the function $d(u, v, \epsilon)$ has to be evaluated.

According to (4.1.8) we have

$$d(u, v, \epsilon) = \gamma (r_1^2 + r_2^2) - 2\gamma \sum_{i=1}^{n} u_i v_i + \xi (r_1^2 - r_2^2)^2 \tag{4.4.9}$$

$$+\alpha (r_1^4 + r_2^4) - 2\alpha (\sum_{i=1}^{n} u_i v_i)^2 + (\delta - 2\alpha) \sum\sum_{i<j} (u_i u_j - v_i v_j)^2 ,$$

or

$$d(u, v, \epsilon) = \gamma (r_1^2 + r_2^2) - 2\gamma \sum_{i=1}^{n} u_i v_i + \xi (r_1^2 - r_2^2)^2 \tag{4.4.10}$$

$$+\tfrac{1}{2}\delta (r_1^4 + r_2^4) - \delta (\sum_{i=1}^{n} u_i v_i)^2 - \tfrac{1}{2} (\delta - 2\alpha) \sum_{i=1}^{n} (u_i^2 - v_i^2)^2 .$$

The expressions (4.4.9) and (4.4.10) can be used in proving the following lemma.

Lemma 4.4.3

Let ϵ be the design consisting of the pairs of $SP((w, -rw))$ with weights $\nu = 1/(2^n n!)$.

If r and w are such that $\max_{u,v} d(u,v,\epsilon)$ is minimized, then r and w satisfy

$$\sum_{i=1}^{n} w_i^4 = \frac{3}{n+2} \ , \tag{4.4.4}$$

$$r = \tfrac{1}{2} n + 2 - \tfrac{1}{2} \sqrt{n^2 + 8n + 12} \ . \tag{4.4.11}$$

Proof

We shall prove that $2\alpha = \delta$, which is equivalent to (4.4.4), by showing that $2\alpha \leqslant \delta$ implies $2\alpha = \delta$ and that $2\alpha \geqslant \delta$ also implies $2\alpha = \delta$. The values of p, z, t and s are given by (4.4.2).

Suppose $2\alpha \leqslant \delta$, so $\sum_{i=1}^{n} w_i^4 \geqslant \frac{3}{n+2}$. From (4.4.10) it can be seen that

$$d(u,v,\epsilon) \leqslant d_1(u,v,\epsilon) \ ,$$

where

$$d_1(u,v,\epsilon) = \gamma\,(r_1^2 + r_2^2) - 2\gamma \sum_{i=1}^{n} u_i v_i + \xi\,(r_1^2 - r_2^2)^2$$
$$+ \tfrac{1}{2}\delta\,(r_1^4 + r_2^4) - \delta\,(\sum_{i=1}^{n} u_i v_i)^2 \ ;$$

$d_1(u,v,\epsilon)$ attains its maximal value if u and v satisfy (4.4.6), and the maximal value of $d(u,v,\epsilon)$ is given in (4.4.7). So,

$$d(u,v,\epsilon) \leqslant 2\gamma + \delta + \frac{\gamma^2}{\delta} \ .$$

According to (4.4.2) we have $\delta > \gamma$.
Therefore, it is possible to choose

$$u_0 = ((\frac{\delta+\gamma}{2\delta})^{\frac{1}{2}}, (\frac{\delta-\gamma}{2\delta})^{\frac{1}{2}}, 0, \ldots, 0)' \ ,$$

and

$$v_0 = (-(\frac{\delta+\gamma}{2\delta})^{\frac{1}{2}}, (\frac{\delta-\gamma}{2\delta})^{\frac{1}{2}}, 0, \ldots, 0)' \ .$$

and it is easily seen that

$$d(u_0, v_0, \epsilon) = 2\gamma + \delta + \frac{\gamma^2}{\delta} \ .$$

So, we have to minimize the expression

$$\frac{2n}{(1+r)^2} + \frac{n(n-1)}{(1-r^2)^2}\,\frac{1}{1-w_0} + \frac{n(1-r^2)^2}{(n-1)(1+r)^4}\,(nw_0-1)$$

with respect to r and w_0, where $w_0 = \sum_{i=1}^{n} w_i^4$.

This is an increasing function of w_0 for all values of r. Therefore w_0 has to be chosen as small as possible, so $w_0 = \frac{3}{n+2}$ and $2\alpha = \delta$.

Now suppose $2\alpha \geqslant \delta$, so $\sum_{i=1}^{n} w_i^4 \leqslant \frac{3}{n+2}$.

From (4.4.9) it follows that

$$d(u,v,\epsilon) \leqslant d_2(u,v,\epsilon),$$

where

$$d_2(u,v,\epsilon) = \gamma\,(r_1^2+r_2^2) - 2\gamma \sum_{i=1}^{n} u_i v_i + \xi\,(r_1^2-r_2^2)^2$$

$$+ \alpha\,(r_1^4+r_2^4) - 2\alpha\,(\sum_{i=1}^{n} u_i v_i)^2 .$$

In a similar way it can be seen that $d(u,v,\epsilon)$ is maximal at the pair (u_1,v_1) where

$$u_1 = ([\tfrac{1}{2}+\tfrac{1}{2}(\frac{4\alpha^2-\gamma^2}{4\alpha^2})^{\frac{1}{2}}]^{\frac{1}{2}}, [\tfrac{1}{2}-\tfrac{1}{2}(\frac{4\alpha^2-\gamma^2}{4\alpha^2})^{\frac{1}{2}}]^{\frac{1}{2}}, 0, \ldots, 0)' ,$$

$$u_1 = (-[\tfrac{1}{2}-\tfrac{1}{2}(\frac{4\alpha^2-\gamma^2}{4\alpha^2})^{\frac{1}{2}}]^{\frac{1}{2}}, -[\tfrac{1}{2}+\tfrac{1}{2}(\frac{4\alpha^2-\gamma^2}{4\alpha^2})^{\frac{1}{2}}]^{\frac{1}{2}}, 0, \ldots, 0)' ,$$

and that

$$d(u_1,v_1,\epsilon) = 2\gamma + 2\alpha + \frac{\gamma^2}{2\alpha} .$$

This last function is decreasing in w_0, and therefore we find

$$w_0 = \frac{3}{n+2}, \text{ and } 2\alpha = \delta .$$

Hence

$$\gamma = \frac{n}{(1+r)^2} ,$$

$$\delta = 2\alpha = \frac{n(n+2)}{(1-r^2)^2} ,$$

and

$$2\gamma + \delta + \frac{\gamma^2}{\delta} = \frac{2n}{(1+r)^2} + \frac{n(n+2)}{(1-r^2)^2} + \frac{n^2(1-r^2)^2}{n(n+2)(1+r)^4} .$$

This last function has a unique maximum at

$$r = \tfrac{1}{2}n + 2 - \tfrac{1}{2}\sqrt{n^2+8n+12}$$

This completes the proof. □

The D- and $\mathring{G}$-efficiencies of the exact designs given in lemma 4.4.3 are listed in table 4.4.4. Again, the results are not satisfactory, since the $\mathring{G}$-efficiency has a value between 40% and 50%. As could be expected, the $\mathring{G}$-efficiency is higher than the value found when using the D-criterion to determine r and w. The value of the D-efficiency, of course, is lower.
In general the number of pairs of the designs given in corollary 4.4.2 and lemma 4.4.3 equals $2^n n!$. This number can be reduced by choosing w in a suitable way.
Choose

$$w = (w_1, w_2, 0, \ldots, 0)'.$$

Now w must satisfy the conditions $w_1^2 + w_2^2 = 1$ and (4.4.4), the latter condition being equivalent to

$$w_1^4 + w_2^4 = \frac{3}{n+2}.$$

The only relevant solution of these equations is

$$w_1 = [\tfrac{1}{2} + \tfrac{1}{2}(\frac{4-n}{n+2})^{\frac{1}{2}}]^{\frac{1}{2}},$$

$$w_2 = [\tfrac{1}{2} - \tfrac{1}{2}(\frac{4-n}{n+2})^{\frac{1}{2}}]^{\frac{1}{2}}.$$

This choice is possible if $n \leqslant 4$. The results are given in table 4.4.4, where ϕ is such that

$$w = (\cos\phi, \sin\phi, 0, \ldots, 0)'.$$

Now we consider the case $n \geqslant 5$.
We choose

$$w = (w_1, w_2, \ldots, w_n)',$$

where

$$w_2 = w_3 = \cdots = w_n.$$

Now w_1 and w_2 must satisfy the conditions

$$w_1^2 + (n-1)\, w_2^2 = 1,$$

$$w_1^4 + (n-1)\, w_2^4 = \frac{3}{n+2}.$$

The only relevant solution of these equations is

$$w_1^2 = \frac{1}{n} + \frac{n-1}{n}\left(\frac{n}{n+2}\right)^{\frac{1}{2}},$$

and

$$w_2^2 = \frac{1}{n} - \frac{1}{n}\left(\frac{n}{n+2}\right)^{\frac{1}{2}}.$$

In general the number of pairs of these designs equals $n\ 2^n$ again. We give some further results in the case $n = 5$. The number of pairs of the design given above is 160. With a method to be discussed in section 5.4.2 the number of pairs can be reduced to 80. In the following we construct a design that does not satisfy conditon (4.4.4). Therefore the D-efficiency and $\mathring{G}$-efficiency is less than the efficiencies of the designs given above. However, the number of pairs equals 40. Choose

$$w = (\tfrac{1}{2}\sqrt{2}, \tfrac{1}{2}\sqrt{2}, 0, \ldots, 0)' .$$

This choice of z gives

$$\gamma = \frac{5}{(1+r)^2},$$

$$\delta = \frac{40}{(1-r^2)^2},$$

$$\alpha = \frac{40}{3(1-r^2)^2},$$

$$\alpha + 5\xi = \frac{5}{(1-r^2)^2}.$$

The maximal value of the variance function equals

$$2\gamma + \delta + \frac{\gamma^2}{\delta} = \frac{80(1-r)^2 + 320 + 5(1-r)^4}{8(1-r^2)^2}.$$

Minimizing this function with respect to r yields the condition

$$r^4 - 12r^3 + 30r^2 - 92r + 9 = 0 ,$$

or

$$r = 5 - 2\sqrt{6} = 0.1010 .$$

Maximizing the determinant of the information matrix leads to the same value of r as given in the condition (4.4.3), so $r = \frac{1}{7}$.

The results of section 4.4.1 are given in table 4.4.4. In this table is

w the choice made above to reduce the number of pairs of the design,

ϕ is such that $w = (\cos\phi_1, \sin\phi_1, 0, \ldots, 0)'$, and

N is the number of pairs of the design.

Table 4.4.4

Values of constants determining the exact designs $SP((w, -rw))$ given in section 4.4.1 , and found by using the D- and $\overset{*}{G}$-criteria.

n	2		3		4	
Criterion	D	$\overset{*}{G}$	D	$\overset{*}{G}$	D	$\overset{*}{G}$
r	0.25	0.1716	0.20	0.1459	0.1667	0.1270
$\sum_{i=1}^{n} w_i^4$	0.75	0.75	0.60	0.60	0.50	0.50
α	4.5511	4.2463	8.1380	7.8298	12.6955	12.3968
δ	9.1022	8.4926	16.2760	15.6596	25.3910	24.7935
γ	1.2800	1.4571	2.0833	2.2847	2.9388	3.1492
ξ	−1.1378	−1.0616	−1.6276	−1.5660	−2.1159	−2.0661
$\det(M^{-1}(\epsilon))$	154.44	162.56	$8.41\ 10^6$	$8.79\ 10^6$	$1.73\ 10^{14}$	$1.79\ 10^{14}$
D-eff	68.04%	67.35%	59.53%	59.23%	55.59%	55.44%
$\overset{*}{G}$-eff	42.22%	42.89%	43.46%	43.77%	44.29%	44.46%
w	(w_1, w_2)		$(w_1, w_2, 0)$		$(w_1, w_2, 0, 0)$	
w_1^2	$\frac{1}{2} + \frac{1}{4}\sqrt{2}$		$\frac{1}{2} + \frac{1}{10}\sqrt{2}$		$\frac{1}{2}$	
w_2^2	$\frac{1}{2} - \frac{1}{4}\sqrt{2}$		$\frac{1}{2} - \frac{1}{10}\sqrt{2}$		$\frac{1}{2}$	
ϕ	22.5°		31.72°		45°	
N	8		24		24	

n	5			
Criterion	D	$\overset{*}{G}$	only with respect to r: D	only with respect to r: $\overset{*}{G}$
r	0.1429	0.1125	0.1429	0.1010
$\sum_{i=1}^{n} w_i^4$	0.4286	0.4286	0.50	0.50
α	18.2368	17.9517	13.8947	13.6097
δ	36.4735	35.9033	41.6840	40.8291
γ	3.8281	4.0398	3.8281	4.1246
ξ	−2.6053	−2.5645	−1.7368	−1.7012
det $(M^{-1}(\epsilon))$	1.974 10^{24}	2.04 10^{24}	2.53 10^{24}	2.69 10^{24}
D-eff	53.42%	53.34%	52.77%	52.61%
$\overset{*}{G}$-eff	44.91%	45.01%	40.25%	40.41%
w	(w_1,w_2,w_2,w_2,w_2)		$(w_1,w_2,0,0,0)$	
w_1^2	$\frac{1}{5}+\frac{4}{5}\sqrt{\frac{5}{7}}$		$\frac{1}{2}$	
w_2^2	$\frac{1}{5}-\frac{1}{5}\sqrt{\frac{5}{7}}$		$\frac{1}{2}$	
N	80		40	

4.4.2. Exact designs consisting of pairs of SP((w, -rw)) and pairs of SP((x,y))

Let x, y and w be points for which condition (4.2.11) holds and let θ be such that

$$\cos\theta = \sum_{i=1}^{n} x_i y_i . \tag{4.4.12}$$

Consider the sets $SP((x,y))$ and $SP((w,-rw))$, where $0 \leqslant r < 1$. In this section we construct exact designs consisting of pairs of $SP((x,y))$ and of pairs of $SP((w,-rw))$. In general we choose m_1 pairs of $SP((x,y))$ and m_2 pairs of $SP((w,-rw))$. The values of m_1 and m_2 must be chosen such that the information matrix of the design has the structure of (4.1.5). Then, in view of (4.2.20) and (4.2.23) the information matrix of the normalized design can be expressed by (4.2.22), where

$$p_1 = \frac{m_1}{m_1+m_2}\,\frac{1}{n}\,2(1-\cos\theta) ,$$

$$
\begin{aligned}
s_1 + nt_1 &= 0 , \\
t_1 &= \frac{2m_1}{m_1+m_2} \frac{1}{n(n-1)} \sum_{i<j}\sum (x_i^2 - y_i^2)(x_j^2 - y_j^2) , \\
z_1 &= \frac{2m_1}{m_1+m_2} \frac{1}{n(n-1)} \sum_{i<j}\sum (x_i x_j - y_i y_j)^2 ,
\end{aligned}
$$

(4.4.13)

$$
\begin{aligned}
p_2 &= \frac{m_2}{m_1+m_2} \frac{1}{n} (1+r)^2 , \\
s_2 + nt_2 &= \frac{m_2}{m_1+m_2} \frac{1}{n} (1-r^2)^2, \\
z_2 &= \frac{m_2}{m_1+m_2} \frac{1}{n(n-1)} (1-r^2)^2 (1-\sum_{i=1}^{n} w_i^4) , \\
t_2 &= z_2 .
\end{aligned}
$$

From this it follows that

$$
s_1 = 2\frac{m_1}{m_1+m_2} \frac{1}{n-1} \sin^2\theta - nz_1 . \tag{4.4.14}
$$

Now r and w have to be chosen according to some criterion. First we consider the D-criterion. In lemma 4.4.5 conditions for r and w are given.

Lemma 4.4.5

Let ϵ be the design defined above and let θ and r be fixed; det $(M(\epsilon))$ *is maximized if $2\alpha = \delta$, or equivalently*

$$
\sum_{i=1}^{n} w_i^4 = -2\frac{m_1}{m_2} \frac{n}{n+2} \frac{\sin^2\theta}{(1-r^2)^2} + \frac{3}{n+2} \tag{4.4.15}
$$

$$
+2\frac{m_1}{m_2} \frac{1}{(1-r^2)^2} \sum_{i<j}\sum (x_i x_j - y_i y_j)^2 .
$$

If the condition (4.4.15) is satisfied, then

(4.4.16)

$$
\begin{aligned}
z &= \frac{1}{(m_1+m_2)(n+2)} [\frac{2m_1}{n-1} \sin^2\theta + \frac{m_2}{n} (1-r^2)^2] , \\
s &= 2z , \\
s + nt &= \frac{m_2}{m_1+m_2} \frac{1}{n} (1-r^2)^2 , \\
p &= \frac{1}{n(m_1+m_2)} [2m_1(1-\cos\theta) + m_2(1+r)^2] ,
\end{aligned}
$$

Proof

As can be seen by investigating the expressions given in (4.4.13) the quantities p_1, p_2, $s_1 + nt_1$ and $s_2 + nt_2$ only depend on θ and r. So det $(M(\epsilon))$ is maximal when the expression

$$(s_1 + s_2)^{n-1} (z_1 + z_2)^{\frac{1}{2}n(n-1)}$$

is maximal. This expression only depends on $\sum_{i=1}^{n} w_i^4$ and r. This leads to

$$(z_1 + z_2)\frac{\partial(s_1+s_2)}{\partial w_0} + \tfrac{1}{2}n(s_1 + s_2)\,\frac{\partial(z_1+z_2)}{\partial w_0} = 0\,,$$

where

$$w_0 = \sum_{i=1}^{n} w_i^4$$

Solving for w_0 we obtain

$$w_0 = \frac{-s_1 + 2z_1 + 3\dfrac{m_1}{m_1+m_2}\,\dfrac{(1-r^2)^2}{n(n-1)}}{(n+2)\dfrac{m_2}{m_1+m_2}\,\dfrac{(1-r^2)^2}{n(n-1)}}\,.$$

Using (4.4.14) we find condition (4.4.15) and the expressions (4.4.16). □

Lemma 4.4.5 shows that under condition (4.4.15) the determinant of the information matrix depends only on θ and r. We maximize the determinant of the information matrix with respect to θ and r. Now it is not clear that θ and r should satisfy the conditions

$$\cos\theta = -\frac{\gamma}{2\alpha}\,, \tag{4.4.17}$$

and

$$r = \tfrac{1}{2} - \tfrac{1}{2}\,[1-\frac{2\gamma}{\alpha+\xi}]^{\frac{1}{2}}\,. \tag{4.4.18}$$

For discrete D-optimal designs this has been proved by use of the fact that a D-optimal design is G-optimal as well. A computerprogram has been written that determines the values of $\cos\theta$ and r for which the determinant of the information matrix is maximal. This program uses the procedure MINIFUN, described in THE-RC38859a (1980). MINIFUN has been designed for non-linear optimalization with non-linear constraints.

Results are given in table 4.4.6. Note that θ and r do satisfy the equations (4.4.17) and (4.4.18).

Let us now consider the $\mathring{G}$-criterion . We have to choose r and w such that the maximal value of the variance function is minimized. Again the condition $2\alpha = \delta$ plays an important role as can be seen intuitively as follows. We have

$$\max_{u,v} d(u,v,\epsilon) = \max\{d_1, d_2\},$$

where

$$d_1 = \max_{u_1,v_1} d(u_1,v_1,\epsilon) \text{ with } \sum_{i=1}^{n} u_{1,i}^2 = \sum_{i=1}^{n} v_{1,i}^2 = 1,$$

and

$$d_2 = \max_{u_2,v_2} d(u_2,v_2,\epsilon) \text{ with } \sum_{i=1}^{n} u_{2,i}^2 = 1,$$

$$\text{and} v_2 = -r_2 u_2 \ , \quad 0 \leqslant r_2 < 1 \ .$$

If $d_1 \geqslant d_2$,
then

$$\max_{u,v} d(u,v,\epsilon) = \begin{cases} 2\gamma + \delta + \dfrac{\gamma^2}{\delta} & ,\text{if } 2\alpha \leqslant \delta, \\ \\ 2\gamma + 2\alpha + \dfrac{\gamma^2}{2\alpha} & ,\text{if } 2\alpha > \delta . \end{cases}$$

Now the same argument as given in the proof of lemma 4.4.3 suggests $2\alpha = \delta$. An argument analogous to this can be given in the case $d_2 > d_1$.

Assuming $2\alpha = \delta$, and using lemma 4.2.5 we find,

$$\max_{u,v} d(u,v,\epsilon) = \max\{2\gamma + 2\alpha + \frac{\gamma^2}{2\alpha}, \gamma(1+r_2)^2 + (\alpha + \xi)(1-r_2^2)^2\},$$

where

$$r_2 = \tfrac{1}{2} - \tfrac{1}{2}[1 - \frac{2\gamma}{\alpha+\xi}]^{\frac{1}{2}} .$$

A computerprogram has been written that determines the values of r and $\cos\theta$ for which the maximal value of the variance function is minimized, given m_1 and m_2 .

Results are given in table 4.4.6. Note that θ and r do *not* satisfy the equations (4.4.17) and (4.4.18). The two equations above are given for fixed m_1 and m_2. To construct exact designs we have to specify x, y, w, m_1 and m_2 . The values of m_1 and m_2 have to be chosen such that the matrix can be expressed by (4.2.22). For practical reasons it is useful to choose m_1 and m_2 as small as

possible. Moreover, m_1 and m_2 have to be chosen so that the efficiency of the designs is high. The design constructed is D-optimal if it satisfies the conditions (4.4.15), (4.4.17), (4.4.18) and $m_1/m_2 = \nu_1/\nu_2$. This can be seen as follows. If one wants to compute the efficiency of such a design, one has to consider the normalized design. Expressions for its information matrix are given in (4.4.13).

Using $m_1/m_2 = \nu_1/\nu_2$, one finds $\frac{m_1}{m_1+m_2} = \nu_1 \, 2^n \, n!$ and

$\frac{m_2}{m_1+m_2} = \nu_2 \, 2^n \, n!$ Substitution of this in (4.4.13) and verification of the conditions (4.4.15), (4.4.17), (4.4.18) shows that such a design is D-optimal. As can be seen from table 4.2.10 the values of the ratio of ν_1 and ν_2 are:

n	2	3	4	5
ν_1/ν_2	2.316	4.408	7.163	10.413

If we choose x , y and w as below, m_2 is small relative to m_1 .

Choose $w = (1,0, \ldots, 0)'$,

so $m_2 = q_2 \, 2n$ with $q_2 \in$ N ;

$x = (\cos\phi_1, \sin\phi_1, 0, \ldots, 0)'$,

$y = (\cos\phi_2, \sin\phi_2, 0, \ldots, 0)'$,

so $m_1 = q_1 N$ with $q_1 \in$ N and

$$N = \begin{cases} 4n\,(n-1) & \text{,if } n \text{ even ,} \\ 2n\,(n-1) & \text{,if } n \text{ odd .} \end{cases}$$

Condition (4.4.15) gives

$$\cos^2(\phi_1+\phi_2) = \frac{n}{n+2} + \frac{n-1}{2(n+2)} \frac{m_2}{m_1} \frac{(1-r^2)^2}{\sin^2\theta} . \tag{4.4.19}$$

It is useful to consider another choice of w . If w is chosen as $w = \frac{1}{\sqrt{n}}(1,1, \ldots, 1)'$, then the ratio of m_1 and m_2 differs from the ratio of m_1 and m_2 of the design mentioned above. Therefore the designs with $w = \frac{1}{\sqrt{n}}(1,1, \ldots, 1)'$ might have a higher efficiency than the designs mentioned above. However, the number of pairs is larger. Choose

x , y as above ,

and

$$w = \frac{1}{\sqrt{n}}(1,1, \ldots, 1)' ,$$

so

$$m_2 = q_2\, 2^n \text{ with } q_2 \in \mathbb{N}.$$

Condition (4.4.15) now gives

$$\cos^2(\phi_1+\phi_2) = \frac{n}{n+2} - \frac{(n-1)}{n(n+2)} \frac{m_2}{m_1} \frac{(1-r^2)^2}{\sin^2\theta} \tag{4.4.20}$$

Results are given in table 4.4.6.
In this table r_0, d_1 and d_2 are defined by

$$r_0 = \tfrac{1}{2} - \tfrac{1}{2}[1-\frac{2\gamma}{\alpha+\xi}]^{\frac{1}{2}} ,$$

$$d_1 = \max_{u,v} d(u,v,\epsilon) \quad \text{with } \sum_{i=1}^{n} u_i^2 = \sum_{i=1}^{n} v_i^2 = 1 ,$$

$$d_2 = \max_{r,w} d(w,-rw,\epsilon) \quad \text{with } 0 \leqslant r < 1 \text{, and } \sum_{i=1}^{n} w_i^2 = 1 .$$

The results are satisfactory. The efficiency of the designs is good and the number of pairs is relatively small, although the number of pairs is larger than the number of pairs of the designs given in table 4.4.4.

Table 4.4.6
Values of constants, determining the designs given in section 4.4.2, and found by using the D- and $\mathring{G}$-criteria

n	2				4	
Criterion	D		$\mathring{G}$		D	$\mathring{G}$
w	(1,0)	w [1]	(1,0)	w [1]	(1,0,0,0)	(1,0,0,0)
m_1	8	8	8	8	48	48
m_2	4	4	4	4	8	8
m_1+m_2	12	12	12	12	56	56
r	0.1381		0.2026		0.0918	0.2918
$\cos(\phi_1-\phi_2)$	−0.3125		−0.3046		−0.1790	−0.1700
$\cos^2(\phi_1+\phi_2)$	0.5666	0.4334	0.5666	0.4334	0.7090	0.7090
ϕ_1	74.69°	78.52°	74.45°	78.28°	66.48°	66.22°
ϕ_2	−33.52°	−29.69°	−33.28°	−29.45°	−33.83°	−33.57°
α	1.4668		1.4675		5.0999	5.1300
δ	2.9336		2.9350		10.1999	10.2600
γ	0.9167		0.9003		1.8253	1.7824
ξ	2.3844		2.5285		5.8446	7.0812
$\gamma/2\alpha$	0.3125		0.3067		0.1790	0.1737
r_0	0.1381		0.1294		0.0918	0.0793
d_1	5.0535		5.0116		14.1772	14.1344
d_2	4.8931		5.0116		12.9367	14.1344
$\det(M^{-1}(\epsilon))$	22.548		22.776		$4.72\ 10^{10}$	$5.32\ 10^{10}$
D-eff	99.98%		99.78%		99.91%	99.06%
$\mathring{G}$-eff	98.94%		99.77%		98.75%	99.05%

1) $w = (\frac{1}{2}\sqrt{2}, \frac{1}{2}\sqrt{2})$.

n	3					
Criterion w m_1 m_2 m_1+m_2	D (1,0,0) 12 6 18	D (1,0,0) 24 6 30	D w [1] 36 8 44	$\mathring{G}$ (1,0,0) 12 6 18	$\mathring{G}$ (1,0,0) 24 6 30	$\mathring{G}$ w [1] 36 8 44
r $\cos(\phi_1-\phi_2)$ $\cos^2(\phi_1+\phi_2)$ ϕ_1 ϕ_2	0.1596 −0.2151 0.6996 67.83° −34.59°	0.1068 −0.2245 0.6515 69.58° −33.40°	0.0984 −0.2255 0.5694 72.02° −31.01°	0.4098 −0.1613 0.6999 66.25° −33.03°	0.2269 −0.2289 0.6517 69.70° −33.54°	0.0580 −0.2626 0.5688 73.14° −32.09°
α δ γ ξ	3.3722 6.7444 1.4505 2.0348	3.0309 6.0619 1.3610 4.1056	2.9903 5.9807 1.3485 4.6112	3.4424 6.8848 1.3569 3.1861	3.0560 6.1121 1.3231 4.5387	3.0416 6.0832 1.3218 4.5234
$\gamma/2\alpha$ r_0	0.2151 0.1596	0.2245 0.1068	0.2255 0.0984	0.1971 0.1158	0.2165 0.0964	0.2173 0.0967
d_1 d_2 $\det(M^{-1}(\epsilon))$	9.9573 7.0855 $1.01\ 10^5$	9.0895 8.6420 $7.92\ 10^4$	8.9818 9.0820 $7.89\ 10^4$	9.8660 8.1412 $1.26\ 10^5$	9.0448 9.0448 $8.24\ 10^4$	9.0139 9.0139 $7.99\ 10^4$
D-eff $\mathring{G}$-eff	97.31% 90.39%	99.96% 99.02%	99.998% 99.10%	94.97% 91.22%	99.53% 99.50%	99.86% 99.85%

1) $w = \frac{1}{3}\sqrt{3}(1,1,1)$.

n	5			
Criterion	D			
w	(1,0,0,0,0)			$\frac{1}{5}\sqrt{5}(1,0,0,0,0)$
m_1 m_2 m_1+m_2	40 10 50	80 10 90	120 10 130	160 16 176
r $\cos(\phi_1-\phi_2)$ $\cos^2(\phi_1+\phi_2)$ ϕ_1 ϕ_2	0.1165 −0.1474 0.7853 63.04° −35.22°	0.0821 −0.1499 0.7503 64.30° −34.32°	0.0632 −0.1506 0.7384 64.71° −33.95°	0.0714 −0.1504 0.7027 65.84° −32.81°
α δ γ ξ	8.1351 16.2703 2.3979 3.5116	7.6691 15.3381 2.2995 7.5887	7.5055 15.0109 2.2612 11.6032	7.5714 15.1428 2.2769 9.5987
$\gamma/2\alpha$ r_0	0.1474 0.1165	0.1499 0.0821	0.1506 0.0632	0.1504 0.0714
d_1 d_2 $\det(M^{-1}(\epsilon))$	21.4195 14.3219 $1.16\ 10^{19}$	20.2818 17.7454 $7.31\ 10^{18}$	19.8740 21.5124 $7.14\ 10^{18}$	20.0391 19.6092 $7.09\ 10^{18}$
D-eff $\hat{G}$-eff	97.56% 93.37%	99.84% 98.61%	99.96% 92.97%	99.996% 99.81%

n	5			
Criterion	$\overset{*}{G}$			
w	(1,0,0,0,0)			$\frac{1}{5}\sqrt{5}(1,0,0,0,0)$
m_1 m_2 m_1+m_2	40 10 50	80 10 90	120 10 130	160 16 176
r $\cos(\phi_1-\phi_2)$ $\cos^2(\phi_1+\phi_2)$ ϕ_1 ϕ_2	0.2196 −0.1370 0.7853 62.74° −35.14°	0.2338 −0.1433 0.7503 64.11° −34.13°	0.0037 −0.1731 0.7386 65.35° −34.61°	0.1539 −0.1511 0.7027 65.87° −32.82°
α δ γ ξ	8.1638 16.3275 2.3621 3.8868	7.6893 15.3786 2.2710 8.5330	7.5579 15.1159 2.2289 11.4888	7.5840 15.1681 2.2584 10.0235
$\gamma/2\alpha$ r_0	0.1447 0.1101	0.1477 0.0757	0.1475 0.0624	0.1489 0.0689
d_1 d_2 $\det(M^{-1}(\epsilon))$	21.3935 14.6710 $1.21\ 10^{19}$	20.2560 18.6647 $7.87\ 10^{18}$	19.9023 21.4144 $7.27\ 10^{18}$	20.0211 20.0211 $7.23\ 10^{18}$
D-eff $\overset{*}{G}$-eff	97.34% 93.49%	99.47% 98.74%	99.87% 93.40%	99.90% 99.89%

4.5. Robustness of the designs

In this section we discuss the robustness of the designs given in section 4.3 against violation of the condition $\beta = 0$. In general condition (1.8.6) is not satisfied and the designs, that are D-optimal in the case $\beta = 0$ are not D-optimal when $\beta \neq 0$. However, β is the vector of parameters which should be estimated from the experiment which is being designed. Results given in this section concerning the robustness of these designs are satisfactory. Therefore, the D-optimal designs in the case $\beta = 0$ are useful in practical applications. We shall discuss the D-efficiency of some of these designs for several values of β.
Let ϵ_0 be a design and $\beta = \beta_0$. The information matrix is denoted by $M(\epsilon_0 | \beta = \beta_0)$. The D-efficiency of this design equals

$$\left(\frac{\det (M(\epsilon_0 \mid \beta = \beta_0))}{\max\limits_{\epsilon} \det (M(\epsilon \mid \beta = \beta_0))} \right)^{\frac{1}{k}} . \qquad (4.5.1)$$

In order to compute the value

$$\max_{\epsilon} \det (M(\epsilon \mid \beta = \beta_0))$$

D-optimal designs have to be constructed in the case $\beta = \beta_0$. This is a rather cumbersome task and it seems that it can only be done by maximizing $\det (M(\epsilon \mid \beta = \beta_0))$ numerically. But then one cannot be sure that the absolute maximum has been found; the procedure may lead to a local maximum. It is easy, however, to compute a lower bound for the D-efficiency by using the following lemma.

Lemma 4.5.1
A lower-bound for the D-efficiency of the design ϵ_0 in the case $\beta = \beta_0$ is given by

$$\left(\frac{\det M(\epsilon_0 \mid \beta = \beta_0))}{\max\limits_{\epsilon} \det (M(\epsilon \mid \beta = 0))} \right)^{\frac{1}{k}} \qquad (4.5.2)$$

Proof
We prove that

$$\max_{\epsilon} \det (M(\epsilon \mid \beta = \beta_0)) \leqslant \max_{\epsilon} \det (M(\epsilon \mid \beta = 0)) .$$

Let ϵ_1, consisting of the pairs (u_i, v_i) with weight $p(u_i, v_i)$, $i = 1, \ldots, N$, be a design where $\det (M(\epsilon \mid \beta = \beta_0))$ is maximal. Let $\lambda(u, v)$ be as defined in (2.3.19) and (2.3.20). Now it is easy to see that

$$\lambda(u, v) \leqslant \tfrac{1}{4} ,$$

and

$$\lambda(u,v) = \tfrac{1}{4} \text{ for all } u,v \text{ if and only if } \beta = 0 .$$

Define

$$\overset{*}{p}(u_i,v_i) = 4p(u_i,v_i)\,\lambda(u_i,v_i) ,$$

and

$$\bar{p}(u_i,v_i) = \overset{*}{p}(u_i,v_i)/(\sum_{i=1}^{N} \overset{*}{p}(u_i,v_i)) .$$

Now we have

$$\det(M(\epsilon_1 \mid \beta = \beta_0))$$
$$= \det(\sum_{i=1}^{N} p(u_i,v_i)\,\lambda(u_i,v_i)(f(u_i) - f(v_i))\,(f(u_i) - f(v_i))')$$
$$= \det(\sum_{i=1}^{n} \overset{*}{p}(u_i,v_i)\,\tfrac{1}{4}(f(u_i) - f(v_i))\,(f(u_i) - f(v_i))')$$
$$\leqslant \det(\sum_{i=1}^{N} \bar{p}(u_i,v_i)\,\tfrac{1}{4}(f(u_i) - f(v_i))\,(f(u_i) - f(v_i))')$$
$$= \det(M(\epsilon_2 \mid \beta = 0)) \leqslant \max_{\epsilon} \det(M(\epsilon \mid \beta = 0)) ,$$

where ϵ_2 is a design consisting of the pairs (u_i,v_i) with weight $\bar{p}(u_i,v_i)$, $i = 1, \ldots, N$. □

In table 4.5.2 lower bounds for the D-efficiency of some designs are given for several values of β. The designs considered are designs which are D-optimal when $\beta = 0$. For $n = 2$ three designs are given for each value of β. The lower bounds for the D-efficiency of these designs are approximately the same. Therefore only one design has been chosen in the cases $n = 3, 4, 5$. It is the design for which

$$w = \frac{1}{\sqrt{n}}(1, \ldots, 1)' .$$

In this table the smallest value of $\pi_{i.ij}$ is listed. This is the smallest value of

$$\frac{\pi_u}{\pi_u + \pi_v},$$

where

$$\log \pi_x = (f(x))'\,\beta_0$$

and (u,v) is a pair of the design.

It is also possible to compute lower bounds for the D-efficiency by using theorem 2.3.9. Doing so, one has to compute $\max_{u,v} \lambda(u,v)\,d(u,v,\epsilon)$. This is not easy, though it is not as difficult as computing $\max_{\epsilon} \det(M(\epsilon))$. For $n = 2$

lower bounds are computed by means of theorem 2.3.9 and the procedure MINIFUN to determine the maximal value of $\lambda(u,v)\,d(u,v,\epsilon)$.
Results are given in table 4.5.2. The lower bounds found by this method are approximately the same as the lower bounds found with lemma 4.5.1. In view of this, lemma 4.5.1 is used to find lower bounds in the cases $n = 3, 4, 5$.

Table 4.5.2
Lower bounds for the D-efficiency of some designs

$n=2$					smallest	lower bounds			
β_0					value	using(4.5.2)			(2.3.28)
β_1	β_2	β_{11}	β_{12}	β_{12}	of $\pi_{i,ij}$	$\omega=0°$	22.5°	45°	$\omega=0°$
0.05	0.05	0.05	0.05	0.05	0.4650	0.998	0.998	0.998	0.997
−0.05	0.05	0.05	0.05	0.05	0.4650	0.998	0.998	0.998	0.997
0.05	0.05	−0.05	0.05	0.05	0.4495	0.998	0.998	0.998	0.997
0.1	0.1	0.1	0.1	0.1	0.4304	0.993	0.993	0.993	0.993
−0.1	0.1	0.1	0.1	0.1	0.4304	0.993	0.993	0.993	0.993
0.1	0.1	−0.1	0.1	0.1	0.3999	0.990	0.990	0.990	0.991
0.3	0.3	0.3	0.3	0.3	0.3014	0.940	0.940	0.941	0.935
−0.3	0.3	0.3	0.3	0.3	0.3014	0.940	0.940	0.940	0.938
0.3	0.3	−0.3	0.3	0.3	0.2284	0.921	0.921	0.921	0.927
0.5	0.5	0.5	0.5	0.5	0.1977	0.851	0.853	0.854	0.824
−0.5	0.5	0.5	0.5	0.5	0.1977	0.851	0.851	0.850	0.844
0.5	0.5	−0.5	0.5	0.5	0.1162	0.813	0.814	0.815	0.813
1	1	1	1	1	0.0572	0.597	0.608	0.616	0.410
−1	1	1	1	1	0.0572	0.602	0.596	0.587	0.595
1	1	−1	1	1	0.0170	0.546	0.554	0.558	0.453
0.1	0	0	0	0	0.4622	0.997	0.997	0.997	0.997
0.3	0	0	0	0	0.3882	0.976	0.976	0.976	0.980
0.5	0	0	0	0	0.3190	0.936	0.936	0.935	0.945
1	0	0	0	0	0.1800	0.786	0.784	0.782	0.801
0	0	0.1	0	0	0.4755	0.999	0.999	0.999	0.992
0	0	0.3	0	0	0.4268	0.991	0.991	0.991	0.990
0	0	0.5	0	0	0.3796	0.974	0.974	0.974	0.972
0	0	1	0	0	0.2724	0.903	0.903	0.902	0.892
0	0	0	0	0.1	0.4822	0.999	0.999	0.999	0.999
0	0	0	0	0.3	0.4468	0.992	0.992	0.992	0.991
0	0	0	0	0.5	0.4119	0.979	0.979	0.979	0.975
0	0	0	0	1	0.3291	0.920	0.919	0.918	0.903

$n=3$									smallest	
β_0									value	lower
β_1	β_2	β_3	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}	of $\pi_{i,ij}$	bound
0.05									0.4817	0.9995
0.1									0.4634	0.9982
0.2									0.4272	0.9927
0.3									0.3918	0.9837
0.5									0.3245	0.9560
1									0.1875	0.8467
			0.05						0.4920	0.9999
			0.1						0.4840	0.9994
			0.2						0.4681	0.9976
			0.3						0.4522	0.9946
			0.5						0.4207	0.9850
			1						0.3453	0.9424
						0.05			0.4908	0.9999
						0.1			0.4816	0.9996
						0.2			0.4633	0.9983
						0.3			0.4451	0.9963
						0.5			0.4092	0.9897
						1			0.3241	0.9604
0.05	0.05	0.05							0.4748	0.9986
0.1	0.1	0.1							0.4498	0.9948
0.2	0.2	0.2							0.4006	0.9782
0.3	0.3	0.3							0.3533	0.9522
0.5	0.5	0.5							0.2675	0.8765
1	1	1							0.1176	0.6296
0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.4516	0.9982
0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.4041	0.9928
0.2	0.2	0.2	0.2	0.2	0.2	0.2	0.2	0.2	0.3150	0.9720
0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.2377	0.9394
0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.1254	0.8505
1	1	1	1	1	1	1	1	1	0.0201	0.5980
−0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3047	0.9388
−0.3	0.3	0.3	0.3	0.3	−0.3	0.3	0.3	0.3	0.3047	0.9272
−0.3	0.3	0.3	−0.3	0.3	0.3	−0.3	0.3	0.3	0.3169	0.9241

The entries that are not given in this table are zero.

$n=4$			
β_0	value of the	smallest	
non zero parameters	non zero parameters	value of $\pi_{i,ij}$	lower bound
β_1	0.05	0.4818	0.9996
	0.1	0.4636	0.9986
	0.2	0.4275	0.9945
	0.3	0.3923	0.9878
	0.5	0.3253	0.9673
	1	0.1886	0.8878
β_{11}	0.05	0.4927	0.9999
	0.1	0.4854	0.9996
	0.2	0.4709	0.9984
	0.3	0.4564	0.9965
	0.5	0.4276	0.9903
	1	0.3583	0.9624
β_{12}	0.05	0.4901	0.9999
	0.1	0.4802	0.9998
	0.2	0.4605	0.9990
	0.3	0.4408	0.9978
	0.5	0.4022	0.9939
	1	0.3166	0.9766
β_i ,$1 \leqslant i \leqslant 4$	0.1	0.4461	0.9945
	0.3	0.3432	0.9524
	0.5	0.2532	0.8776
	1	0.1031	0.6364
β_{ii} ,$1 \leqslant i \leqslant 4$	0.1	0.4752	0.9997
	0.3	0.4260	0.9973
	0.5	0.3783	0.9926
	1	0.2703	0.9726
β_{ij} ,$1 \leqslant i < j \leqslant 4$	0.1	0.4628	0.9985
	0.3	0.3901	0.9867
	0.5	0.3219	0.9638
	1	0.1839	0.8664
β_i ,β_{ij} ,$1 \leqslant i \leqslant j \leqslant 4$	0.05	0.4422	0.9982
	0.1	0.3859	0.9927
	0.2	0.2831	0.9718
	0.3	0.1988	0.9393
	0.5	0.0892	0.8515
	1	0.0095	0.6117

$n=5$			
β_0	value of the	smallest	
non zero parameters	non zero parameters	value of $\pi_{i.ij}$	lower bound
β_1	0.05	0.4818	0.9989
	0.1	0.4637	0.9973
	0.2	0.4278	0.9956
	0.3	0.3926	0.9903
	0.5	0.3258	0.9736
	1	0.1893	0.9060
	1.5	0.1014	0.8202
	2	0.0517	0.7345
β_{11}	0.05	0.4933	0.9999
	0.1	0.4865	0.9997
	0.2	0.4731	0.9990
	0.3	0.4597	0.9976
	0.5	0.4331	0.9932
	1	0.3685	0.9735
	1.5	0.3083	0.9425
	2	0.2540	0.9028
β_{12}	0.05	0.4896	0.99996
	0.1	0.4793	0.9998
	0.2	0.4586	0.9993
	0.3	0.4381	0.9985
	0.5	0.3978	0.9959
	1	0.3039	0.9844
	1.5	0.2238	0.9672
	2	0.1600	0.9469

β_i ,$1 \leqslant i \leqslant 5$	0.05	0.4701	0.9986
	0.1	0.4405	0.9945
	0.2	0.3827	0.9784
	0.3	0.3280	0.9525
	0.5	0.2322	0.8767
	1	0.0838	0.6243
	1.5	0.0269	0.3988
	2	0.0083	0.2446
β_{ii} ,$1 \leqslant i \leqslant 5$	0.05	0.4876	0.99995
	0.1	0.4751	0.9998
	0.2	0.4504	0.9991
	0.3	0.4259	0.9981
	0.5	0.3781	0.9947
	1	0.2699	0.9803
	1.5	0.1835	0.9600
	2	0.1202	0.9370
β_{ij} ,$1 \leqslant i < j \leqslant 5$	0.05	0.4751	0.9996
	0.1	0.4504	0.9984
	0.2	0.4018	0.9934
	0.3	0.3550	0.9853
	0.5	0.2699	0.9599
	1	0.1202	0.8531
	1.5	0.0481	0.7093
	2	0.0183	0.5590
β_i ,β_{ij} ,$1 \leqslant i \leqslant j \leqslant 5$	0.05	0.4332	0.9982
	0.1	0.3687	0.9927
	0.2	0.2544	0.9715
	0.3	0.1662	0.9385
	0.5	0.0637	0.8482
	1	0.0046	0.5946
	1.5	0.0003	0.4052
	2	0.0000	0.2830

5. Designs in the case of a quadratic model with a hypercube as experimental region

5.1. Introduction

In this chapter the parameters of the model are the same as in chapter 4, but the experimental region is now a hypercube. So, we have

$$f(x) = (x_1, \ldots, x_n, x_1^2, \ldots, x_n^2, x_1x_2, \ldots, x_{n-1}x_n)' , \tag{5.1.1}$$

$$x \in X , X \subset \mathbf{R}^n , x = (x_1, \ldots, x_n)' ,$$

where

$$X = \{ x \in X \mid -1 \leqslant x_i \leqslant 1 \text{ for all } i \} . \tag{5.1.2}$$

For the construction of optimal designs the assumption $\pi_t = (1, \ldots, 1)'$ is made. In section 5.2 D-optimal designs are given. The D-optimality is proved in section 5.3. Discrete D-optimal designs with a relatively small number of pairs are given in section 5.4. Exact designs are considered in section 5.5 and in section 5.6 we will discuss the robustness of the discrete designs constructed in section 5.2 against violation of the assumption $\pi_t = (1, \ldots, 1)'$.

Again (4.1.4) holds and the assumptions (4.1.5) and (4.1.6) concerning the structure of the covariance matrix are made. The variance function can be expressed by (4.1.8).

5.2. Discrete D-optimal designs

Again it is important to investigate the variance function. If the variance function $d(x, y, \epsilon)$ of a design ϵ can be expressed by (4.1.8), then $d(x, y, \epsilon)$ satisfies (3.1.8) and (3.1.9). In chapter 4 D-optimal designs were proved to be strongly rotatable. In the case of a hypercube as experimental region D-optimal designs have the following property.

$$d((x_1, \ldots, x_i, \ldots, x_n),(y_1, \ldots, y_i, \ldots, y_n),\epsilon) \tag{5.2.1}$$

$$= d((x_1, \ldots, y_i, \ldots, x_n),(y_1, \ldots, x_i, \ldots, y_n),\epsilon)$$

$$\text{for all } x , y \text{ and } 1 \leqslant i \leqslant n .$$

In the next lemma a condition equivalent to property (5.2.1) is given.

Lemma 5.2.1

Let ϵ be a design with covariance matrix of type (4.1.6). The design ϵ has property (5.2.1) if and only if

$$\delta = -4\xi \tag{5.2.2}$$

Proof

Let d_1 and d_2 be defined by $d_1 = d(x,y,\epsilon)$ and
$d_2 = d((x_1, \ldots, y_i, \ldots, x_n),(y_1, \ldots, x_i, \ldots, y_n),\epsilon)$.
Then, using (4.1.8) we find

$$d_1 - d_2 =$$
$$= \delta \sum_{j \neq i} (x_i^2 x_j^2 + y_i^2 y_j^2 - y_i^2 x_j^2 - x_i^2 y_j^2) + 4\,\xi\,(x_i^2 - y_i^2) \sum_{j \neq i} (x_j^2 - y_j^2)$$
$$= (\delta + 4\xi)(x_i^2 - y_i^2) \sum_{j \neq i} (x_j^2 - y_j^2) .$$

The last expression vanishes for all $x, y \in X$ if and only if $\delta = 4\xi$. □

The lemmas 5.2.2 and 5.2.3 are useful in finding pairs where the variance function is maximal. The proofs of these lemmas are given in section 5.3, because they can be regarded as part of the proof of the D-optimality of the designs considered in this section.

Lemma 5.2.2

Let ϵ be a design with covariance matrix of type (4.1.6). If $d(x,y,\epsilon)$ is maximal at $(x,y) = (u,v)$, then for all $1 \leqslant i \leqslant n$

$$|u_i| = 1 \quad \textit{or} \quad |v_i| = 1 .$$

According to lemma 3.2.1 we have $|u_i| = |v_i| = 1$ for all $1 \leqslant i \leqslant n$. This does not hold in the case of a quadratic model as can be seen as follows. Suppose that it holds, then a D-optimal design consists of pairs of this type. However, such a design does not measure the quadratic effects, since $u_i^2 = v_i^2 = 1$ for all $1 \leqslant i \leqslant n$.

Having obtained one pair where the variance function is maximal, one can find more pairs having this property. This might be useful in the construction of optimal designs. Let (u,v) be a pair where the variance function is maximal and let k_1 be the number of pairs of coordinates (u_i,v_i) for which $u_i = v_i$, and k_2 the number of pairs (u_i,v_i) for which $u_i = -v_i$. Now, using (3.1.8), (3.1.9) and -if it holds- (5.2.1), other pairs can be found where the variance function is maximal ; for example the pair $(\bar{u},\bar{v})$ with

$$\bar{u} = (1, \ldots, 1)' ,$$
$$\bar{v}_i = 1 \quad \text{for } 1 \leqslant i \leqslant k_1 ,$$
$$\bar{v}_i = -1 \quad \text{for } k_1 < i \leqslant k_2 ,$$

and

$$-1 < \bar{v}_i < 1 \quad \text{for } k_1 + k_2 < i \leqslant k_2 .$$

This will be used in the next lemma and definition.

Lemma 5.2.3

Let ϵ be a design with covariance matrix of type (4.1.6) and $\delta = -4\xi$. Let (u,v) be a pair where the variance function is maximal and assume (without loss of generality) that

$$u = (1, \ldots, 1)' \ ,$$

$$v = (1, \ldots, 1, -1, \ldots, -1, v_{k_1+k_2+1}, \ldots, v_n)' \ ,$$

where

k_1 *is the number of* 1's *in* v ,

k_2 *is the number of* -1's *in* v ,

and

$$-1 < v_i < 1 \text{ for } k_1 + k_2 < i \leqslant n \ .$$

Then

$$v_i = v_j \text{ for all } i,j \text{ with } k_1 + k_2 < i,j \leqslant n \ .$$

In the light of these lemmas it is useful to define the following sets of pairs.

Definition 5.2.4

Let the pair (u,v) be as defined in lemma 5.2.3 , with $v_i = w$ for $k_1 + k_2 < i \leqslant n$ if $k_1 + k_2 < n$, and let $v = (1, \ldots, 1, -1, \ldots, -1)$ if $k_1 + k_2 = n$. Let $k_3 = n - k_1 - k_2$. Now define

$$S(k_1,k_2,k_3; w) := S((u,v)) \ ,$$
$$SP(k_1,k_2,k_3; w) := SP((u,v)) \ ,$$

and

$SP_l(0,0,n; w)$ is the set containing the pairs of $SP(0,0,n; w)$ and all pairs that can be obtained by replacing l pairs of coordinates (u_i,v_i) by (v_i,u_i) as is done in (5.2.1).

The information matrices of these sets are denoted by replacing the letter S by the letter M, so $MP(k_1,k_2,k_3; w)$ is the information matrix of $SP(k_1,k_2,k_3; w)$.

The number of pairs of the above sets is as follows

$$S(k_1,k_2,k_3; w) \text{ contains } \begin{cases} 2^n \text{ pairs} & \text{,if } k_3 \neq 0 \ , \\ 2^{n-1} \text{ pairs} & \text{,if } k_3 = 0 \ . \end{cases}$$

$$SP(k_1,k_2,k_3; w) \text{ contains } \begin{cases} \dfrac{n!}{k_1!k_2!k_3!} 2^n \text{ pairs} & \text{,if } k_3 \neq 0 \ , \\ \dfrac{n!}{k_1!k_2!} 2^{n-1} \text{ pairs} & \text{,if } k_3 = 0 \ . \end{cases}$$

$$SP_l(0,0,n\,;w) \text{ contains } \begin{cases} \binom{n}{l}2^n \text{ pairs} & ,\text{if } l \neq \tfrac{1}{2}n\ , \\ \binom{n}{\frac{1}{2}n}2^{n-1} \text{ pairs} & ,\text{if } l = \tfrac{1}{2}n\ . \end{cases}$$

The set $SP(k_1,k_2,0;w)$ coincides with the set $S(k_1,k_2)$ given in definition 3.2.2. Expressions for the information matrices of the sets given in definition 5.2.4 are presented in lemma 5.2.5.

Lemma 5.2.5

Let (5.2.3)

$$\begin{aligned} p_1 &= \frac{(n-1)!}{k_1!k_2!k_3!}(4k_2 + g\ k_3)2^n\ , \\ s_1 + t_1 &= \frac{(n-1)!}{k_1!k_2!k_3!}k_3\, gh\, 2^n\ , \\ t_1 &= \frac{2(n-2)!}{k_1!k_2!k_3!}\binom{k_3}{2}\, gh\ 2^n\ , \\ z_1 &= \frac{2(n-2)!}{k_1!k_2!k_3!}\left(4k_1k_2 + k_2k_3\, h + k_1k_3\, g + \binom{k_3}{2}\, gh\right)2^n\ , \end{aligned}$$

with

$$g = (1-w)^2\ , h = (1+w)^2\ .$$

Then

$$MP(k_1,k_2,k_3;w) = \left[\begin{array}{c|c|c} p_1 I & & \\ \hline & s_1 I + t_1 J & \\ \hline & & z_1 I \end{array}\right] ,if\ \ k_3 > 0,$$

and (5.2.4)

$$MP(k_1,k_2,k_3;w) = \frac{1}{2}\left[\begin{array}{c|c|c} p_1 I & & \\ \hline & s_1 I + t_1 J & \\ \hline & & z_1 I \end{array}\right] ,if\ \ k_3 = 0.$$

Let (5.2.5)

$$p_2 \qquad = \binom{n}{l}\, g\ 2^n\ ,$$

$$
\begin{aligned}
s_2 + t_2 &= \binom{n}{l} gh\ 2^n , \\
t_2 &= \left[\binom{n}{l} - 4\binom{n-2}{l-1} \right] gh\ 2^n , \\
z_2 &= \left[\binom{n}{l} - 2\binom{n-2}{l-1} \right] gh\ 2^n .
\end{aligned}
$$

Then

$$
MP_l(0,0,n\,;w) = \left[\begin{array}{c|c|c} p_2 I & & \\ \hline & s_2 I + t_2 J & \\ \hline & & z_2 I \end{array} \right] ,\text{if } l \neq \tfrac{1}{2}n ,
$$

and (5.2.6)

$$
MP_{\frac{1}{2}n}(0,0,n\,;w) = \frac{1}{2} \left[\begin{array}{c|c|c} p_2 I & & \\ \hline & s_2 I + t_2 J & \\ \hline & & z_2 I \end{array} \right] .
$$

Proof

It is easy to prove these results by applying the general expression for $MP((u,v))$ given in (4.2.20). Note that the results of (4.2.20) are related to the case where $MP((u,v))$ contains $n!2^n$ pairs. □

Let ϵ be a design for which the variance function can be expressed by (4.1.8). For all pairs (x,y) belonging to $SP(k_1,k_2,k_3;w)$ the variance function $d(x,y,\epsilon)$ has the same value. The value that is attained by the variance function at the pairs of $SP(k_1,k_2,k_3;w)$ is denoted by $d(k_1,k_2,k_3;w)$ and can be expressed by

$$
\begin{aligned}
d(k_1,k_2,k_3;w) = {} & 4k_2\,\gamma + k_3\, g\ \gamma + 4k_1 k_2\,\delta \qquad (5.2.7) \\
& + k_1 k_3\, g\ \delta + k_2 k_3\, h\ \delta + \binom{k_3}{2} gh\ \delta + k_3\, gh\ \alpha + k_3^2\ gh\ \xi ,
\end{aligned}
$$

where

$$
g = (1-w)^2 \ , \text{and} \ h = (1+w)^2 .
$$

Moreover, if ϵ is a design of type (4.1.6), and if $\delta = -4\xi$ holds, then -by lemma 5.2.1- the value of the variance function is the same for all pairs belonging to $SP_l(0,0,n\,;w)$. This value can be expressed by

$$
d(0,0,n\,;w) = n\ g\ \gamma + \binom{n}{2} gh\ \delta + n\ gh\ \alpha + n^2\, gh\ \xi . \qquad (5.2.8)
$$

If $k_3 = 0$, then $d(k_1,k_2,k_3;w)$ is denoted by $d(k_1,k_2)$, and we have

$$d(k_1,k_2) = 4k_2\gamma + 4k_1k_2\delta\,. \tag{5.2.9}$$

Note that contrary to (3.2.7) in (5.2.7)-(5.2.9) reference to the design ϵ has been suppressed. Whenever the above notations are used, it will be clear to what design ϵ they are related. It will appear that a D-optimal discrete design can be found by choosing a combination of sets as defined in definition 5.2.4 and suitable weights. Such a combination can be obtained by using a procedure similar to procedure 2.3.8. Start with some combination of sets and compute weights by maximizing the determinant of the information matrix. Leave out those sets for which the weights are not positive. Compute the maximal value of the variance function using lemma 5.2.3 and add the sets that contain pairs where $d(x,y,\epsilon)$ is maximal. Now a new combination has been found, and this step is repeated with the new combination. This process converges and a D-optimal discrete design can be found. Again it is not a priori obvious that this procedue converges, because the condition $\delta = -4\xi$ is used. In section 5.3 it will be proved that $\delta = -4\xi$. Then, it is clear that the procedure converges in the same way as procedure 2.3.8. In the following sections D-optimal designs will be presented. A method to prove the D-optimality of these designs will be given in section 5.3. In this section some remarks are made about computing the information matrices of these D-optimal designs. We distinguish between three cases:

i) $n \geqslant 6$, n even ,

ii) $n \geqslant 3$, n odd ,

iii) $n = 2$ or $n = 4$.

The information matrix and covariance matrix of the designs given in section 5.2.1, 5.2.2 and 5.2.3 are given by (4.1.5) and (4.1.6).

5.2.1. Discrete D-optimal designs in the case $n \geqslant 6$, n even.

We shall present a D-optimal design ϵ that consists of 4 sets of the type given in definition 5.2.4. The information matrices of these sets are denoted by M_i , $i = 1, 2, 3, 4$, where

$$M_i = \left[\begin{array}{c|c|c} p_i I & & \\ \hline & s_i I + t_i J & \\ \hline & & z_i I \end{array}\right], \tag{5.2.10}$$

Consider the design, consisting of

i) the pairs of $S(\frac{1}{2}n-1,\frac{1}{2}n+1)$ with weights ν_1;

the number of these pairs is $\binom{n}{\frac{1}{2}n-1}2^{n-1}$,

$p_1 = 2\binom{n-1}{\frac{1}{2}n-1}2^n$,

$s_1 = t_1 = 0$,

$z_1 = 4\binom{n-2}{\frac{1}{2}n-2}2^n$,

$$d(\tfrac{1}{2}n-1, \tfrac{1}{2}n+1) = (2n+4)\,\gamma + (n-2)(n+2)\,\delta\,, \tag{5.2.11}$$

ii) the pairs of $S(\frac{1}{2}n, \frac{1}{2}n)$ with weights ν_2;

the number of these pairs is $\binom{n}{\frac{1}{2}n}2^{n-1}$,

$p_2 = 2\binom{n-1}{\frac{1}{2}n}2^n$,

$s_2 = t_2 = 0$,

$z_2 = 4\binom{n-2}{\frac{1}{2}n-1}2^n$,

$$d(\tfrac{1}{2}n, \tfrac{1}{2}n) = 2n\;\gamma + n^2\,\delta\,, \tag{5.2.12}$$

iii) the pairs of $SP(0,0,n\,;w_1)$ with weights μ ;

the number of these pairs is 2^n ,

$p_3 = g_1\, 2^n$,

$s_3 = 0$,

$t_3 = g_1 h_1\, 2^n$,

$z_3 = g_1 h_1\, 2^n$,

with $g_1 = (1-w_1)^2$, $h_1 = (1+w_1)^2$.

$$d(0,0,n\,;w_1) = n\;g_1\,\gamma + \binom{n}{2} g_1 h_1\,\delta + n\;g_1 h_1\,\alpha + n^2\,g_1 h_1\,\xi\,, \tag{5.2.13}$$

iv) the pairs of $SP_{\frac{1}{2}n}(0,0,n\,;w_1)$ with weights λ ;

the number of these pairs is $\binom{n}{\frac{1}{2}n}2^{n-1}$,

$p_4 = \binom{n}{\frac{1}{2}n}\,g_1\, 2^{n-1}$,

$s_4 = 2\binom{n-2}{\frac{1}{2}n-1}\,g_1 h_1\, 2^n$,

$s_4 + t_4 = \binom{n}{\frac{1}{2}n}\,g_1 h_1\, 2^{n-1}$,

$z_4 = [\binom{n}{\frac{1}{2}n} - 2\binom{n-2}{\frac{1}{2}n-1}]\,g_1 h_1\, 2^{n-1}$;

the value of the variance function in the pairs of this set equals

$d(0,0,n\,;w_1)$ if and only if $\delta = -4\xi$.

The total number of pairs of the design ϵ equals

$$N = [1 + \frac{3n+4}{n} \binom{n}{\frac{1}{2}n-1}]2^n \ . \tag{5.2.14}$$

If one assumes that the design ϵ is D-optimal then the information matrix $M(\epsilon)$ can be derived without computing the weights of the pairs of the design. The variance function is maximal at the pairs of the design and the maximal value equals $\frac{1}{2}n(n+3)$. Using (5.2.11), (5.2.12), (5.2.13) and lemma 5.2.1 , we find

$$(2n+4)\gamma + (n-2)(n+2)\delta = \tfrac{1}{2}n(n+3) , \tag{5.2.15}$$

$$4\gamma + 2n\ \delta = n+3 , \tag{5.2.16}$$

$$g_1\gamma + \tfrac{1}{2}(n-1)g_1h_1\delta + g_1h_1\alpha + n\ g_1h_1\xi = \tfrac{1}{2}(n+3) , \tag{5.2.17}$$

$$\delta = -4\,\xi \tag{5.2.18}$$

The function $d(0,0,n\,;v)$ considered as a function of v is maximal at $v = w_1$; this yields

$$w_1 = -\tfrac{1}{2} + \tfrac{1}{2}[1-\frac{2\gamma}{\alpha+n\xi+\frac{1}{2}(n-1)\delta}]^{\frac{1}{2}} . \tag{5.2.19}$$

Solving the equations (5.2.15)-(5.2.19) we obtain

$$\gamma = \delta = \frac{n+3}{2n+4} , \tag{5.2.20}$$

$$(1-w_1)^3 + 2(n+2)w_1 = 0 ; \tag{5.2.21}$$

the value of α can be computed by means of (5.2.17).

Now, the weights ν_1, ν_2, μ and λ can be computed from the equation

$$M(\epsilon) = \nu_1 M_1 + \nu_2 M_2 + \mu M_3 + \lambda M_4 . \tag{5.2.22}$$

This yields

$$\begin{vmatrix} p \\ s \\ t \\ z \end{vmatrix} = b \begin{vmatrix} 2(n-1) & 2(n-1) & g_1 & (n-1)g_1 \\ 0 & 0 & 0 & n\ g_1h_1 \\ 0 & 0 & g_1h_1 & -g_1h_1 \\ 2(n-2) & 2n & g_1h_1 & \frac{1}{2}(n-2)g_1h_1 \end{vmatrix} \begin{vmatrix} \nu_1 \\ \nu_2 \\ \mu \\ \lambda \end{vmatrix} , \tag{5.2.23}$$

where

$$b = 2^{n+1}\frac{1}{n}\binom{n-2}{\frac{1}{2}n-1},$$

and

$$\overset{*}{\mu} = \frac{2^n}{b}\,\mu .$$

Solving for ν_1, ν_2, λ and μ we find

$$\nu_1 = \frac{1}{b}\left[\frac{n+2}{2(n-1)(n+3)} + \tfrac{1}{8}s + \tfrac{1}{4}t - \frac{(s+t)n}{4(n-1)}\frac{1}{h_1}\right], \tag{5.2.24}$$

$$\nu_2 = \frac{1}{b}\left[\frac{n+2}{2(n-1)(n+3)} - \tfrac{1}{8}s - \tfrac{1}{4}t + \frac{(s+t)(n-2)}{4(n-1)}\frac{1}{h_1}\right],$$

$$\lambda = \frac{s}{n\ b\ g_1 h_1}$$

$$\mu = \frac{s+nt}{n\ g_1 h_1\ 2^n}.$$

Results for $n = 6$ are given in table 5.2.7.

In section 5.3 it will be shown that the set of pairs of any discrete D-optimal design is contained in the union of the sets $S(\frac{1}{2}n-1,\frac{1}{2}n+1)$, $S(\frac{1}{2}n,\frac{1}{2}n)$ and all $SP_l(0,0,n;w_1)$ with $0 \leqslant l < n$. The design ϵ is not D-optimal in the case $n = 2$ or $n = 4$. Solving the equations (5.2.24) in the case $n = 2$ yields a negative value for ν_1. The results in the case $n = 4$ are

$$\begin{aligned}
\alpha &= 2.5580\\
\delta &= 0.5833\\
\gamma &= 0.5833\\
\xi &= -0.1458
\end{aligned}$$

It can be shown that the variance function is maximal at the pairs of the set $SP(1,2,1;0)$ and that the maximal value is equal to 14.079. Therefore, the design is not D-optimal.

5.2.2. Discrete D-optimal designs in the case $n \geqslant 3$, n odd.

We will give a D-optimal design consisting of 3 sets of the type given in definition 5.2.4. The information matrices of these sets are again given by (5.2.10). Consider the design consisting of

i) the pairs of $S(\frac{1}{2}(n-1),\frac{1}{2}(n+1))$ with weights ν_1;

   the number of these pairs is $\binom{n}{\frac{1}{2}n-\frac{1}{2}}2^{n-1}$,

   $$p_1 = 2\binom{n-1}{\frac{1}{2}n-\frac{1}{2}}2^n,$$

   $$s_1 = t_1 = 0,$$

$$z_1 = 4\binom{n-2}{\frac{1}{2}n-\frac{3}{2}}2^n \ ,$$

$$d\left(\tfrac{1}{2}(n-1),\tfrac{1}{2}(n+1)\right) = (2n+2)\,\gamma + (n-1)(n+1)\,\delta \ , \tag{5.2.25}$$

ii) the pairs of $SP(0,0,n\,;w_1)$ with weights μ;
the information matrix of this design has been given in section 5.2.1.

iii) the pairs of $SP_{\frac{1}{2}(n-1)}(0,0,n\,;w_1)$ with weights λ ;

the number of these pairs is $\binom{n}{\frac{1}{2}n-\frac{1}{2}}2^n$,

$$p_3 = \binom{n}{\frac{1}{2}n-\frac{1}{2}}\,g_1\,2^n \ ,$$

$$s_3 = 4\binom{n-2}{\frac{1}{2}n-\frac{3}{2}}\,g_1 h_1\,2^n \ ,$$

$$s_3 + t_3 = \binom{n}{\frac{1}{2}n-\frac{1}{2}}\,g_1 h_1\,2^n \ ,$$

$$z_3 = \left[\binom{n}{\frac{1}{2}n-\frac{1}{2}} - 2\binom{n-2}{\frac{1}{2}n-\frac{3}{2}}\right] g_1 h_1\,2^n \ .$$

The total number of pairs of the design equals

$$N = \left[\,1 + \tfrac{3}{2}\binom{n}{\frac{1}{2}n-\frac{1}{2}}\right]2^n \ .$$

Recalling the fact that a D-optimal design is G-optimal, we find

$$2(n+2)\,\gamma + (n-1)(n+1)\,\delta = \tfrac{1}{2}\,n\,(n+3)\ , \tag{5.2.26}$$

$$4\,\gamma + 2n\,\delta = n+3\ , \tag{5.2.27}$$

$$\delta = -4\,\xi \tag{5.2.28}$$

$$w_1 = -\tfrac{1}{2} + \tfrac{1}{2}\left[1-\frac{2\gamma}{\alpha+n\,\xi+\frac{1}{2}(n-1)\delta}\right]^{\frac{1}{2}} . \tag{5.2.29}$$

These are four equations with five unknown variables. As a fifth equation we use

$$M(\epsilon) = \nu_1\,M_1 + \mu\,M_2 + \lambda\,M_3\ , \tag{5.2.30}$$

i.e.,

$$\begin{bmatrix} p \\ s \\ t \\ z \end{bmatrix} = \begin{bmatrix} p_1 & p_2 & p_3 \\ 0 & 0 & s_3 \\ 0 & t_2 & t_3 \\ z_1 & z_2 & z_3 \end{bmatrix} \begin{bmatrix} \nu \\ \mu \\ \lambda \end{bmatrix} . \tag{5.2.31}$$

This yields

$$\begin{bmatrix} \nu \\ \mu \\ \lambda \end{bmatrix} = \begin{bmatrix} \frac{-z_3 t_2 + z_2 t_3}{z_1 t_2 s_3} & -\frac{z_2}{z_1 t_2} & \frac{1}{z_1} \\ -\frac{t_3}{t_2 s_3} & \frac{1}{t_2} & 0 \\ \frac{1}{s_3} & 0 & 0 \end{bmatrix} \begin{bmatrix} s \\ t \\ z \end{bmatrix} . \tag{5.2.32}$$

Substituting this in $p = p_1 \nu_1 + p_2 \mu + p_3 \lambda$, we obtain

$$p = z + (\frac{1}{h_1} - 1) t + (\frac{1}{h_1} - \tfrac{1}{2}) s , \tag{5.2.33}$$

or

$$\frac{1}{\gamma} = \frac{1}{\delta} - (\frac{1}{h_1} - 1) \frac{\xi}{\alpha(\alpha + n\xi)} + (\frac{1}{h_1} - \tfrac{1}{2}) \frac{1}{\alpha} . \tag{5.2.34}$$

The five equations (5.2.26)-(5.2.29), and (5.2.34) can be solved numerically. The weights can be computed by means of (5.2.30). The set of pairs of any discrete D-optimal design is contained in the union of the sets $S(\frac{1}{2}n-1, \frac{1}{2}n+1)$ and all $SP_l(0,0,n\,;w_1)$ with $0 \leqslant l < n$. Some results are given in table 5.2.7.

5.2.3. Discrete D-optimal designs in the case $n = 2, 4$

We give a D-optimal design consisting of 4 sets of the type given in section 5.2.4. The information matrix of these sets are denoted by (5.2.10). Consider the design consisting of

i) the pairs of $S(\frac{1}{2}n, \frac{1}{2}n)$ with weights ν_2 ,

ii) the pairs of $SP(0,0,n\,;w_1)$ with weights μ ,

iii) the pairs of $SP_{\frac{1}{2}n}(0,0,n\,;w_1)$ with weights λ ;

results concerning the information matrices of these sets are given in section 5.2.1 and 5.2.2 ,

iv) the pairs of $SP(\frac{1}{2}n-1, \frac{1}{2}n, 1;\, w_2)$ with weights ρ ;

the number of these pairs, say N_4, equals

$$N_4 = \begin{cases} 8 \text{ ,if } n = 2 , \\ 192 \text{ ,if } n = 4 , \end{cases}$$

$$M_4 = \left|\begin{array}{c|c|c} (16+4g_2)I & & \\ \hline & 4g_2h_2I & \\ \hline & & 8h_2I \end{array}\right| \quad , \text{ if } n = 2 \,,$$

$$M_4 = \left|\begin{array}{c|c|c} (384+48g_2)I & & \\ \hline & 48g_2h_2I & \\ \hline & & (256+32g_2+64h_2)I \end{array}\right| \quad , \text{ if } n = 4 \,,$$

where

$$g_2 = (1-w_2)^2 \ , h_2 = (1+w_2)^2 \ ,$$

$$d(\tfrac{1}{2}n-1, \tfrac{1}{2}n, 1; w_2) = 2n\ \gamma + g_2\gamma + n(n-2)\,\delta + (\tfrac{1}{2}n-1)\,g_2\,\delta$$

$$+ \tfrac{1}{2}n\ h_2\,\delta + \alpha\ g_2h_2 + \xi\ g_2h_2\,. \tag{5.2.35}$$

Using similar arguments as in section 5.2.1 and 5.2.2 we find the equations

$$2\,\gamma + n\ \delta = \tfrac{1}{2}\,(n+3)\,, \tag{5.2.36}$$

$$g_1\,\gamma + \tfrac{1}{2}(n-1)\,g_1h_1\,\delta + g_1h_1\,\alpha + n\ g_1h_1\,\xi = \tfrac{1}{2}(n+3)\,, \tag{5.2.37}$$

$$\delta = -4\,\xi\,, \tag{5.2.38}$$

$$2n\ \gamma + g_2\,\gamma + n(n-2)\,\delta + (\tfrac{1}{2}n-1)g_2\,\delta$$

$$+ \tfrac{1}{2}n\ h_2\,\delta + \alpha\ g_2h_2 + \xi\ g_2h_2 = \tfrac{1}{2}n\,(n+3)\,, \tag{5.2.39}$$

$$w_1 = -\tfrac{1}{2} + \tfrac{1}{2}\,[1 - \frac{2\gamma}{\alpha + n\,\xi + \frac{1}{2}(n-1)\delta}]^{\frac{1}{2}}\,, \tag{5.2.40}$$

$$2(\alpha + \xi)\,w_2^3 + [(n-1)\,\delta + \gamma - 2(\alpha+\xi)]w_2 + \delta - \gamma = 0\,. \tag{5.2.41}$$

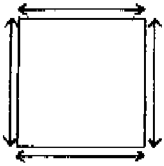
The equations (5.2.36)-(5.2.41) can be solved numerically. Results are given in table 5.2.7, and for $n = 2$ in figure 5.2.6; the arrows indicate the pairs. In table 5.2.7 NP denotes the number of pairs of the corresponding subset of ϵ. In the row marked with % the total weights of the subsets are given as percentages. ND denotes the number of pairs of the design ϵ, and $ND^{\dagger}$ equals $\frac{1}{8}n\,(n+1)(n+2)(n+3)(n+4)$, the number given in (4.1.4).

Figure 5.2.6
A D-optimal design in the case $n = 2$

Pairs

$S(1,1)$

$\nu_2 = 0.02480$



$((1,1),(1,-1))$

$((1,1),(-1,1))$

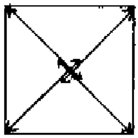
$((1,1),(-1,1))$

$((1,1),(1,-1))$

$SP(0,0,2;\, w_1)$

$w_1 = -0.15029$

$\mu = 0.04621$



$((1,1),(w_1,w_1))$

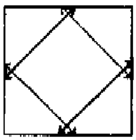
$((-1,1),(-w_1,w_1))$

$((1,-1),(w_1,-w_1))$

$((1,1),(-w_1,-w_1))$

$SP_1(0,0,2;\, w_1)$

$\lambda = 0.02975$



$((1,w_1),(w_1,1))$

$((-1,w_1),(-w_1,1))$

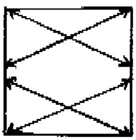
$((1,-w_1),(w_1,-1))$

$((-1,-w_1),(-w_1,-1))$

$SP(0,1,1;\, w_2)$

$w_2 = -0.12002$

$\rho = 0.07462$

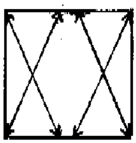


$((1,1),(-1,w_2))$

$((-1,-1),(1,-w_2))$

$((-1,1),(1,w_2))$

$((1,-1),(-1,-w_2))$



$((1,1),(w_2,-1))$

$((-1,-1),(-w_2,1))$

$((1,-1),(w_2,1))$

$((-1,1),(-w_2,-1))$

Table 5.2.7
Values of constants determining discrete D-optimal designs and the information matrices of these designs

n	2	3	4	5	6	7
α	1.933	2.279	2.589	3.015	3.331	3.760
δ	0.756	0.618	0.599	0.578	0.563	0.559
γ	0.494	0.507	0.553	0.510	0.563	0.510
ξ	−0.189	−0.155	−0.150	−0.145	−0.141	−0.140
w_1	−0.150	−0.118	−0.107	−0.080	−0.078	−0.061
w_2	0.120		0.018			
det[1]	0.5541	0.2901	0.1484	$0.2737\ 10^{-1}$	$0.5771\ 10^{-2}$	$0.3522\ 10^{-3}$
ν_1		$0.425\ 10^{-1}$		$0.402\ 10^{-2}$	$0.146\ 10^{-3}$	$0.321\ 10^{-3}$
NP		12		160	480	2240
%		51.0%		64.3%	7.0%	71.9%
ν_2	$0.248\ 10^{-1}$		$0.711\ 10^{-2}$		$0.952\ 10^{-3}$	
NP	4		48		640	
%	9.9%		34.1%		60.9%	
μ	$0.462\ 10^{-1}$	$0.189\ 10^{-1}$	$0.678\ 10^{-2}$	$0.241\ 10^{-2}$	$0.106\ 10^{-2}$	$0.516\ 10^{-6}$
NP	4	8	16	32	64	128
%	18.5%	15.1%	10.8%	7.7%	6.8%	0.007%
λ	$0.298\ 10^{-1}$	$0.141\ 10^{-1}$	$0.492\ 10^{-2}$	$0.875\ 10^{-3}$	$0.396\ 10^{-3}$	$0.105\ 10^{-3}$
NP	4	24	48	320	640	4480
%	11.9%	33.8%	23.6%	28.0%	25.3%	28.1%
ρ	$0.746\ 10^{-1}$		$0.164\ 10^{-2}$			
NP	8		192			
%	59.7%		31.4%			
ND	20	44	304	512	1824	6848
ND^{*}	15	45	105	210	378	630

1) det = det $(M^{-1}(\epsilon))$

5.3. A method to prove the D-optimality of the designs given in section 5.2

There are two reasons for calling this section "A method to prove the $\cdots$" and not "Proof of the $\cdots$".

1. The D-optimality of a design is proved by computing the maximum of the variance function. In this section it is proved that this maximum can be found by determining the maximum element of a set of $\frac{1}{2}(n+2)(n+1)$ numbers. It seems not possible to give a general expression for these values. Therefore for given n it is necessary to compute all these values. This has been done for all $n \leqslant 20$.
2. The values of α, δ, γ and ξ determining the covariance matrix are computed numerically. Therefore statements concerning the proof of the D-optimality for given n are numerical results.

Throughout this section ϵ is a design with covariance matrix of type 4.1.6 and (u,v) denotes a pair where the variance function $d(x,y,\epsilon)$ is maximal. A necessary and sufficient condition for D-optimality is

$$d(u,v,\epsilon) = \tfrac{1}{2}n(n+3)\,. \tag{5.3.1}$$

When giving the method to prove the D-optimality of the designs of section 5.2, we do not use the condition $\delta = -4\xi$ until the very end of this section. In that way results are achieved that can also be used for the construction of exact designs. Using $\delta = -4\xi$ from the beginning would have made the proof of the D-optimality slightly shorter.
We recall lemma 5.2.2, which we did not prove.

Lemma 5.2.2
Let ϵ and (u,v) be as defined above. Then

$$|u_i| = 1 \quad or \quad |v_i| = 1 \qquad (1 \leqslant i \leqslant n)\,.$$

Proof
Assume that $|u_i| < 1$ and $|v_i| < 1$ for some i. Using (3.1.8) and (3.1.9) we suppose without loss of generality that $i = 1$.
Consider

$$\begin{aligned}
d_1 &= d((1,u_2,\ldots,u_n),v,\epsilon)\,,\\
d_2 &= d((-1,u_2,\ldots,u_n),v,\epsilon)\,,\\
d_3 &= d(u,(1,v_2,\ldots,v_n),\epsilon)\,,\\
d_4 &= d(u,(-1,v_2,\ldots,v_n),\epsilon)\,.
\end{aligned}$$

Since $d(x,y,\epsilon)$ is maximal at (u,v) we have

$$d_i - d(u,v,\epsilon) \leqslant 0\,.$$

So,

$$d_1 - d =$$

$$= \gamma\, [(1-v_1)^2 - (u_1 - v_1)^2] + \delta \sum_{j=2}^{n} [(u_j - v_1 v_j)^2 - (u_1 u_j - v_1 v_j)^2]$$

$$+\alpha\, [(1-v_1^2)^2 - (u_1^2 - v_1^2)^2]$$

$$+ \xi \left[(1-v_1^2)^2 - (u_1^2 - v_1^2)^2 + 2 \sum_{j=2}^{n} [(1-v_1^2)(u_j^2 - v_j^2) - (u_1^2 - v_1^2)(u_j^2 - v_j^2)] \right]$$

$$= \gamma\, [1 - u_1^2 - 2v_1(1-u_1)] + \delta \sum_{j=2}^{n} [u_j^2(1-u_1^2) - 2v_1 v_j u_j (1-u_1)]$$

$$+\alpha\, [(1-u_1^4) - 2v_1^2(1-u_1^2)]$$

$$+ \xi\, [(1-u_1^4) - 2v_1^2(1-u_1^2) + 2(1-u_1^2) \sum_{j=2}^{n} (u_j^2 - v_j^2)] \leqslant 0.$$

This yields

$$\gamma\, (1+u_1 - 2v_1) + \delta \sum_{j=2}^{n} [(1+u_1)u_j^2 - 2v_1 u_j v_j] +$$

$$\alpha\, [1 + u_1 + u_1^2 + u_1^3 - 2v_1^2(1+u_1)]$$

$$+\xi\, [1 + u_1 + u_1^2 + u_1^3 - 2v_1^2(1+u_1) + 2(1+u_1) \sum_{j=2}^{n} (u_j^2 - v_j^2)] \leqslant 0. \qquad \text{(i)}$$

Similarly we find using $d_2 - d(u, v, \epsilon) \leqslant 0$

$$\gamma\, (1-u_1 + 2v_1) + \delta \sum_{j=2}^{n} [(1-u_1)u_j^2 + 2v_1 u_j v_j] +$$

$$\alpha\, [1 - u_1 + u_1^2 - u_1^3 - 2v_1^2(1-u_1)]$$

$$+\xi\, [1 - u_1 + u_1^2 - u_1^3 - 2v_1^2(1-u_1) + 2(1-u_1) \sum_{j=2}^{n} (u_j^2 - v_j^2)] \leqslant 0. \qquad \text{(ii)}$$

From (i) and (ii) it follows that

$$2\gamma + 2\delta \sum_{j=2}^{n} u_j^2 + 2(\alpha + \xi)(1 + u_1^2 - 2v_1^2) + 4\xi \sum_{j=2}^{n} (u_j^2 - v_j^2) \leqslant 0,$$

or

$$2(\alpha + \xi)(1 + u_1^2 - 2v_1^2) + 4\xi \sum_{j=2}^{n} (u_j^2 - v_j^2) \leqslant 0. \qquad \text{(iii)}$$

Since $d_3 - d(x, y, \epsilon) \leqslant 0$ and $d_4 - d(x, y, \epsilon) \leqslant 0$ we have

$$2(\alpha + \xi)(1 + v_1^2 - 2u_1^2) - 4\xi \sum_{j=2}^{n} (u_j^2 - v_j^2) \leqslant 0. \qquad \text{(iv)}$$

From (iii) and (iv) it follows that

$$2(\alpha + \xi)(2-u_1^2-v_1^2) \leqslant 0 \, ,$$

Since $\alpha + \xi > 0$ this contradicts our assumptions. $\square$

We have to find a pair (u,v) where the variance function is maximal. Using (3.1.8), (3.1.9) and lemma 5.2.2 we can assume without loss of generality that u and v are such that

$$\tag{5.3.2} \begin{array}{llll} u_i & = 1 & \text{for} & 1 \leqslant i \leqslant k_1 + k_2 + l_2 \, , \\ -1 < u_i < 1 & & \text{for} & k_1 + k_2 + l_2 < i \leqslant n \, , \\ v_i & = 1 & \text{for} & 1 \leqslant i \leqslant k_1 \, , \\ v_i & = -1 & \text{for} & k_1 < i \leqslant k_1 + k_2 \, , \\ -1 < v_i < 1 & & \text{for} & k_1 + k_2 < i \leqslant k_1 + k_2 + l_2 \, , \\ v_i & = 1 & \text{for} & k_1 + k_2 + l_2 < i \leqslant k_1 + k_2 + l_2 + l_1 \, , \end{array}$$

for some k_1, k_2, l_1 and l_2, with $k_1 + k_2 + l_1 + l_2 = n$.

We define

$$k_3 := l_1 + l_2 \, ,$$

$$L_1 := \{ \, i \mid k_1 + k_2 + l_2 < i \leqslant n \, \} \, ,$$

$$L_1 := \{ \, i \mid k_1 + k_2 < i \leqslant k_1 + k_2 + l_2 \} \, ,$$

$$K_3 := L_1 \cup L_2 \, .$$

Throughout the rest of this section (u,v) denotes a pair as defined in (5.3.2). If we write $v_i = w_i$ for all $i \in L_2$,
and $u_i = w_i$ for all $i \in L_1$, then u and v can be expressed by

$$u = (1, \ldots, 1, w_{k_1+k_2+l_2+1}, \ldots, w_n)' \, , \tag{5.3.3}$$

$$v = (1, \ldots, 1, -1, \ldots, -1, w_{k_1+k_2+1}, \ldots, w_{k_1+k_2+l_2}, 1, \ldots, 1)' \, .$$

We give some further results

Lemma 5.3.1 *Let (u,v) be as in (5.3.3). Then*

$$\begin{aligned} d(u,v,\epsilon) = {} & 4k_2\gamma + \gamma \sum_{i \in K_3} (1-w_i)^2 + 4k_1k_2\delta + k_1\delta \sum_{i \in K_3} (1-w_i)^2 \\ & + k_2\delta \sum_{i \in K_3} (1+w_i)^2 + \delta \sum_{\substack{i,j \in K_3 \\ i<j}}\sum (1-w_iw_j)^2 + \alpha \sum_{i \in K_3} (1-w_i^2)^2 \\ & + \xi \, [\sum_{i \in K_3} (1-w_i^2)]^2 - (\delta + 4\xi) \sum_{i \in L_1} \sum_{j \in L_2} (1-w_i^2)(1-w_j^2) \, . \end{aligned} \tag{5.3.4}$$

Proof
Using (4.1.8) we obtain

$$d(u,v,\epsilon) = 4k_2\gamma + \gamma \sum_{i\in L_2}(1-w_i)^2 + \gamma \sum_{i\in L_1}(w_i-1)^2 + 4k_1k_2\delta$$
$$+ k_1\delta \sum_{i\in L_1}(1-w_i)^2 + k_2\delta \sum_{i\in L_2}(1+w_i)^2 + k_1\delta \sum_{i\in L_1}(w_i-1)^2$$
$$+ k_2\delta \sum_{i\in L_1}(w_i+1)^2 + \delta \sum_{i\in L_1}\sum_{j\in L_2}(w_i-w_j)^2$$
$$+ \delta \sum\sum_{\substack{i,j\in L_1\\ i<j}}(w_iw_j-1)^2 + \delta \sum\sum_{\substack{i,j\in L_2\\ i<j}}(1-w_iw_j)^2 + \alpha \sum_{i\in L_1}(w_i^2-1)^2$$
$$+ \alpha \sum_{i\in L_2}(1-w_i^2)^2 + \xi\,[l_2+\sum_{i\in L_1}w_i^2-(l_1+\sum_{i\in L_2}w_i^2)]^2 . \tag{i}$$

We have

$$\delta \sum_{i\in L_1}\sum_{j\in L_2}(w_i-w_j)^2 =$$
$$\delta \sum_{i\in L_1}\sum_{j\in L_2}[(1-w_iw_j)^2-(1-w_i^2)(1-w_j^2)] , \tag{ii}$$

and

$$\xi\,[\,l_2+\sum_{i\in L_1}w_i^2-(l_1+\sum_{i\in L_2}w_i^2)\,]^2 =$$
$$\xi\,[\sum_{i\in K_3}(1-w_i^2)]^2-4\xi \sum_{i\in L_1}\sum_{j\in L_2}(1-w_i^2)(1-w_j^2) . \tag{iii}$$

Substitution of (ii) and (iii) in (i) completes the proof. $\square$

Remark 5.3.2
From lemma 5.3.1 we conclude that

if $\delta + 4\xi > 0$, then $L_1 = \varnothing$ or $L_2 = \varnothing$,

if $\delta + 4\xi = 0$, then $L_1 = \varnothing$ without loss of generality .

Lemma 5.3.3
Let (x,y) *have the same structure as* (u,v) *in (5.5.3) and let* $k \in L_1$, $l \in L_1$. *Consider* $d(x,y,\epsilon)$ *as function of* w_k *and* w_l . *Then*

$$\frac{\partial d(x,y,\epsilon)}{\partial w_k} = -2\gamma + 2(k_2-k_1)\delta + [2\gamma+2\delta(k_1+k_2)-4(\alpha+4k_3\xi)]w_k$$
$$+ 4(\alpha+\xi)w_k^3 - 2\delta \sum_{\substack{j\in K_3\\ j\neq k}} w_j + 2(\delta+2\xi)\,w_k \sum_{\substack{j\in K_3\\ j\neq k}} w_j^2 \tag{5.3.5}$$
$$+ 2(\delta+4\xi)\,w_k \sum_{j\in L_2}(1-w_j^2) ,$$

$$\frac{\partial d(x,y,\epsilon)}{\partial w_k} - \frac{\partial d(x,y,\epsilon)}{\partial w_l} = 2(w_k - w_l)\, g(w_k, w_l)\,, \tag{5.3.6}$$

where

$$g(w_k,w_l) = \gamma + (k_1+k_2+1)\,\delta - 2(\alpha + k_3\xi) + l_2(\delta + 4\xi)$$
$$+ (w_k^2 + w_k w_l + w_l^2)(2\alpha - \delta) + (\delta + 2\xi) \sum_{j \in K_3} w_j^2 - (\delta + 4\xi) \sum_{j \in L_2} w_j^2 .$$

Proof

The first part follows immediately from (5.3.4). Using (5.3.5) we obtain

$$\frac{\partial d(x,y,\epsilon)}{\partial w_k} - \frac{\partial d(x,y,\epsilon)}{\partial w_l} = (w_k - w_l)[2\gamma + 2(k_1+k_2)\delta - 4(\alpha + k_3\xi)]$$
$$+ 4(w_k^3 - w_l^3)(\alpha + \xi) - 2\delta\,(w_l - w_k) + 2(\delta + 2\xi)(w_k - w_l) \sum_{j \in K_3} w_j^2$$
$$- 2(\delta + 2\xi)(w_k^3 - w_l^3) + 2l_2(\delta + 4\xi)(w_k - w_l)$$
$$- 2(\delta + 4\xi)(w_k - w_l) \sum_{j \in L_2} w_j^2 .$$

This yields (5.3.6). □

Lemma 5.3.3

Let (u,v) *be as defined in (5.3.3) and* $l_2 \geqslant 1$. *Then for all* i *with* $k_1 + k_2 < i \leqslant k_1 + k_2 + l_2$,

$$\gamma + (k_1+k_2)\,\delta + 2\xi - 2k_3\,\xi + l_2\,(\delta + 4\xi) \tag{5.3.7}$$
$$+ (\alpha + \xi)(3w_i^2 + 2|w_i| - 1) + (\delta + 2\xi) \sum_{\substack{j \in K_3 \\ j \neq i}} w_j^2 - (\delta + 4\xi) \sum_{j \in L_2} w_j^2 \leqslant 0 .$$

If $\delta + 2\xi \geqslant 0$ *and* $\xi \leqslant 0$, *then* $|w_i| < \frac{1}{3}$. (5.3.8)

Proof

Without loss of generality we choose $i = k_1 + k_2 + 1$ and $w_{k_1+k_2+1}$ is denoted by w. Consider $d_2 = d(u,\bar{v},\epsilon)$, where $\bar{v}$ is defined by $\bar{v}_{k_1+k_2+1} = 1$ and $\bar{v}_j = v_j$ for $j \neq k_1+k_2+1$. Using (5.3.4) we get

$$d_2 = 4(k_2+1)\,\gamma + \gamma \sum_{\substack{j \in K_3 \\ j \neq i}} (1-w_j)^2 + 4k_1(k_2+1)\,\delta + k_1\,\delta \sum_{\substack{j \in K_3 \\ j \neq i}} (1-w_j)^2$$
$$+ (k_2+1)\,\delta \sum_{\substack{j \in K_3 \\ j \neq i}} (1+w_j)^2 + \delta \sum_{\substack{j \in K_3 \\ j \neq i}} \sum_{\substack{k \in K_3 \\ k \neq i,\, j<k}} (1 - w_j w_k)^2 + \alpha \sum_{\substack{j \in K_3 \\ j \neq i}} (1-w_j^2)^2$$
$$+ \xi\, [\sum_{\substack{j \in K_3 \\ j \neq i}} (1-w_j^2)\,]^2 - (\delta + 4\xi) \sum_{\substack{j \in L_1 \\ j \neq i}} \sum_{\substack{k \in L_2 \\ k \neq i}} (1-w_j^2)(1-w_k^2)\,,$$

and therefore

$$d_2 - d(u,v,\epsilon) = 4\gamma - \gamma(1-w)^2 + 4k_1\delta - k_1\delta(1-w)^2 - k_2\delta(1+w)^2$$
$$+ \delta \sum_{\substack{j\in K_3\\ j\neq i}} (1+w_j)^2 - \delta \sum_{\substack{j\in K_3\\ j\neq i}} (1-w_i w_j)^2 - (\alpha+\xi)(1-w^2)^2$$
$$+ (\delta+4\xi)(1-w^2) \sum_{j\in L_2} (1-w_j^2) - 2\xi(1-w^2) \sum_{\substack{j\in K_3\\ j\neq i}} (1-w_j^2).$$

Using $d_2 - d(u,v,\epsilon) \leqslant 0$ and $1+w > 0$ we obtain

$$\gamma(3-w) + k_1\delta(3-w) - k_2\delta(1+w) - \alpha(1-w)(1-w^2)$$
$$- \xi\,[(1-w)(1-w^2) + 2(k_3-1)(1-w)] + \delta \sum_{\substack{j\in K_3\\ j\neq i}} [(1-w)w_j^2 + 2w_j]$$
$$+ 2\xi(1-w) \sum_{\substack{j\in K_3\\ j\neq i}} w_j^2 + (\delta+4\xi)(1-w) \sum_{j\in L_2} (1-w_j^2) \leqslant 0.$$

Using the fact that (u,v) is a pair where $d(x,y,\epsilon)$ is maximal, we may add

$$\left.\frac{\partial d(x,y,\epsilon)}{\partial w}\right|_{(x,y)=(u,v)}$$

to the left side of the last inequality. It follows that

$$\gamma + \gamma w + (k_1+k_2)\delta + (k_1+k_2)\delta w + (\alpha+\xi)(-1-3w+w^2+3w^3)$$
$$-2(k_3-1)\xi(1+w) + [\delta(1-w) + 2\xi(1-w) + 2(\delta+2\xi)w] \sum_{\substack{j\in K_3\\ j\neq i}} w_j^2$$
$$+ [(\delta+4\xi)(1-w) + 2(\delta+4\xi)w] \sum_{j\in L_2} (1-w_j^2) \leqslant 0.$$

This yields, again using $1+w > 0$,

$$\gamma + (k_1+k_2)\delta + (\alpha+\xi)(3w^2-2w-1) - 2(k_3-1)\xi + l_2(\delta+4\xi)$$
$$+ (\delta+2\xi) \sum_{\substack{j\in K_3\\ j\neq i}} w_j^2 - (\delta+4\xi) \sum_{j\in L_2} w_j^2 \leqslant 0. \qquad \text{(i)}$$

Consider $d_1 = d(\bar{u},v,\epsilon)$, where $\bar{u}$ is defined by

$$\bar{u}_j = 1 \text{ for } 1 \leqslant j \leqslant k_1+1,$$
$$\bar{u}_j = -1 \text{ for } k_1+1 < j \leqslant k_1+k_2+1,$$

and

$$\bar{u}_j = u_j \text{ for } k_1+k_2+1 < j \leqslant n.$$

Analogously we find

$$\gamma + (k_1+k_2)\,\delta + (\alpha + \xi)(3w^2+2w-1) - 2(k_3-1)\,\xi + l_2(\delta + 4\xi)$$
$$+ (\delta + 2\xi) \sum_{\substack{j \in K_3 \\ j \neq i}} w_j^2 - (\delta + 4\xi) \sum_{j \in L_2} w_j^2 \leqslant 0\,. \tag{ii}$$

Use of expressions (i) and (ii) and of the conditions $\delta + 2\xi \geqslant 0$ and $\xi \leqslant 0$ completes the proof of (5.3.7). Now it follows that

$$(\alpha + \xi)(3w^2+2|w|-1) \leqslant -\gamma - (k_1+k_2)\,\delta + 2(k_3-1)\xi - l_2\,(\delta + 4\xi)$$
$$- (\delta + 2\xi) \sum_{\substack{j \in K_3 \\ j \neq i}} w_j^2 + (\delta + 4\xi) \sum_{j \in L_2} w_j^2$$
$$= -\gamma - (k_1+k_2)\,\delta + 2(k_3-l_2-1)\,\xi - l_2(\delta + 2\xi) - (\delta + 2\xi) \sum_{\substack{j \in K_3 \\ j \neq i}} w_j^2$$
$$+ 2\xi \sum_{j \in L_2} w_j^2 < 0\,,$$

because

$$\delta + 2\xi \geqslant 0\,,\ \gamma > 0\,,\ \xi \leqslant 0 \text{ and } \delta > 0\,.$$

Since $\alpha + \xi > 0$ we have

$$3w^2 + 2|w| - 1 < 0\,,$$
$$(3|w|-1)(|w|+1) < 0\,,$$
$$|w| < \tfrac{1}{3}\,.$$

∎

Now we can prove a theorem that is important in proving the D-optimality of the designs of section 5.2.

Theorem 5.3.4

Let ϵ be a design with covariance matrix of type (4.1.6) and let (u,v) be a pair where the variance function is maximal, having the structure of (5.3.2).
If

$$\delta + 2\xi \geqslant 0\,,\ \xi \leqslant 0 \text{ and } \alpha - 2\delta \geqslant 0\,,$$

then

$$u_i = u_j \text{ for all } k_1 + k_2 + l_2 < i,j \leqslant n\,,$$
$$v_k = v_l \text{ for all } k_1 + k_2 < k,l \leqslant k_1 + k_2 + l_2\,.$$

Proof

Let $\delta + 2\xi \geqslant 0$, $\xi \leqslant 0$ and $\alpha - 2\delta \geqslant 0$. We prove that $u_i = u_j$ for all $k_1 + k_2 + l_2 < i,j \leqslant n$, or in the notation of (5.3.3) that $w_i = w_j$ for all $i,j \in L_1$. Consider the function $g(w_i,w_j)$ defined in (5.3.6). Using (5.3.7) we find

$$g(w_i,w_j) \leqslant \gamma + (k_1+k_2+1)\,\delta - 2(\alpha + k_3\,\xi) + l_2(\delta + 4\xi)$$

$$+ (w_i^2+w_i w_j+w_j^2)(2\alpha - \delta) + (\delta + 2\xi) \sum_{l \in K_3} w_l^2 - (\delta + 4\xi) \sum_{l \in L_2} w_l^2$$

$$- \gamma - (k_1+k_2)\,\delta + 2(k_3-1)\,\xi - l_2\,(\delta + 4\xi) - (\alpha + \xi)(3w_i^2+2\,|w_i\,|-1)$$

$$- (\delta + 2\xi) \sum_{\substack{l \in K_3 \\ l \neq i}} w_l^2 + (\delta + 4\xi) \sum_{l \in L_2} w_l^2$$

$$= \delta - (\alpha + \xi) - (\alpha + \xi)\,w_i^2 - 2(\alpha + \xi)\,|w_i\,| + (2\alpha - \delta)\,w_i w_j$$

$$+ (2\alpha - \delta)\,w_j^2 =: h(w_i,w_j)\;.$$

Using (5.3.8) we obtain $|w_i\,| \leqslant \frac{1}{3}$ and $|w_j\,| \leqslant \frac{1}{3}$. The function $h(w_i,w_j)$ is maximal for $w_i = 0$ and $w_j = \frac{1}{3}$. This yields

$$g(w_i,w_j) \leqslant \delta - (\alpha + \xi) + \tfrac{1}{9}\,(2\alpha - \delta) = -\tfrac{7}{9}\alpha + \tfrac{8}{9}\delta - \xi$$

$$= -\tfrac{1}{9}[7(\alpha - 2\delta) + \tfrac{9}{2}\,(\delta + 2\xi) + \tfrac{3}{2}\delta] < 0\;.$$

From (5.3.6) and the fact that

$$\left(\frac{\partial d\,(x,y,\epsilon)}{\partial w_i} - \frac{\partial d\,(x,y,\epsilon)}{\partial w_j} \right)\Bigg|_{(x,y)\,=\,(u,v)} = 0\;,$$

it follows that

$$w_i = w_j \text{ for all } i\,,\,j \in L_1\;.$$

Use of (3.1.8) and (3.1.9) proves that

$$w_k = w_l \text{ for all } k\,,\,l \in L_2\;. \qquad \square$$

Lemma 5.3.5
Let (x, y) have the same structure as (u, v) in (5.3.3) and let

$$x_i = w_1 \text{ for all } i \text{ with } k_1 + k_2 + l_2 < i \leqslant n , \tag{5.3.9}$$

$$y_i = w_2 \text{ for all } i \text{ with } k_1 + k_2 < i \leqslant k_1 + k_2 + l_2 .$$

Then

$$\begin{aligned} d(x, y, \epsilon) &= 4k_2 \gamma + l_1 \gamma (1-w_1)^2 + l_2 \gamma (1-w_2)^2 + 4k_1 k_2 \delta \\ &+ k_1 l_1 \delta (1-w_1)^2 + k_1 l_2 \delta (1-w_2)^2 + k_2 l_1 \delta (1+w_1)^2 + k_2 l_2 \delta (1+w_2)^2 \\ &+ l_1 l_2 \delta (w_1 - w_2)^2 + \binom{l_1}{2} \delta (1-w_1^2)^2 + \binom{l_2}{2} \delta (1-w_2^2)^2 + l_1 \alpha (1-w_1^2)^2 \\ &+ l_2 \alpha (1-w_2^2)^2 + [l_1 (1-w_1^2) - l_2 (1-w_2^2)]^2 \xi . \end{aligned} \tag{5.3.10}$$

If w_1 and w_2 are such that the function given in (5.3.10) is maximal at w_1 and w_2, then

$$\begin{aligned} & w_i^3 [4\binom{l_i}{2} \delta + 4l_i \alpha + 4l_i^2 \xi] \\ &+ w_i [2l_i \gamma + 2(k_1+k_2) l_i \delta + 2l_i l_j \delta - 4\binom{l_i}{2} \delta - 4l_i \alpha - 4l_i^2 \xi \\ &+ 4l_i l_j \xi (1-w_j^2)] - 2l_i \gamma - 2k_1 l_i \delta + 2k_2 l_i \delta - 2l_i l_j \delta w_j = 0 , \\ & \text{for } (i, j) = (1,2) \text{ and } (i, j) = (2,1) . \end{aligned} \tag{5.3.11}$$

Proof
It is easy to show that (5.3.9) holds by using (5.3.4). Equation (5.3.11) can be proved by using the fact that (u, v) is a pair where $d(x, y, \epsilon)$ is maximal. So

$$\left. \frac{\partial d(x, y, \epsilon)}{\partial w_1} \right|_{(x, y) = (u, v)} = \left. \frac{\partial d(x, y, \epsilon)}{\partial w_2} \right|_{(x, y) = (u, v)} = 0 . \qquad \square$$

In view of lemma 5.3.5 it is useful to give the following definition.

Definition 5.3.6
Let k_1, k_2, l_1 and l_2 be fixed. The maximal value of the functions given in (5.3.10) is denoted by $d(k_1, k_2, l_1, l_2; \epsilon)$.

Now it is possible to prove that the designs ϵ given in section 5.2 are D-optimal. The procedure is as follows. It is sufficient to prove that $d(x, y, \epsilon) \leqslant \frac{1}{2} n (n+3)$. If the conditions $\delta + 2\xi \geqslant 0$, $\xi \leqslant 0$, and $\alpha - 2\delta \geqslant 0$ are satisfied, then one just has to consider the pairs (u, v) as defined in theorem 5.3.4. The values $d(k_1, k_2, l_1, l_2; \epsilon)$ can be computed by use of lemma 5.3.5. The maximal value of $d(x, y, \epsilon)$ can be found by computing these values for all combinations (k_1, k_2, l_1, l_2) with $k_1 + k_2 + l_1 + l_2 = n$. This seems a rather cumbersome task.

However, many combinations can be omitted using trivial arguments. If $\delta - 4\xi$, then the combinations $(k_1, k_2, 0, k_3)$ have to be investigated. In that case w_2 satisfies the equation

$$\begin{aligned} & w_2^2\ [2(k_3-1)\,\delta + 4(\alpha + k_3\,\xi)] \\ & + w_2\,[2\gamma + 2(k_1 + k_2)\,\delta - 2(k_3-1)\,\delta - 4(\alpha + k_3\,\xi)] \\ & -2\gamma + 2(k_2-k_1)\,\delta = 0\,. \end{aligned} \tag{5.3.12}$$

If $k_1 = k_2 = 0$, then

$$w_2 = -\tfrac{1}{2} + \tfrac{1}{2}\,[1 - \frac{2\gamma}{\alpha + n\,\xi + \frac{1}{2}(n-1)\delta}]^{\frac{1}{2}}\,. \tag{5.3.13}$$

Theorem 5.3.7

The designs ϵ given in section 5.2 in table 5.2.7 are D-optimal.

Proof

The procedure given above is used. The conditions $\delta + 2\xi \geqslant 0$, $\xi \leqslant 0$ and $\alpha - 2\delta \geqslant 0$ hold. Moreover $\delta = -4\xi$. This means that the maximal value of $d(x, y, \epsilon)$ is equal to one of the values $d(k_1, k_2, 0, k_3; \epsilon)$. By computing these values one finds that the variance function is maximal at the pairs of the design ϵ and that the maximal value is equal to $\frac{1}{2}n\,(n+3)$. $\square$

5.4. Reduction of the number of pairs of discrete D-optimal designs

The number of pairs ND of the design given in table 5.2.7 is large compared to the number ND^* given in that table. We recall these numbers here

Table 5.4.1

Number of pairs of the D-optimal designs given in section 5.2

n	2	3	4	5	6	7
ND	20	44	304	512	1824	6848
ND^*	15	45	105	210	378	630

According to theorem 2.3.6 ND^* is such that a D-optimal design exists with m pairs and such that $m \leqslant ND^*$. As can be seen in table 5.4.1 it is possible to reduce considerably the number of pairs of the designs given in section 5.2 , especially when n is large. When $n = 3$ the number of pairs is smaller than ND^*. Therefore we will exclude this case. In section 5.4.1 a D-optimal design for $n = 2$ is given with 15 pairs. Section 5.4.2 contains some general remarks and results. In section 5.4.3 and 5.4.4 we discuss the cases $n = 5$ and $n = 4$.

5.4.1. A discrete D-optimal design with 15 pairs when $n=2$

As a result of the proof of the D-optimality of the design given in section 5.2, the set of pairs of any discrete D-optimal design is contained in the set of 20 pairs of the D-optimal design given in that section. These 20 pairs are given in figure 5.2.6. The information matrix M of a discrete D-optimal design is denoted by (4.1.5). We shall construct a D-optimal design with 15 pairs by choosing new weights τ_i, $1 \leqslant i \leqslant 20$ in such a way that five of them are zero, whereas $0 \leqslant \tau_i \leqslant 1$ for all i with $1 \leqslant i \leqslant 20$.
Further

$$\sum_{i=1}^{20} \tau_i = 1 \quad , \tag{5.4.1}$$

and

$$\sum_{i=1}^{20} \tau_i M(\epsilon_i) = M \quad , \tag{5.4.2}$$

where $M(\epsilon_i)$ is the information matrix of the i-th pair of the design. The pairs are numbered in the order in which they are given in figure 5.2.6. So the pair $((1,1),(1,-1))$ is given number 1 and weight τ_1, and the pair $((-1,1),(-w_2,-1))$ is given number 20 and weight τ_{20}, etc. We define

$$\begin{aligned}\overline{M} = (&M_{11},M_{22},M_{55},M_{33},M_{44},M_{34},M_{12},M_{13},M_{14},M_{23},M_{24},\\ &M_{15},M_{25},M_{35},M_{45})' \quad ,\end{aligned} \tag{5.4.3}$$

so

$$\overline{M} = (p\ ,p\ ,z\ ,s+t\ ,s+t\ ,t\ ,0,0,0,0,0,0,0,0,0)' \quad , \tag{5.4.4}$$

and

$$\tau = (\tau_1,\tau_2,\ .\ .\ .\ ,\tau_{20})' \ . \tag{5.4.5}$$

Now the equation (5.4.2) can be rewritten as the following system of 15 equations

$$\overline{M} = B\ \tau \quad , \tag{5.4.6}$$

where

$$
B=\left|\begin{array}{c|c|cc}
0\;4\;4\;0 & a_1^2(1\;1\;1\;1\;1\;1\;1\;1) & 4(1\;1\;1\;1) & a_2^2(1\;1\;1\;1) \\
4\;0\;0\;4 & a_1^2(1\;1\;1\;1\;1\;1\;1\;1) & a_2^2(1\;1\;1\;1) & 4(1\;1\;1\;1) \\
4\;4\;4\;4 & a_1^2b_1^2(1\;1\;1\;1\;0\;0\;0\;0) & b_2^2(1\;1\;1\;1) & b_2^2(1\;1\;1\;1) \\
\hline
 & a_1^2b_1^2(1\;1\;1\;1\;1\;1\;1\;1) & 0 & a_2^2b_2^2(1\;1\;1\;1) \\
 & a_1^2b_1^2(1\;1\;1\;1\;1\;1\;1\;1) & a_2^2b_2^2(1\;1\;1\;1) & 0 \\
 & a_1^2b_1^2(1\;1\;1\;1\;-1\;-1\;-1\;-1) & 0 & 0 \\
\hline
 & a_1^2(0\;0\;0\;0\;-1\;1\;1\;-1) & 2a_2(1\;1\;-1\;-1) & 2a_2(-1\;-1\;1\;1) \\
 & a_1^2b_1(1\;-1\;1\;-1\;1\;-1\;1\;-1) & 0 & a_2^2b_2(1\;-1\;1\;-1) \\
 & a_1^2b_1(1\;-1\;1\;-1\;-1\;1\;-1\;1) & 2a_2b_2(1\;-1\;-1\;1) & 0 \\
 & a_1^2b_1(1\;-1\;-1\;1\;-1\;-1\;1\;1) & 0 & 2a_2b_2(-1\;1\;1\;-1) \\
 & a_1^2b_1(1\;-1\;-1\;1\;1\;1\;-1\;-1) & a_2^2b_2(1\;-1\;1\;-1) & 0 \\
\hline
0\;4\;-4\;0 & & 2b_2(1\;-1\;1\;-1) & a_2b_2(-1\;1\;1\;-1) \\
4\;0\;0\;-4 & & a_2b_2(1\;-1\;1\;-1) & 2b_2(1\;-1\;1\;-1) \\
\hline
 & a_1^2b_1^2(1\;1\;-1\;-1\;0\;0\;0\;0) & 0 & a_2b_2^2(-1\;-1\;1\;1) \\
 & a_1^2b_1^2(1\;1\;-1\;-1\;0\;0\;0\;0) & a_2b_2^2(1\;1\;-1\;-1) & 0
\end{array}\right| ,
$$

with $a_i = (1-w_i)$ and $b_i = (1+w_i)$, $i=1,2$. By investigating the structure of the information matrix, one can show that the first 6 of these 15 equations are equivalent with the following 6:

$$
\begin{aligned}
&\tau_1 + \tau_4 = 2\nu , \\
&\tau_2 + \tau_3 = 2\nu , \\
&\tau_5 + \tau_6 + \tau_7 + \tau_8 = 4\mu , \\
&\tau_9 + \tau_{10} + \tau_{11} + \tau_{12} = 4\lambda , \\
&\tau_{13} + \tau_{14} + \tau_{15} + \tau_{16} = 4\rho , \\
&\tau_{17} + \tau_{18} + \tau_{19} + \tau_{20} = 4\rho ,
\end{aligned}
\tag{5.4.7}
$$

where ν, μ, λ and ρ are the weights corresponding to the discrete D-optimal design given in section 5.2. From this it follows that for any D-optimal design at least one of the pairs of each of the 6 subsets, defined by the 6 equations above, has a positive weight. From (5.4.7) it is clear that condition (5.4.2) is satisfied. Now we have a set of 15 equations -the 6 equations of (5.4.7) and the last 9 equations of (5.4.6)- in 20 variables τ_i .

We choose $\tau_3 = \tau_4 = \tau_6 = \tau_{10} = \tau_{11} = 0$. Then we obtain

$$\tau_1 = 2\nu = 0.04960 \ ,$$

$$\tau_2 = 2\nu = 0.04960 \ ,$$

$$\tau_3 = 0 \ ,$$

$$\tau_4 = 0 \ ,$$

$$\tau_5 = 2\mu - 2\lambda \left[4\frac{(1+\nu_1)^2}{(1+\nu_2)^2} - 1\right]^{-1} = 0.04673 \ ,$$

$$\tau_6 = 0 \ ,$$

$$\tau_7 = \tau_8 = \mu + \lambda \left[4\frac{(1+\nu_1)^2}{(1+\nu_2)^2} - 1\right]^{-1} = 0.06906 \ ,$$

$$\tau_9 = \frac{8\nu(1-\nu_2)^2}{(1-\nu_1)(1-\nu_1)^2(3-\nu_2)(1+\nu_2)} - \mu + \lambda \left[2 + \left(4\frac{(1+\nu_1)^2}{(1+\nu_2)^2} - 1\right)^{-1}\right] = 0.07850 \ ,$$

$$\tau_{10} = \tau_{11} = 0 \ ,$$

$$\tau_{12} = \frac{-8\nu(1-\nu_2)^2}{(1-\nu_1)(1-\nu_1)^2(3-\nu_2)(1+\nu_2)} + \mu + \lambda \left[2 - \left(4\frac{(1+\nu_1)^2}{(1+\nu_2)^2} - 1\right)^{-1}\right] = 0.04050 \ ,$$

$$\tau_{15} = \tau_{19} = \rho - \frac{2\nu}{(1+\nu_2)^2} + \mu \frac{(1-\nu_1)(1-\nu_1)^2}{2(1-\nu_2)^2} - \lambda \frac{(1-\nu_1)(1-\nu_1)^2}{2(1-\nu_2)} \frac{1}{2(1+\nu_1)-(1+\nu_2)} = 0.02864 \ ,$$

$$\tau_{16} = \tau_{20} = \rho + \frac{2\nu}{(1+\nu_2)^2} - \mu \frac{(1-\nu_1)(1-\nu_1)^2}{2(1-\nu_2)^2} - \lambda \frac{(1-\nu_1)(1-\nu_1)^2}{2(1-\nu_2)} \frac{1}{2(1+\nu_1)+(1+\nu_2)} = 0.08106 \ ,$$

$$\tau_{17} = \tau_{13} = \rho - \frac{2\nu}{(1+\nu_2)^2} - \mu \frac{(1-\nu_1)(1-\nu_1)^2}{2(1-\nu_2)^2} + \lambda \frac{(1-\nu_1)(1-\nu_1)^2}{2(1-\nu_2)} \frac{1}{2(1+\nu_1)-(1+\nu_2)} = 0.06569 \ ,$$

$$\tau_{18} = \tau_{14} = \rho + \frac{2\nu}{(1+\nu_2)^2} + \mu \frac{(1-\nu_1)(1-\nu_1)^2}{2(1-\nu_2)^2} + \lambda \frac{(1-\nu_1)(1-\nu_1)^2}{2(1-\nu_2)} \frac{1}{2(1+\nu_1)+(1+\nu_2)} = 0.12309 \ .$$

All weights are between 0 and 1. So, we have found a discrete D-optimal design with 15 pairs. However, this design is not very useful for the construction of exact designs: the weights have 9 different values, whereas in an exact design consisting of these 15 pairs all these pairs have the same weights. The information matrix of such a design does not have the structure given in (4.1.5).

5.4.2. Half-replicates and quarter-replicates of $S((u,v))$.

In this section some general remarks are made concerning the reduction of the number of pairs of the designs of the type given in section 5.2. We shall consider the reduction of the number of pairs of the set $S((u,v))$ in general and of the set $S(k_1,k_2)$ in particular. As we have seen in (4.2.16), there is a relation between the design matrix of the set $S((u,v))$ and the design matrix of a 2^n-factorial experiment, where all interactions between three or more factors are assumed negligible. The method to construct fractional factorial experiments can be used to reduce the numbers of pairs of $S((u,v))$ as follows. Let a half-replicate of a 2^n-factorial experiment exists, for which all main effects and all two-factor interactions are clear of one another. Now, by using the expressions (4.2.16) and (4.2.18) it is easy to see that a design can be constructed consisting of 2^{n-1} pairs of $S((u,v))$ and having an information matrix equal to $\frac{1}{2}M((u,v))$. The designmatrix $\bar{D}$ of this set of 2^{n-1} pairs is

$$\bar{D} = \bar{X}_1(n)(U - V) \ . \tag{5.4.8}$$

Here U and V are as defined in (4.2.17) and $\bar{X}_1(n)$ consists of the rows of $X_1(n)$ which are related to the pairs chosen in the half-replicate of the 2^n-factorial. A method to construct fractional factorial experiments is given in chapter 10 of Davies (1963). As is pointed out there a relation exists between fractional factorial experiments and confounding. When a design is confounded in blocks, any block constitutes a fractional factorial design and any block can be obtained by applying a set of defining contrasts. So, when a design is confounded in four blocks any block constitutes a quarter-replicate. However, some effects and (higher-order) interactions are confounded. To construct a half-replicate of $S((u,v))$ it is necessary to construct a half-replicate for which all main effects and all two-factor interactions, which are measured in the set $S((u,v))$, are clear of one another. A half-replicate of a 2^n-factorial experiment for which all main effects and $\binom{n}{2}$ two-factor interactions are clear of one another can be found for $n \geqslant 5$. We give the defining contrast of the principal block of the corresponding confounded design for $n = 5, 6, 7$. See also chapter 10 of Davies (1963).

Table 5.4.2
Defining contrast of a half-replicate of a 2^n-factorial,for which all main effects and all two-factor interactions are clear of one another

n	Defining contrast	Number of pairs	Principal block
5	I,- ABCDE	16	All treatment combinations for
6	I, ABCDEF	32	which the number of letters con-
7	I,- ABCDEFG	64	stituting that combination is even.

When $n = 5$, the principal block, for example, consists of (1), ab, ac, bc, ad, bd, cd, ae, be, ce, de, abcd, abce, abde, acde, bcde.

Remark

We did not discuss the matrix K in $X_1(n)$, which might disturb the orthogonality of the design matrix of the half-replicate of $S((u,v))$. However, a column of K consists of +1's, and therefore it is orthogonal to the other columns of the design matrix of the half-replicate of the 2^n-factorial, each column having the same number of +1's and -1's. Actually, a column of the matrix K plays the same role as the constant factor in the 2^n-factorial experiment. $\square$

One might be tempted to construct a quarter-replicate of a 2^7-factorial experiment. Since the number of main effects and two order-interactions is equal to 28, which is less than 32, a quarter-replicate might be found for which the main effects are clear of one another. However, this is not possible. Choose for example as defining contrasts I, ABCDE, DEFG, ABCFG. Note that the product of ABCDE and DEFG is equal to the last defining contrast where $D^2 = E^2 = I$, as usual. It is clear that we cannot do better than this, because if a letter is added to the four-factor interaction the product with one of the other will be a four-factor interaction. So in every set of defining contrasts a four-factor interaction is contained. This means that 3 two-factor interactions are confounded with 3 other two-factor interactions. In this case DE = FG, DF = EG and DG = EF .
Let us now consider the reduction of the number of pairs of $S(k_1,k_2)$. In general the number of pairs of a half-replicate of $S((u,v))$ is 2^{n-1}. However, if $|u_i| = |v_i| = 1$ for all i, $1 \leqslant i \leqslant n$, then the number of pairs of $S((u,v))$ is equal to 2^{n-1} since all pairs occur twice. So at first sight it seems that nothing has been gained. However, by investigating the design more carefully, some results can be achieved. We shall discuss this for $n = 5$, 6 and 7. $S(k_1,k_2)$ consists of $\binom{n}{k_1}$ sets of the type $S((u,v))$, where $|u_i| = |v_i| = 1$ for all i, $1 \leqslant i \leqslant n$. We apply the method described above to construct half-replicates

of the sets $S(k_1,k_2)$.

i) First we consider the case $n = 5$.

We use the defining contrasts given in table 5.4.2 to obtain half-replicates of the sets $S((u,v))$ of which $S(k_1,k_2)$ is composed. By investigating these half-replicates of the sets $S((u,v))$ we see that in the case of $S(1,4)$ and $S(3,2)$ all pairs occur twice in these half-replicates, since all treatment combinations with an even number of letters occur in the principal block. The other treatment combinations occur in the second block. The objects of any pair of $S(1,4)$ or $S(3,2)$ are elements of the same block. For example (1) and ab occur in the principal block and the pair ((1),ab) is a pair of $S(3,2)$. So, by the method described above a half-replicate of $S(1,4)$ and of $S(3,2)$ is obtained. In the case of $S(0,5)$, $S(2,3)$ and $S(4,1)$ the objects of the principal block are compared with objects of the second block. Therefore, in these cases the number of pairs is not reduced by using this half-replicate. It is possible to reduce the number of pairs of $S(0,5)$ by using a quarter-replicate of a 2^5-factorial experiment, defined by the contrasts I, -BCE, -ADE, ABCD. In this quarter-replicate all main effects are clear of one another, but they are confounded with two-factor interactions. This does not affect the structure of the information matrix of the design, because two-factor interactions are not measured in $S(0,5)$. It is not possible to reduce the number of pairs of $S(2,3)$ by reducing the numbers of pairs of each subset $S((u,v))$ of which it is composed without confounding some main effects or two-factor interactions, which are measured in this set, with one another. However, it is possible to reduce the number of pairs of the set $S(2,3)$. This will be shown in section 5.4.3.

ii) $n = 6$

We consider the sets $S(k_1,k_2)$ and the sets $S((u,v))$ of which is composed. Using the defining contrast given in table 5.4.2 one can obtain half-replicates of the sets $S((u,v))$. By investigating these half-replicates it can be seen that in the cases $S(0,6)$, $S(2,4)$ and $S(4,2)$ pairs occur twice in these half-replicates. The objects of any pair of these sets occur in the same block. This does not hold in the cases $S(1,5)$, $S(3,3)$ and $S(5,1)$. In these cases other defining contrasts have to be used. Consider the defining contrasts I, -ABCDE. All main effects and two-factor interactions are clear of one another. The principal block consists of the treatment combinations mentioned in table 5.4.2, together with all treatment combinations that can be found by multiplying these combinations by f. Using these defining contrasts to construct half-replicates of the set $S((u,v))$ where $u = (-1,-1,-1,-1,-1,-1)'$ and $v = (-1,1,1,1,1,1)'$, we obtain half-replicates in which all pairs occur twice. The objects (1) and bcdef, for example, are elements of the principal block, and the pair ((1),bcdef) is an element of the set $S((-1,-1,-1,-1,-1,-1),(-1,1,1,1,1,1))$. Similarly, using e.g. I,-ABCDF as defining contrasts, one can obtain half-replicates of other subsets $S((u,v))$ of $S(1,5)$ in which all pairs occur twice. So, we have found a half-replicate of

$S(1,5)$. The same defining contrasts yield a half-replicate of $S(3,3)$. Therefore, summarizing the results in the case $n = 6$, we have found half-replicates for all $S(k_1,k_2)$ -cf. table 5.4.3.

iii) $n = 7$

We consider the quarter-replicate of a 2^7-factorial experiment given at the beginning of this section, with defining contrasts I, -ABCDE, DEFG, -ABCFG. It consists of the treatment combinations:

(1), ab, ac, bc, de, abde, acde, bcde, adf, bdf, cdf, abcdf, aef, bef, cef, abcef and all treatment combinations obtained by multiplying these combinations by fg, where $f^2 = 1$. In this quarter-replicate all main effects are clear of two-factor interactions, but three two-factor interactions are confounded with three other two-factor interactions: DE=FG, DF=EG and DG=EF. However, the sets $S((u,v))$ of which the set $S(k_1,k_2)$ is composed, measure k_1 main effects and k_1k_2 two-factor interactions. Therefore this quarter-replicate yields a quarter-replicate of the set $S((u,v))$ with $u = (-1,-1,-1,-1,-1,-1,-1)'$ and $v = (-1,-1,-1,1,1,1,1)'$, in which all main effects and two-factor interactions, that are measured, are clear of one another. Moreover, all pairs occur twice in this set. Using similar defining contrasts for the other subsets, a quarter-replicate can be obtained of $S(3,4)$. Similar methods yield quarter-replicates of the sets $S(k_1,k_2)$, the case $S(3,4)$ being the most difficult one, because 16 main effects and two-factor interactions are measured in this set.

In table 5.4.3 some results of this section are given.

Table 5.4.3
Summary of results concerning the reduction of the number of pairs of $S((u,v))$ and $S(k_1,k_2)$

Set	Number of pairs	Number of pairs after reduction
$S((u,v))$ with $n \geqslant 5$	2^n	2^{n-1}
$S(0,5)$	16	8
$S(1,4)$	80	40
$S(0,6)$	32	16
$S(1,5)$	192	96
$S(2,4)$	480	240
$S(3,3)$	640	320
$S(0,7)$	64	16
$S(1,6)$	448	124
$S(2,5)$	1344	336
$S(3,4)$	2240	560

5.4.3. Reduction of the number of pairs of discrete D-optimal designs for $n=4$ and $n=5$.

We consider the discrete D-optimal designs given in section 5.2. First we discuss the reduction of the number of pairs when $n = 5$.
The design given in section 5.2 consists of

i) $S(2,3)$ with $10\ 2^4 = 160$ pairs ,
ii) $SP(0,0,5;w_1)$ with $2^5 = 32$ pairs ,
iii) $SP_2(0,0,5;w_1)$ with $10\ 2^5 = 320$ pairs .

By the method given in section 5.4.2 half-replicates can be found of $SP(0,0,5;w_1)$ and $SP_2(0,0,5;w_1)$. This yields a D-optimal design with 336 pairs. But a further reduction of the number of pairs is possible. First we consider the set $SP_2(0,0,5;w_1)$. This set consists of the following subsets:

$$
\begin{aligned}
S_1 &= S((w_1,w_1,w_1,\ 1,\ 1),(\ 1,\ 1,\ 1,w_1,w_1))\ ,\\
S_2 &= S((w_1,w_1,\ 1,w_1,\ 1),(\ 1,\ 1,w_1,\ 1,w_1))\ ,\\
S_3 &= S((w_1,w_1,\ 1,\ 1,w_1),(\ 1,\ 1,w_1,w_1,\ 1))\ ,\\
S_4 &= S((w_1,\ 1,w_1,w_1,\ 1),(\ 1,w_1,\ 1,\ 1,w_1))\ ,\\
S_5 &= S((w_1,\ 1,w_1,\ 1,w_1),(\ 1,w_1,\ 1,w_1,\ 1))\ ,\\
S_6 &= S((w_1,\ 1,\ 1,w_1,w_1),(\ 1,w_1,w_1,\ 1,\ 1))\ ,\\
S_7 &= S((\ 1,w_1,w_1,w_1,\ 1),(w_1,\ 1,\ 1,\ 1,w_1))\ ,\\
S_8 &= S((\ 1,w_1,w_1,\ 1,w_1),(w_1,\ 1,\ 1,w_1,\ 1))\ ,\\
S_9 &= S((\ 1,w_1,\ 1,w_1,w_1),(w_1,\ 1,w_1,\ 1,\ 1))\ ,\\
S_{10} &= S((\ 1,\ 1,w_1,w_1,w_1),(w_1,w_1,\ 1,\ 1,\ 1))\ ,
\end{aligned}
$$

Each set S_i consists of 32 pairs. A quarter-replicate of each set can be found by using the defining contrasts I, CDE, ABD, ABCE. The following quarter-replicates of a 2^5-factorial experiment are obtained by using these defining contrasts:

(I): (1), ab, acd, bcd, ce, abce, ade, bde .
Defining contrasts I, -CDE, -ABD, ABCE .

(II): a, b, cd, abcd, ace, bce, de, abde .
Defining contrasts I, -CDE, ABD, -ABCE .

(III): c, abc, ad, bd, e, abe, acde, acde, bcde .
Defining contrasts I, CDE, -ABD, -ABCE .

(IV): ac, bc, d, abd, ae, be, cde, abcde .
Defining contrasts I, CDE, ABD, ABCE .

In these blocks some main effects and two-factor interactions are confounded:
C=DE, D=CE=AB, E=CD, A=BD, B=AD, AC=BE, AE=BC .
All other main effects and two-factor interactions are clear of one another and of the main effects and interactions given above. We compute the information matrices $M_{(I)}$, $M_{(II)}$, $M_{(III)}$ and $M_{(IV)}$. If all main effects and two-factor interactions would have been clear of one another, then the result would have been

$$
M_{(i)} = \tfrac{1}{4}\, 2^n \left[\begin{array}{c|c|c} I & & \\ \hline & I+J & \\ \hline & & I \end{array}\right],
$$

where i = I , II , III , IV . Now, due to the fact that some main effects and two-factor interactions are confounded, we have

$$
|(M_{(i)})_{k,l}| = 8 \quad ,\text{for } i = \text{I , II , III , IV} .
$$

where

$$
(k,l) \in \{\ (3,20),(4,19),(4,11),(11,19),(5,16),(1,15),(2,14),(12,18),(13,17)\ \} .
$$

The signs of $(M_{(i)})_{k,l}$ are given in the following table.

Table 5.4.4
Signs of $(M_{(i)})_{k,l}$

(k,l)	i:I	II	III	IV	confounded effects
(13,17)	+	-	-	+	BC , AE
(12,18)	+	-	-	+	AC , BE
(11,19)	+	-	-	+	AB , CE
(4,11)	-	+	-	+	D , AB
(2,14)	-	+	-	+	B , AD
(1,15)	-	+	-	+	A , BD
(5,16)	-	-	+	-	E , CD
(4,19)	-	-	+	-	D , CE
(3,20)	-	-	+	-	C , DE

These signs can be found as follows. $(M_{(i)})_{13,17}$ is related to BC and AE, which are confounded. The defining contrasts of (I) are I, -CDE, -ABD, ABCE. Therefore, BC = AE and $(M_{(I)})_{13,17} = +8$. Similarly we find $(M_{(II)})_{13,17} = -8$. Now we can compute the information matrices M_i of quarter-replicates of S_i . We define

$$\delta_{i,j} = \begin{cases} +1 & \text{,if the quarter-replicate } (i) \text{ or } (j) \text{ is chosen ,} \\ -1 & \text{,if not } (i) \text{ or } (j) \text{ is chosen.} \end{cases} \tag{5.4.9}$$

The expression (4.2.16) can be used to compute M_i . We find for example for S_1.

$$U = (w_1,w_1,w_1,1,1 \mid w_1^2,w_1^2,w_1^2,1,1 \mid w_1^2,w_1^2,w_1,w_1,w_1,w_1,w_1,w_1,1)'.$$

$$V = (1,1,1,w_1,w_1 \mid 1,1,1,w_1^2,w_1^2 \mid 1,1,w_1,w_1,w_1,w_1,w_1,w_1,w_1^2)'.$$

So

$$U-V = (w_1-1,\ w_1-1,\ w_1-1,\ 1-w_1, 1-w_1 \mid w_1^2-1,\ w_1^2-1,\ w_1^2-1,$$
$$1-w_1^2,\ 1-w_1^2 \mid w_1^2-1,\ w_1^2-1,\ w_1^2-1,\ 0,0,0,0,0,0,1-w_1^2)' ,$$

and

$$(M_1)_{13,17} = 0 ,$$

$$(M_1)_{4,11} = 8(1-w_1)(w_1^2-1)\delta_{II,III} ,$$

$$(M_1)_{3,20} = 8(w_1-1)(1-w_1^2)\delta_{III,IV} .$$

In table 5.4.5 the signs are given of the elements of M_i which are of interest.

Table 5.4.5

Signs of the important elements of M_i

i	(13,17)	(12,18)	(11,19)	(4,11)	(2,14)	(1,15)	(5,16)	(4,19)	(3,20)
1				$\delta_{II,IV}$					$\delta_{III,IV}$
2			$-\delta_{I,IV}$	$-\delta_{II,IV}$	$-\delta_{II,IV}$	$-\delta_{II,IV}$		$\delta_{III,IV}$	
3				$\delta_{II,IV}$			$\delta_{III,IV}$		
4		$-\delta_{I,IV}$			$\delta_{II,IV}$		$\delta_{III,IV}$		
5						$\delta_{II,IV}$		$\delta_{III,IV}$	
6	$-\delta_{I,IV}$				$\delta_{II,IV}$				$\delta_{III,IV}$
7	$-\delta_{I,IV}$					$\delta_{II,IV}$	$\delta_{III,IV}$		
8					$\delta_{II,IV}$			$\delta_{III,IV}$	
9		$-\delta_{I,IV}$				$\delta_{II,IV}$			$\delta_{III,IV}$
10			$-\delta_{I,IV}$	$\delta_{II,IV}$			$-\delta_{III,IV}$	$-\delta_{III,IV}$	$-\delta_{III,IV}$

Now we choose the following quarter-replicate of S_i.

Table 5.4.6

Choice of quarter-replicate of S_i

i	1	2	3	4	5	6	7	8	9	10
quarter-replicate (j)	I	I	I	I	IV	I	III	II	III	II

As can be seen by inspecting table 5.4.5 we have constructed a quarter-replicate of $SP_2(0,0,5;w_1)$ for which the information matrix is equal to $\frac{1}{4}MP_2(0,0,5;w_1)$.

A similar method can be used to reduce the number of pairs of $S(2,3)$ which consists of 160 pairs. First we consider the sets

$$
\begin{aligned}
T_1 &= S((-1,-1,-1,\ 1,\ 1),(\ 1,\ 1,\ 1,\ 1,\ 1))\,,\\
T_2 &= S((-1,-1,\ 1,-1,\ 1),(\ 1,\ 1,\ 1,\ 1,\ 1))\,,\\
T_3 &= S((-1,-1,\ 1,\ 1,-1),(\ 1,\ 1,\ 1,\ 1,\ 1))\,,\\
T_4 &= S((-1,\ 1,-1,-1,\ 1),(\ 1,\ 1,\ 1,\ 1,\ 1))\,,\\
T_5 &= S((-1,\ 1,-1,\ 1,-1),(\ 1,\ 1,\ 1,\ 1,\ 1))\,,\\
T_6 &= S((-1,\ 1,\ 1,-1,-1),(\ 1,\ 1,\ 1,\ 1,\ 1))\,,\\
T_7 &= S((\ 1,-1,-1,-1,\ 1),(\ 1,\ 1,\ 1,\ 1,\ 1))\,,\\
T_8 &= S((\ 1,-1,-1,\ 1,-1),(\ 1,\ 1,\ 1,\ 1,\ 1))\,,\\
T_9 &= S((\ 1,-1,\ 1,-1,-1),(\ 1,\ 1,\ 1,\ 1,\ 1))\,,\\
T_{10} &= S((\ 1,\ 1,-1,-1,-1),(\ 1,\ 1,\ 1,\ 1,\ 1))\,,
\end{aligned}
$$

In each of these sets every pair occurs twice. A quarter-replicate (I), (II), (III) or (IV) of each set T_i is chosen. In a similar way as in the method described above we find for the signs of the important elements of the information matrices M_i of the quarter-replicates:

Table 5.4.7
The signs of the important elements of M_i

i	(13,17)	(12,18)	(11,19)	(4,11)	(2,14)	(1,15)	(5,16)	(4,19)	(3,20)
1					$\delta_{II,IV}$	$\delta_{II,IV}$			
2	$\delta_{I,IV}$	$\delta_{I,IV}$							
3					$\delta_{II,IV}$	$\delta_{II,IV}$			
4	$\delta_{I,IV}$		$\delta_{I,IV}$	$\delta_{II,IV}$		$\delta_{II,IV}$		$\delta_{III,IV}$	$\delta_{III,IV}$
5							$\delta_{III,IV}$		$\delta_{III,IV}$
6		$\delta_{I,IV}$	$\delta_{I,IV}$	$\delta_{II,IV}$		$\delta_{II,IV}$	$\delta_{III,IV}$	$\delta_{III,IV}$	
7		$\delta_{I,IV}$	$\delta_{I,IV}$	$\delta_{II,IV}$	$\delta_{II,IV}$			$\delta_{III,IV}$	$\delta_{III,IV}$
8							$\delta_{III,IV}$		$\delta_{III,IV}$
9	$\delta_{I,IV}$		$\delta_{I,IV}$	$\delta_{II,IV}$	$\delta_{II,IV}$		$\delta_{III,IV}$	$\delta_{III,IV}$	
10	$\delta_{I,IV}$	$\delta_{I,IV}$							

Now we choose the following quarter-replicate of T_i.

Table 5.4.8
Choice of quarter-replicate of T_i

i	1	2	3	4	5	6	7	8	9	10
quarter-replicate (j)	I	I	II	III	II	II	I	III	IV	II

This yields a half-replicate of $S(2,3)$. We have found a discrete D-optimal design consisting of

i) a half-replicate of $S(2,3)$: 80 pairs ,
ii) a half-replicate of $SP(0,0,5;w_1)$: 16 pairs ,
iii) a quarter-replicate of $SP_2(0,0,5;w_1)$: 80 pairs ,
In total : 176 pairs .

This number is smaller than 210, the number ND^* given in table 5.4.1.

Now we consider the case $n = 4$.
The design given in section 5.2 consists of

i) $S(2,2)$ with $6\ 2^3 =$ 48 pairs ,
ii) $SP(0,0,4;w_1)$ with $2^4 =$ 16 pairs ,
iii) $SP_2(0,0,4;w_1)$ with $3\ 2^4 =$ 48 pairs ,
iv) $SP(1,2,1;w_2)$ with $12\ 2^4 =$ 192 pairs ,
In total : 304 pairs .

First we consider the set $SP(1,2,1;w_2)$. This set consists of the following sets:

$S_1 = ((1,1,1,1),(\ 1,-1,-1,\ w_2)),$
$S_2 = ((1,1,1,1),(-1,\ 1,-1,\ w_2)),$
$S_3 = ((1,1,1,1),(-1,-1,\ 1,\ w_2)),$
$S_4 = ((1,1,1,1),(\ 1,-1,w_2,-1\ )),$
$S_5 = ((1,1,1,1),(-1,\ 1,w_2,-1\ )),$
$S_6 = ((1,1,1,1),(-1,-1,w_2,\ 1\ )),$
$S_7 = ((1,1,1,1),(\ 1,\ w_2,-1,-1\ )),$
$S_8 = ((1,1,1,1),(-1,\ w_2,\ 1,-1\ )),$
$S_9 = ((1,1,1,1),(-1,\ w_2,-1,\ 1\ )),$
$S_{10} = ((1,1,1,1),(\ w_2,\ 1\ ,-1,-1\ )),$
$S_{11} = ((1,1,1,1),(\ w_2,-1\ ,\ 1,-1\ )),$
$S_{12} = ((1,1,1,1),(\ w_2,-1\ ,-1,\ 1\ )).$

All pairs of $SP(1,2,1;w_2)$ have weights ρ. It can be shown that the following design has the same information matrix:
-all pairs of S_1, S_6, S_8 and S_{10} with weights 2ρ ,
-all pairs of S_2, S_4, S_9 and S_{11} with weights ρ ,
This design consists of 128 pairs, but it is not very useful for practical applications for the following reason. If one wants to construct an exact design consisting of these pairs and having an information materix of type (4.1.5), then the pairs of S_1, S_6, S_8 and S_{10} must be chosen twice. Therefore no reduction of the number of pairs is achieved when constructing exact designs. We will construct a half-replicate of $SP(1,2,1;w_2)$ using a method similar to the one used in the case $n = 5$. A half-replicate of each set S_1 can be found by using the defining contrast ABCD. We find half-replicates of a 2^4-factorial experiment:

(I): (1),ab,ac,bc,ad,bd,cd,abcd.
Defining contrasts I, ABCD .

(II): a,b,c,abc,d,abd,acd,bcd.
Defining contrasts I, -ABCD .

The confounded interactions are BC = AD, AC = BD, AB = CD . Therefore, in computing the information matrix $M_{(I)}$ and $M_{(II)}$, the following elements are important:

Table 5.4.9
The signs of $(M_{(i)})_{k,l}$

(k,l)	i: I	II	Confounded interactions
(11,12)	+	-	AD , BC
(10,13)	+	-	AC , BD
(9,14)	+	-	AB , CD

We define

$$\delta_I = \begin{cases} +1 & \text{,if the half-replicate I is chosen,} \\ -1 & \text{,if the half-replicate II is chosen.} \end{cases}$$

Table 5.4.10

The signs of the important elements of M_i

i	(11,12)	(10,13)	(9,14)
1		δ_1	δ_1
2	δ_1		δ_1
3	δ_1	δ_1	
4	δ_1		δ_1
5		δ_1	δ_1
6	δ_1	δ_1	
7	δ_1	δ_1	
8		δ_1	δ_1
9	δ_1		δ_1
10	δ_1	δ_1	
11	δ_1		δ_1
12		δ_1	δ_1

We can choose the following half-replicates of S_i: I for $i = 1,2,3,4,5,6$ and II for $i = 7,8,9,10,11,12$. This gives a half-replicate of $SP(1,2,1;w_2)$, for which the information matrix is equal to $\frac{1}{2}MP(1,2,1;w_2)$. We consider the set $SP_2(0,0,4;w_1)$. It is not possible to construct a half-replicate of $SP_2(0,0,4;w_2)$ having an information matrix of type (4.1.5). Therefore, we consider the following D-optimal design.

i) the pairs of $S(2,2)$ with weights $\nu_2 = 0.00711$,
ii) the pairs of $SP(0,0,4;w_1)$ with weights $\dot{\mu} = 0.00186$,
iii) the pairs of $SP_1(0,0,4;w_1)$ with weights $\dot{\lambda} = 0.00492$,
iv) the pairs of $SP(1,2,1;w_2)$ with weights $\rho = 0.00162$.

The number of pairs of $SP_1(0,0,4;w_1)$ is equal to 64, which is 16 more than the number of pairs of $SP_2(0,0,4;w_1)$. However, it is possible to construct a half-replicate of $SP_1(0,0,4;w_1)$, which consists of the sets

$$T_1 = S((1,\ 1,\ 1,w_1),(w_1,w_1,w_1,\ 1)),$$
$$T_2 = S((1,\ 1,w_1,\ 1),(w_1,w_1,\ 1,w_1)),$$
$$T_3 = S((1,w_1,\ 1,\ 1),(w_1,\ 1,w_1,w_1)),$$
$$T_4 = S((w_1,\ 1,\ 1,\ 1),(1,w_1,w_1,w_1)).$$

Choosing the half-replicate (I) for each set T_i we obtain a half-replicate of $SP_1(0,0,4;w_1)$.

Finally we consider the set $S(2,2)$. This set consists of

$$V_1 = S((1,1,1,1),(-1,-1,\ \ 1,\ \ 1))\ ,$$
$$V_2 = S((1,1,1,1),(-1,\ \ 1,-1,\ \ 1))\ ,$$
$$V_3 = S((1,1,1,1),(-1,\ \ 1,\ \ 1,-1))\ ,$$
$$V_4 = S((1,1,1,1),(\ \ 1,-1,-1,\ \ 1))\ ,$$
$$V_5 = S((1,1,1,1),(\ \ 1,-1,\ \ 1,-1))\ ,$$
$$V_6 = S((1,1,1,1),(\ \ 1,\ \ 1,-1,-1))\ ,$$

In each set V_i the pairs occur twice. Therefore, we need a quarter-replicate of v_i to obtain a half-replicate of $S(2,2)$. Consider the defining contrasts I, D, ABC, ABCD . They yield the following quarter-replicates of a 2^4- factorial experiment.

		Defining contrasts
(I)	: (1), ab, ac, bc	I, -D, -ABC, ABCD ,
(II)	: a, b, c, abc	I, -D, ABC, -ABCD ,
(III)	: d, abd, acd, bcd	I, D, -ABC, -ABCD ,
(IV)	: ad, bd, cd, abcd	I, D, ABC, ABCD .

By methods similar to the ones above it can be seen that a half-replicate of $S(2,2)$ for which the information matrix is equal to $\frac{1}{2}M(2,2)$, can be found by choosing the quarter-replicates given in table 5.4.11.

Table 5.4.11

Choice of quarter-replicate of V_i

i	1	2	3	4	5	6
quarter-replicate (j)	IV	I	II	IV	II	II

A discrete D-optimal design has been constructed consisting of

i) a half-replicate of	$S(2,2)$	: 24 pairs ,
ii)	$SP(0,0,4;w_1)$	: 16 pairs ,
iii) a half-replicate of	$SP_1(0,0,4;w_1)$	: 32 pairs ,
iv) a half-replicate of	$SP(1,2,1;w_2)$	: 96 pairs ,
	In total	: 168 pairs .

This number is larger than 105, the number ND^* given in table 5.4.1. Therefore, a further reduction can be achieved. However, this seems to entail many different weights, which is not attractive for practical applications.

5.5. Exact designs when $n = 2, 3, 4, 5$.

5.5.1. General remarks

In this section exact designs are constructed for $n = 2, 3, 4, 5$. Let ϵ be a discrete D-optimal design. As we have seen in sections 5.2 and 5.3 the following holds.

If n is odd, then the set of pairs of the design ϵ is contained in the union of the following sets:

$S(\frac{1}{2}(n-1), \frac{1}{2}(n+1))$,

$SP(0,0,n; w_1)$,

all $SP_l(0,0,n; w_1)$ with $1 \leqslant l \leqslant n$,

where w_1 has the value given in table 5.2.7.

If $n = 2, 4$, then the set of pairs of the design ϵ is contained in the union of the sets

$S(\frac{1}{2}n, \frac{1}{2}n)$,

$SP(0,0,n; w_1)$,

all $SP_l(0,0,n; w_1)$ with $1 \leqslant l \leqslant n$,

$SP(\frac{1}{2}n - 1, \frac{1}{2}n, 1; w_2)$,

where w_1 and w_2 have the values given in table 5.2.7.

It seems useful to consider exact designs, for which the set of pairs is also contained in this union of sets. However, the pairs cannot have the same weights in an exact design as in a discrete design. This can be partly compensated by choosing other values for w_1 and w_2 than the ones given in table 5.2.7. For this reason and in the light of the proof given in section 5.3 it is useful to define the following sets.

Definition 5.5.1

$S(0,0,l_1,l_2; w_1,w_2) := S((x, y))$,

$SP((0,0,l_1,l_2; w_1,w_2) := SP((x, y))$,

where

$x = (1, \ldots, 1, w_1, \ldots, w_1)'$,

$y = (w_2, \ldots, w_2, 1, \ldots, 1)'$,

l_1 *is the number of* w_1*'s in* x ,

$l_1 + l_2 = n$.

In general $SP(0,0,l_1,l_2; w_1,w_2)$ contains $\binom{n}{l_1}2^n$ pairs. If $w_1 = w_2$, then

$SP(0,0,l_1,l_2;\, w_1,w_2) = SP_l(0,0,n\,;\, w_1)$. The information matrices of the sets given in definition 5.5.1 are denoted by

$$M(0,0,l_1,l_2;\, w_1,w_2)$$

and $\quad MP_l(0,0,l_1,l_2;\, w_1,w_2)$.

An expression for $MP(0,0,l_1,l_2;\, w_1,w_2)$ is given in the following lemma.

Lemma 5.5.2

$$MP(0,0,l_1,l_2;\, w_1,w_2) = 2^n \left|\begin{array}{c|c|c} pI & & \\ \hline & sI+tJ & \\ \hline & & zI \end{array}\right| ,$$

where (5.5.1)

$$\begin{aligned} p &= \binom{n-1}{l_1-1} g_1 + \binom{n-1}{l_2-1} g_2 , \\ z &= \binom{n-2}{l_1-2} g_1h_1 + \binom{n-2}{l_2-2} g_2h_2 + 2\binom{n-2}{l_1-1} (w_1-w_2)^2 , \\ t &= \binom{n-2}{l_1-2} g_1h_1 + \binom{n-2}{l_2-2} g_2h_2 - 2\binom{n-2}{l_1-1} g_{12}g_{22} , \\ s+t &= \binom{n-1}{l_1-1} g_1h_1 + \binom{n-1}{l_2-1} g_2h_2 , \end{aligned}$$

with

$$g_i = (1-w_i)^2 ,\; h_i = (1+w_i)^2 ,\; g_{i2} = (1-w_i^2) .$$

Proof

The correctness of the equations (5.5.1) can be proved by use of (4.2.20). This yields

$$\begin{aligned} p &= \binom{n}{l_1} [l_1 g_1 + l_2 g_2]/ n , \\ z &= \binom{n}{l_1} [\binom{l_1}{2} g_1h_1 + \binom{l_2}{2} g_2h_2 + l_1l_2(w_1-w_2)^2]/ \binom{n}{2} , \\ t &= \binom{n}{l_1} [\binom{l_1}{2} g_1h_1 + \binom{l_2}{2} g_2h_2 - l_1l_2\, g_{11}g_{22}]/ \binom{n}{2} , \\ s+t &= \binom{n}{l_1} [l_1 g_1h_1 + l_2 g_2h_2]/ n , \end{aligned}$$

equivalent to (5.5.1). □

We choose exact designs for $n = 2, 3, 4, 5$. If $n = 2$, we choose exact designs with pairs contained in the union of the following sets

-$S(1,1)$,
-$SP(0,0,2;\, w_1)$,
-$SP(0,0,1,1;\, w_2,w_3)$,
-$SP(0,1,1;\, w_4)$.

If $n = 4$, these sets are

-$S(2,2)$,
-$SP(0,0,4;\, w_1)$,
-$SP(0,0,2,2;\, w_2,w_3)$, or $SP(0,0,1,3;\, w_2,w_3)$,
-$SP(1,2,1;\, w_4)$.

If $n = 3, 5$, these sets are

-$S(\frac{1}{2}(n-1),\frac{1}{2}(n+1))$,
-$SP(0,0,n;\, w_1)$,
-$SP(0,0,\frac{1}{2}(n-1),\frac{1}{2}(n+1);\, w_2,w_3)$.

The values of w_1, w_2, w_3 and w_4 have to be chosen according to some criterion. We choose the $\mathring{G}$-criterion and the D-criterion. Exact designs are given in section 5.5.2 for the cases $n = 3, 5$ and in section 5.5.3 for the cases $n = 2, 4$. In this section a lemma is given that can be used when the $\mathring{G}$-criterion is applied. The maximal value of the variance function has to be computed. According to the discussion in section 5.3 the values $d(k_1,k_2,l_1,l_2)$ have to be computed. In many cases the maximal value is one of the values d_1, d_2, d_3 if n is odd and one of the values d_1, d_2, d_3, d_4 if n is even, where

$$
\begin{aligned}
d_1 &= \begin{cases} d(\frac{1}{2}n,\frac{1}{2}n) & \text{,if } n \text{ even ,} \\[2ex] d(\frac{1}{2}(n-1),\frac{1}{2}(n+1)) & \text{,if } n \text{ odd ,} \end{cases} \\
d_2 &= d(0,0,0,n) , \\
d_3 &= \begin{cases} d(0,0,\frac{1}{2}n,\frac{1}{2}n) & \text{,if } n \text{ even ,} \\[2ex] d(0,0,\frac{1}{2}(n-1),\frac{1}{2}(n+1)) & \text{,if } n \text{ odd ,} \end{cases} \\
d_4 &= d(\tfrac{1}{2}n-1,\tfrac{1}{2}n,0,1) \text{ ,if } n \text{ even .}
\end{aligned}
\tag{5.5.2}
$$

The maximal value has to be minimized. The following lemma is useful in achieving this.

Lemma 5.5.3

Let l_1 and l_2 be fixed with $l_1 + l_2 = n$ and let ϵ be a design with covariance matrix of type (4.1.6). Let v_1 be the value that maximizes $d(0,0,0,n)$, and (v_2,v_3) the pair that maximizes $d(0,0,l_1,l_2)$.
Then

$$d(0,0,0,n) = d(0,0,l_1,l_2)$$

if and only if

$$\delta = -4\xi \text{ and } v_1 = v_2 = v_3 .$$

Proof

i) Assume $\delta = -4\xi$ and $v_1 = v_2 = v_3$. By applying lemma 5.2.1 it can be shown that $d(0,0,0,n) = d(0,0,l_1,l_2)$.

ii) Assume $d(0,0,0,n) = d(0,0,l_1,l_2)$. Let $d(k,k_2,l_1,l_2;w_1,w_2)$ denote the function given in (5.3.10). So $d(0,0,l_1,l_2) = d(0,0,l_1,l_2;v_2,v_3)$. In the notation of (5.2.8) we have $d(0,0,0,n) = d(0,0,n;v_1)$. We shall show that $\delta + 4\xi = 0$ by proving that the statements $\delta + 4\xi < 0$ and $\delta + 4\xi > 0$ are both false.

a) Suppose $\delta + 4\xi < 0$.
The maximal value of $d(0,0,l_1,l_2;v_2,v_3)$ is $d(0,0,l_1,l_2)$. Therefore,

$$d(0,0,l_1,l_2;v_2,v_3) \geqslant d(0,0,l_1,l_2;v_1,v_1) .$$

So, using (5.3.10), we find

$$d(0,0,l_1,l_2;v_2,v_3) > d(0,0,l_1,l_2;v_1,v_1) + l_1l_2(\delta + 4\xi)(1-v_1^2)^2$$

$$= l_1\gamma(1-v_1)^2 + l_2\gamma(1-v_1)^2 + \binom{l_1}{2}\delta(1-v_1^2)^2 + \binom{l_2}{2}\delta(1-v_1^2)^2$$

$$+ l_1\alpha(1-v_1^2)^2 + l_2\alpha(1-v_1^2)^2 + \xi[l_1(1-v_1^2) - l_2(1-v_1^2)]^2$$

$$+ l_1l_2\delta(1-v_1^2)^2 + 4l_1l_2\xi(1-v_1^2)^2$$

$$= n\gamma(1-v_1)^2 + \binom{n}{2}\delta(1-v_1^2)^2 + n\alpha(1-v_1^2)^2$$

$$+ \xi[l_1(1-v_1^2) + l_2(1-v_1^2)]^2 = d(0,0,0,n) .$$

This contradicts $d(0,0,0,n) = d(0,0,l_1,l_2)$.

b) Suppose $\delta + 4\xi > 0$.
Similarly we have

$$d(0,0,0,n) > d(0,0,0,n) - l_1l_2(\delta + 4\xi)(1-v_2^2)(1-v_3^2)$$

$$\geqslant l_1\gamma(1-v_2)^2 + l_2\gamma(1-v_3)^2 + \binom{l_1}{2}\delta(1-v_2^2)^2 + \binom{l_2}{2}\delta(1-v_3^2)^2$$

$$+ l_1l_2\delta(1-v_2v_3)^2 + l_1\alpha(1-v_2^2)^2 + l_2\alpha(1-v_3^2)^2$$

$$+ \xi\,[l_1(1-v_2^2) + l_2(1-v_3^2)]^2 - l_1 l_2\,(\delta + 4\xi)\,(1-v_2^2)(1-v_3^2)$$

$$= d\,(0,0,l_1,l_2;\, v_2,v_3)\,.$$

This contradicts $d\,(0,0,0,n) = d\,(0,0,l_1,l_2)$ and completes the proof. □

5.5.2. Exact designs when $n = 3, 5$.

Exact designs are constructed as follows.
If $n = 3$, we choose

i) n_1 times the pairs of $S\,(1,2)$,
ii) n_2 times the pairs of $SP\,(0,0,3;\, w_1)$,
iii) n_3 times the pairs of $SP\,(0,0,1,2;\, w_2,w_3)$.

The information matrix of this design has the structure of (4.1.5) and is determined by

(5.5.3)

$$\begin{aligned}
p &= [32n_1 + 8n_2\,g_1 + 8n_3(g_2 + 2g_3)]\,/\,N\,,\\
s &= [\;0 + 0 + 8n_3(g_{22} + g_{32})^2]\,/\,N\,,\\
t &= [\;0 + 8n_2\,g_1 h_1 + 8n_3(g_3 h_3 - 2g_{22}g_{32})]\,/\,N\,,\\
z &= [32n_1 + 8n_2 g_1 h_1 + 8n_3(g_3 h_3 + 2(w_2 - w_3)^2]\,/\,N\,,
\end{aligned}$$

where g_i, h_i and g_{i2} are defined as usual and $N = 12n_1 + 8n_2 + 24n_3$.

If $n = 5$, we choose

i) n_1 times the pairs of a half-replicate of $S\,(2,3)$,
ii) n_2 times the pairs of a half-replicate of $SP\,(0,0,5;\, w_1)$,
iii) n_3 times the pairs of a quarter-replicate of $SP\,(0,0,2,3;\, w_2,w_3)$;

n_1, n_2 and n_3 have to be chosen such that the covariance matrix of the design has the structure of (4.1.6). By the results of section 5.4 this implies the following inequalities $n_1 \geqslant 1$, $n_2 \geqslant 1$, $n_3 \geqslant 2$ if $w_2 \neq w_3$ and $n_3 \geqslant 1$ if $w_2 = w_3$.
If these conditions are satisfied, then the information matrix is determined by

(5.5.4)

$$\begin{aligned}
p &= [192n_1 + 16n_2\,g_1 + 16n_3(2g_2 + 3g_3)]\,/\,N\,,\\
s &= [\;0 + 0 + 24n_3(g_{22} + g_{32})^2]\,/\,N\,,\\
t &= [\;0 + 16n_2\,g_1 h_1 + 8n_3(g_2 h_2 + 3g_3 h_3 - 6g_{22}g_{32})]\,/\,N\,,\\
z &= [192n_1 + 16n_2\,g_1 h_1 + 8n_3(g_2 h_2 + 3g_3 h_3 + 6(w_2 - w_3)^2]\,/\,N\,,
\end{aligned}$$

where $N = 80n_1 + 16n_2 + 80n_3$.

Let n_1, n_2 and n_3 be fixed. Now w_1, w_2 and w_3 have to be chosen according to the $\mathring{G}$-criterion or the D-criterion. First we consider the $\mathring{G}$-criterion. In many cases minimizing the maximal value of d_1, d_2 and d_3 means that w_1, w_2 and w_3

have to be such that $d_1 = d_2 = d_3$. Therefore lemma 5.5.3 can be used. We have written a computer program that determines w_1, w_2 and w_3 such that $\max\{d_1, d_2\}$ is minimized under the restriction $\delta = -4\xi$. In some cases it is not true that $d_1 = d_2 = d_3$. Then lemma 5.5.3 cannot be applied. So, a computerprogram has been written to determine w_1, w_2 and w_3 without the assumption $\delta = -4\xi$. This program minimizes the maximal value of d_1, d_2 and d_3. In some cases the values of w_1, w_2 and w_3 are also computed under the restriction $w_1 = w_2$ or $w_1 = w_2 = w_3$. This is done for practical applications. In the case $n = 5$ the restriction $w_2 = w_3$ is useful with respect to the number of pairs of the exact design, because now we may choose $n_3 = 1$ without affecting the structure of the information matrix. Moreover, the D-criterion is used to determine the values of w_1, w_2 and w_3. The assumption $\delta = -4\xi$ cannot be made in computing these values, since in general it does not hold as can be seen in table 5.5.4. Again in some cases we assume $w_2 = w_3$ or $w_1 = w_2 = w_3$ when computing these values. Results are given in table 5.5.4 for some choices of n_1, n_2 and n_3. These determine the weights of the pairs of the design. An argument that can be used when choosing n_1, n_2 and n_3 is that these weights should be approximately the same as those in the discrete D-optimal designs. These weights are given in table 5.2.7. However, the number of pairs of the design must be small for practical applications. Some choices are given in table 5.5.4. In the rows where the restrictions are given a 1 means that w_1, w_2 and w_3 are computed under that restriction; a 0 means that no such restriction is made. The results are satisfactory. The efficiency of the designs is good. The number of pairs is small in the case $n = 3$. However, when $n = 5$, some designs have a large number of pairs. The choice $n_1 = n_2 = n_3 = 1$ or $n_1 = 2, n_2 = n_3 = 1$ seems to be a good one, both with the restrictions $w_2 = w_3$ and $w_1 = w_2 = w_3$. The number of pairs of these designs are comparatively small and the information matrices of these designs have the structure of (4.1.5). The $\mathring{G}$-efficiency of these designs is more than 80%, the D-efficiency more than 89%. The efficiencies of the designs constructed without the restriction $\delta + 4\xi = 0$ are approximately the same as the efficiencies of the designs constructed under this restriction.

Table 5.5.4

Constants determining exact designs as given in section 5.5.2

$n = 3$						
Choice of n_1, n_2, n_3 1)	$n_1 = 1$; $n_2 = 1$; $n_3 = 1$; (44)					
Restrictions						
$\delta + 4\xi = 0$	1	0	0	1	0	0
$w_2 = w_3$	0	0	0	1	1	1
$w_1 = w_2 = w_3$	0	0	0	0	0	0
Criterion	$\dot{G}$	$\dot{G}$	D	$\dot{G}$	$\dot{G}$	D
w_1	−0.7352	−0.3762	−0.1590	−0.4720	−0.0988	−0.1398
w_2	−0.7194	0.6087	−0.5222	−0.5944	−0.5904	−0.1987
w_3	0.2333	−0.4324	−0.0425			
α	2.6970	2.6432	1.8475	3.2875	3.2398	1.4904
δ	0.7947	0.7270	0.8585	1.0951	1.0176	0.9348
γ	0.4936	0.5418	0.5593	0.3988	0.4298	0.5723
ξ	−0.1987	−0.3088	−0.2049	−0.2738	−0.5353	−0.0152
d_1	10.3066	10.1503	11.3417	11.9511	11.5794	12.0566
d_2	10.3066	9.1608	8.2145	11.9510	9.3584	9.0933
d_3		10.1503			11.5794	
$\dot{G}$-efficiency	87.3	88.7	79.4	75.3	77.7	74.6
D-efficiency	87.9	90.2	94.9	79.8	83.7	94.3

1) Between brackets the number of pairs is given.

Table 5.5.4

Constants determining exact designs as given in section 5.5.2

$n = 3$						
Choice of n_1, n_2, n_3 1)	$n_1 = 1$; $n_2 = 1$; $n_3 = 1$; (44)			$n_2 = 2$; $n_2 = 1$; $n_3 = 1$; (56)		
Restrictions						
$\delta + 4\xi = 0$	0	0	-	1	0	0
$w_2 = w_3$	1	1	-	0	0	0
$w_1 = w_2 = w_3$	1	1	-	0	0	0
Criterion	$\overset{*}{G}$	D	-	$\overset{*}{G}$	$\overset{*}{G}$	D
w_1			0	−0.4247	−0.3365	−0.1212
w_2	−0.3640	0.1809	0	−0.5431	−0.5473	−0.2114
w_3			0	−0.0043	−0.0200	−0.1238
α	1.8270	1.4696	1.3750	2.4079	2.4221	1.8599
δ	0.9991	0.9368	0.9167	0.6828	0.6769	0.7031
γ	0.4807	0.5742	0.6875	0.4852	0.4908	0.5283
ξ	0	0	0	−0.1707	−0.2307	−0.0279
d_1	11.8380	12.0880	12.8333	9.3434	9.3416	9.8512
d_2	10.0551	9.1777	9.3087	9.3434	8.8619	9.2136
d_3					9.3416	
$\overset{*}{G}$-efficiency	76.0	74.5	70.1	96.3	96.3	91.4
D-efficiency	91.0	94.3	91.4	96.5	97.3	99.1

1) Between brackets the number of pairs is given.

Table 5.5.4
Constants determining exact designs as given in section 5.5.2

$n = 3$						
Choice of n_1, n_2, n_3 1)	$n_1 = 2$; $n_2 = 1$; $n_3 = 1$; (56)					
Restrictions						
$\delta + 4\xi = 0$	1	0	0	0	0	-
$w_2 = w_3$	1	1	1	1	1	-
$w_1 = w_2 = w_3$	0	0	0	1	1	-
Criterion	$\overset{*}{G}$	$\overset{*}{G}$	D	$\overset{*}{G}$	D	-
w_1	—0.1192	—0.1192	—0.1195			0
w_2	—0.3989	—0.3989	—0.1509	—0.2386	—0.1419	0
w_3						0
α	2.4748		1.8325	1.9677	1.8226	1.75
δ	0.7232		0.7052	0.7158	0.7056	0.70
γ	0.4629		0.5292	0.4952	0.5297	0.5833
ξ	—0.1808		—0.0079	0	0	0
d_1	9.4887		9.8751	9.6880	9.8825	10.2666
d_2	9.4887		9.3180	9.6880	9.3612	9.3390
d_3						
$\overset{*}{G}$-efficiency	94.8		91.1	92.9	91.1	87.7
D-efficiency	95.4		99.1	98.3	99.0	97.5

1) Between brackets the number of pairs is given.

Table 5.5.4

Constants determining exact designs as given in section 5.5.2

$n = 5$						
Choice of n_1, n_2, n_3 1)	$n_1 = n_2 = n_3 = 2$; (352)			$n_1 = n_2 = n_3 = 1$; (176) or $n_1 = n_2 = n_3 = 2$; (352)		
Restrictions						
$\delta + 4\xi = 0$	1	0	0	1	0	0
$w_2 = w_3$	0	0	0	1	1	1
$w_1 = w_2 = w_3$	0	0	0	0	0	0
Criterion	$\overset{*}{G}$	$\overset{*}{G}$	D	$\overset{*}{G}$	$\overset{*}{G}$	D
w_1	—0.6165	—0.2309	—0.0951	—0.0888	—0.1083	—0.0926
w_2	—0.6521	—0.6507	—0.2604	—0.4602	—0.4068	—0.1299
w_3	0.3151	0.3154	—0.0540			
α	3.3687	3.3612	1.9702	2.9511	2.6327	1.8968
δ	0.6637	0.6441	0.7316	0.7732	0.7655	0.7375
γ	0.5121	0.5400	0.5581	0.4613	0.4757	0.5619
ξ	—0.1659	—0.3524	—0.0381	—0.1933	—0.1323	—0.0053
d_1	22.0750	21.9375	24.2557	24.0919	24.0807	24.4417
d_2	22.0750	17.4170	19.2704	20.1229	20.0642	19.7946
d_3		21.9375			18.6622	
$\overset{*}{G}$-efficiency	90.6	91.2	82.5	83.0	83.1	81.8
D-efficiency	90.7	93.1	95.9	89.7	91.6	95.8

1) Between brackets the number of pairs is given.

Table 5.5.4

Constants determining exact designs as given in section 5.5.2

$n = 5$						
Choice of n_1, n_2, n_3 1)	$n_1 = n_2 = n_3 = 1$; (176) or $n_1 = n_2 = n_3 = 2$; (352)			$n_1 = 4$; $n_2 = 2$; $n_3 = 2$; (412)		
Restrictions						
$\delta + 4\xi = 0$	0	0	-	1	0	0
$w_2 = w_3$	1	1	-	0	0	0
$w_1 = w_2 = w_3$	1	1	-	0	0	0
Criterion	$\overset{*}{G}$	D	-	$\overset{*}{G}$	$\overset{*}{G}$	D
w_1			0	−0.0930	−0.0051	−0.0715
w_2	−0.3048	−0.1220	0	−0.3892	−0.3891	−0.1008
w_3			0	−0.0059	−0.0028	−0.0814
α	2.2281	1.8891	1.8333	3.1218	3.1215	2.7120
δ	0.7603	0.7377	0.7333	0.5861	0.5859	0.5934
γ	0.4952	0.5626	0.6111	0.5013	0.5018	0.5148
ξ	0	0	0	−0.1465	−0.1465	−0.0046
d_1	24.1885	24.4555	24.9333	20.0817	20.0833	20.4204
d_2	21.3947	19.8932	19.8692	20.5040	20.5042	22.1378
d_3	16.9017				20.5042	
$\overset{*}{G}$-efficiency	82.7	81.8	80.2	97.5	97.5	90.3
D-efficiency	93.5	95.8	94.8	98.9	98.9	99.8

1) Between brackets the number of pairs is given.

Table 5.5.4

Constants determining exact designs as given in section 5.5.2

$n = 5$						
Choice of n_1, n_2, n_3 1)	$n_1 = 2 : n_2 = 1 ; n_3 = 1$; (206) or $n_1 = 4 : n_2 = 2 ; n_3 = 2$; (206)					
Restrictions						
$\delta + 4\xi = 0$	1	0	0	0	0	-
$w_2 = w_3$	1	1	1	1	1	-
$w_1 = w_2 = w_3$	0	0	0	1	1	-
Criterion	$\overset{*}{G}$	$\overset{*}{G}$	D	$\overset{*}{G}$	D	-
w_1	—0.0029	—0.0042	—0.0719			0
w_2	—0.3626	—0.0999	—0.0887	—0.0223	—0.0100	0
w_3						0
α	3.5350	2.7207	2.7092	2.6693	2.7208	2.6667
δ	0.6036	0.5935	0.5935	0.5927	0.5939	0.5926
γ	0.4666	0.5152	0.5149	0.5286	0.5118	0.5333
ξ	—0.1509	—0.0090	—0.00250	0	0	0
d_1	20.0853	20.4253	20.4228	20.5666	20.3958	20.6222
d_2	22.4169	22.0731	22.1756	22.1111	22.2821	22.1249
d_3		18.7722		18.6052		
$\overset{*}{G}$-efficiency	89.2	90.6	90.2	90.5	89.8	90.4
D-efficiency	96.0	99.7	99.8	99.6	99.8	99.4

1) Between brackets the number of pairs is given.

Table 5.5.4

Constants determining exact designs as given in section 5.5.2

$n = 5$						
Choice of n_1, n_2, n_3 1)	$n_1 = n_2 = 4;\ n_3 = 2;$ (544)			$n_1 = n_2 = 2;\ n_3 = 1;$ (272) or $n_1 = n_2 = 4;\ n_3 = 2;$ (544)		
Restrictions						
$\delta + 4\xi = 0$	1	0	0	1	0	0
$w_2 = w_3$	0	0	0	1	1	1
$w_1 = w_2 = w_3$	0	0	0	0	0	0
Criterion	$\overset{*}{G}$	$\overset{*}{G}$	D	$\overset{*}{G}$	$\overset{*}{G}$	D
w_1	−0.4980	−0.2121	−0.1049	−0.4599	−0.2003	−0.1050
w_2	−0.3267	−0.3122	−0.0798	−0.2360	−0.2350	−0.0869
w_3	0.0043	−0.1040	−0.0920			
α	3.1619	3.1669	2.8758	3.1775	3.1743	2.8766
δ	0.6214	0.6109	0.6088	0.6290	0.6153	0.6088
γ	0.4860	0.4994	0.5255	0.4735	0.4926	0.5255
ξ	−0.1554	−0.3987	−0.2591	−0.1576	−0.2984	−0.2595
d_1	20.7445	20.6541	20.9164	20.7783	20.6794	20.9163
d_2	20.7445	19.9645	16.8917	20.7783	17.2558	16.8847
d_3		20.6541			20.6794	
$\overset{*}{G}$-efficiency	96.4	96.8	95.6	96.3	96.7	95.6
D-efficiency	96.5	98.5	99.5	96.5	98.3	99.5

1) Between brackets the number of pairs is given.

Table 5.5.4

Constants determining exact designs as given in section 5.5.2

$n = 5$						
Choice of n_1, n_2, n_3 1)	$n_1 = n_2 = 2$; $n_3 = 1$; (272) or $n_1 = n_2 = 4$; $n_3 = 2$; (544)			$n_1 = 2$; $n_2 = 1$; $n_3 = 2$; (336)		
Restrictions						
$\delta + 4\xi = 0$	0	0	-	1	0	0
$w_2 = w_3$	1	1	-	0	0	0
$w_1 = w_2 = w_3$	1	1	-	0	0	0
Criterion	$\hat{G}$	D	-	$\hat{G}$	$\hat{G}$	D
w_1			0	−0.4671	−0.1683	−0.0773
w_2	−0.2351	−0.1000	0	−0.6720	−0.6725	−0.4593
w_3			0	0.2911	0.2911	0.0277
α	3.1746	2.8909	2.8333	3.2677	3.2707	2.1890
δ	0.6166	0.6089	0.6071	0.6365	0.6301	0.6993
γ	0.4902	0.5236	0.5483	0.5204	0.5307	0.5337
ξ	−0.2886	−0.2628	−0.2576	−0.1591	−0.2411	0.0304
d_1	20.6813	20.8957	21.1521	21.5224	21.4905	23.1875
d_2	17.4970	16.8629	16.8452	21.5224	19.5115	21.5711
d_3	20.6813		19.3326		21.4905	
$\hat{G}$-efficiency	96.7	95.7	94.6	92.9	93.1	86.3
D-efficiency	98.2	99.5	99.0	93.0	93.8	95.8

1) Between brackets the number of pairs is given.

Table 5.5.4

Constants determining exact designs as given in section 5.5.2

$n = 5$						
Choice of n_1, n_2, n_3 1)	$n_1 = 3$; $n_2 = 2$; $n_3 = 2$; (432)			$n_1 = 3$; $n_2 = 1$; $n_3 = 2$; (416)		
Restrictions						
$\delta + 4\xi = 0$	1	0	0	1	0	0
$w_2 = w_3$	.0	0	0	0	0	0
$w_1 = w_2 = w_3$	0	0	0	0	0	0
Criterion	$\overset{*}{G}$	$\overset{*}{G}$	D	$\overset{*}{G}$	$\overset{*}{G}$	D
w_1	−0.4135	−0.1596	−0.0817	−0.0105	−0.0132	−0.0575
w_2	−0.5341	−0.5673	−0.1318	−0.5907	−0.5909	−0.2117
w_3	0.1729	0.0311	−0.0905	0.0019	−0.0046	−0.0559
α	3.1704	3.1993	2.3087	3.1794	3.1800	2.2744
δ	0.6177	0.6207	0.6444	0.6113	0.6120	0.6336
γ	0.5045	0.4986	0.5336	0.4895	0.4887	0.5233
ξ	−0.1544	−0.2770	−0.0083	−0.1528	−0.1530	0.2573
d_1	20.8802	20.8796	21.8685	20.5451	20.5515	21.4874
d_2	20.8802	17.9946	20.6661	20.8138	20.8148	26.9090
d_3		20.8796			20.8148	
$\overset{*}{G}$-efficiency	95.8	95.8	91.5	96.1	96.1	74.3
D-efficiency	95.8	97.1	98.9	97.0	97.0	98.2

5.5.3. Exact designs when $n=2, 4$.

Exact designs will be constructed as follows.
If $n = 2$, we choose

i) n_1 times the pairs of $S(1,1)$,
ii) n_2 times the pairs of $SP(0,0,2;\ w_1)$,
iii) n_3 times the pairs of a half-replicate of $SP(0,0,1,1;\ w_2,w_3)$
iv) n_4 times the pairs of $SP(0,1,1;\ w_4)$.

The information matrix of this design has the structure given in (4.1.5) if $n_1 \geqslant 1, n_2 \geqslant 1, n_4 \geqslant 1$ and $n_3 \geqslant 1$ if $w_2 = w_3$ or $n_3 \geqslant 2$ if $w_2 \neq w_3$.
If these conditions are satisfied we have

$$
\begin{aligned}
p &= [\,8n_1 + 4n_2 g_1 + 2n_3(g_2 + g_3) + 4n_4(4 + g_4)]\,/\,N\ ,\\
s &= [\ 0 + 0 + 2n_3(g_{22} + g_{32})^2 + 4n_4(g_4 + h_4)]\,/\,N\ ,\\
t &= [\ 0 + 4n_2\, g_1 h_1 - 4n_3\, g_{22} g_{32} + 0]\,/\,N\ ,\\
z &= [16n_1 + 4n_2\, g_1 h_1 + 4n_3(w_2 - w_3)^2 + 8n_4 h_4]\,/\,N\ ,
\end{aligned}
\tag{5.5.5}
$$

where $N = 4n_1 + 4n_2 + 4n_3 + 8n_4$.

If $n = 4$, we choose

i) n_1 times the pairs of a half-replicate of $S(2,2)$,
ii) n_2 times the pairs of $SP(0,0,4;\ w_1)$,
iiiA) n_3 times the pairs of a half-replicate of $SP(0,0,1,3;\ w_2,w_3)$,
or
iiiB) n_3 times the pairs of a half-replicate of $SP(0,0,2,2;\ w_2,w_3)$,
iv) n_4 times the pairs of a quarter-replicate of $SP(1,2,1;\ w_4)$.

The information matrix of this design has the structure given in (4.1.5) if $n_1 \geqslant 1, n_2 \geqslant 1, n_4 \geqslant 2$ and $n_3 \geqslant 1$ if $w_2 = w_3$ or $n_3 \geqslant 2$ if $w_2 \neq w_3$.
If these conditions are satisfied we have

$$
\begin{aligned}
p &= [48n_1 + 16n_2\, g_1 + 8n_3[(2q_4 - 1)g_2 + 3g_3] + 12n_4(8 + g_4)]\,/N\ ,\\
s &= [\ 0 + 0 + 8n_3 q_4(g_{22} + g_{32})^2 + 12n_4(g_4 + h_4)]\,/N\ ,\\
t &= [\ 0 + 16n_2\, g_1 h_1 + 8n_3[(q_4 - 1)g_2 h_2 + (3 - q_4)g_3 h_3 - 2q_4 g_{22} g_{32}]]/N\ ,\\
z &= [64n_1 + 16n_2\, g_1 h_1 + 8n_3[(q_4 - 1)g_2 h_2 + (3 - q_4)g_3 h_3 + 2q_4(w_2 - w_3)^2)]\\
&\qquad + 8n_4(8 + g_4 + 2h_4)]\,/N\ ,
\end{aligned}
\tag{5.5.6}
$$

where

$$
q_4 = \begin{cases} 1\ , \text{ if } iiiA\text{) is chosen}\ ,\\ 2\ , \text{ if } iiiB\text{) is chosen}\ ,\end{cases}
$$

and

$$N = 24n_1 + 16n_2 + 16(1+q_4)n_3 + 48n_4.$$

Again for fixed n_1, n_2, n_3 and n_4 the values of w_1, w_2, w_3 and w_4 have been computed according to the $\overset{*}{G}$-criterion or the D-criterion. When using the $\overset{*}{G}$-criterion we make the assumption $\delta + 4\xi = 0$, because we did not find better results when this assumption was not made in the case $n = 3, 5$. Again in some cases designs are constructed with $w_2 = w_3$ or $w_1 = w_2 = w_3$. Some results are given in table 5.5.5. For both $n = 2$ and $n = 4$ designs are found for which the number of pairs is comparatively small and which have a high efficiency. The designs given in this table for $n = 4$ are designs with $q_4 = 1$. Using $q_2 = 2$ does not lead to better results.

Table 5.5.5

Constants determining exact designs as given in section 5.5.3

$n = 2$					
Choice of n_1, n_2, n_3, n_4 and q_4 1)	$q_4 = 1$; $n_1 = 0$; $n_2 = 0$; $n_3 = 0$; $n_4 = 1$; (8)			$q_4 = 1$; $n_1 = 2$; $n_2 = 2$; $n_3 = 2$; $n_4 = 2$; (40)	
Restrictions					
$\delta + 4\xi = 0$	0	0	-	1	0
$w_2 = w_3$	-	-	-	0	0
$w_1 = w_2 = w_3$	-	-	-	0	0
Criterion	$\dot{G}$	D	-	$\dot{G}$	D
w_1	-	-	-	—0.0407	—0.1483
w_2	-	-	-	—0.0558	—0.1826
w_3	-	-	-	—0.5128	—0.1826
w_4	0.0754	0.1279	0	0.0061	0.0741
α	2.0229	2.0671	2	1.9975	1.7495
δ	0.8647	0.6860	1	0.6916	0.6884
γ	0.4120	0.4201	0.4	0.5116	0.5222
ξ	0	0	0	—0.1729	—0.0133
d_1	5.1066	4.8246	5.6	4.8127	4.8423
d_2	5.8103	5.8393	5.8700	5.1706	5.3316
d_3					
d_4	5.0230	5.0000	5.1454	5.0877	5.0479
$\dot{G}$-efficiency	86.1	85.6	85.2	96.7	93.8
D-efficiency	98.4	98.7	97.2	98.5	99.6

1) Between brackets the number of pairs is given.

Table 5.5.5

Constants determining exact designs as given in section 5.5.3

$n = 2$					
Choice of n_1, n_2, n_3, n_4 and q_4 1)	$q_4 = 1$ $n_1 = n_2 = n_3 = n_4 = 1$; (20) , or $n_1 = n_2 = n_3 = n_4 = 2$; (40) .				
Restrictions					
$\delta + 4\xi = 0$	1	0	0	0	-
$w_2 = w_3$	1	1	1	1	-
$w_1 = w_2 = w_3$	0	0	1	1	-
Criterion	$\overset{*}{G}$	D	$\overset{*}{G}$	D	-
w_1	−0.0343	−0.1483	−0.0751	−0.1639	0
w_2	−0.3765	−0.1826			0
w_3					0
w_4	0.0224	0.0741	0.0193	0.0744	0
α	2.0225	1.7495	1.6797	1.7344	1.6667
δ	0.7054	0.6884	0.7076	0.6891	0.7143
γ	0.5040	0.5222	0.5392	0.5227	0.5556
ξ	−0.1764	−0.0133	0	0	0
d_1	4.8377	4.8423	4.9869	4.8472	5.0794
d_2	5.1983	5.3316	5.3124	5.3554	5.3383
d_3					
d_4	5.0881	5.0479	5.0966	5.0492	5.1710
$\overset{*}{G}$-efficiency	96.2	93.8	94.1	93.4	93.7
D-efficiency	98.3	99.6	99.1	99.6	98.0

1) Between brackets the number of pairs is given.

Table 5.5.5

Constants determining exact designs as given in section 5.5.3

$n = 2$					
Choice of n_1, n_2, n_3 n_4 and q_4 1)	$q_4 = 1$ $n_1 = 1; n_2 = 2; n_3 = 1; n_4 = 3$; (40) , or $n_1 = 2; n_2 = 4; n_3 = 2; n_4 = 6$; (80) .				
Restrictions					
$\delta+4\xi=0$	1	0	0	0	-
$w_2=w_3$	1	1	1	1	-
$w_1=w_2=w_3$	0	0	1	1	-
Criterion	$\mathring{G}$	D	$\mathring{G}$	D	-
w_1	—0.3182	—0.1567			0
w_2			—0.1380	—0.1502	0
w_3	—0.0333	—0.1384			0
w_4	0.0688	0.1138	—0.0369	0.1136	0
α	2.0132	2.0631	2.0340	2.0687	2
δ	0.8019	0.7493	0.8081	0.7490	0.8333
γ	0.4729	0.4919	0.4838	0.4920	0.5
ξ	—0.2005	—0.2885	—0.2861	—0.2930	—0.2857
d_1	5.0995	4.9649	5.1676	4.9641	5.3333
d_2	5.0995	4.8575	4.8453	4.8506	4.8496
d_3		5.2447	5.1676	5.2555	5.1446
d_4	5.0261	5.0126	5.0236	5.0135	5.1019
$\mathring{G}$-efficiency	98.0	95.3	96.8	95.1	97.2
D-efficiency	99.0	99.9	99.7	99.9	98.6

1) Between brackets the number of pairs is given.

Table 5.5.5

Constants determining exact designs as given in section 5.5.3

$n = 2$			$n = 4$			
Choice of n_1, n_2, n_3 n_4 and q_4 1)	$q_4 = 1$ $n_1 = 2; n_2 = 4;$ $n_3 = 2; n_4 = 6;$ (80)		$q_4 = 1$ $n_1 = 1; n_2 = 0; n_3 = 2; n_4 = 0;$ (88)			
Restrictions						
$\delta + 4\xi = 0$	1	0	1	0	0	-
$w_2 = w_3$	0	0	0	0	1	-
$w_1 = w_2 = w_3$	0	0	0	0	0	-
Criterion	$\mathring{G}$	D	$\mathring{G}$	D	D	-
w_1	—0.3181	—0.1568	-	-	-	-
w_2	—0.0317	—0.1384	0.6118	—0.6193	—0.1802	0
w_3	—0.0315	—0.1384	—0.5250	—0.0366		0
w_4	0.0689	0.1138	-	-	-	-
α	2.0132	2.0631	3.0171	2.1083	1.4689	1.375
δ	0.8018	0.7493	0.7205	0.8241	0.9366	0.9167
γ	0.4730	0.4919	0.5431	0.6218	0.6416	0.7857
ξ	—0.2005	—0.2885	—0.1801	—0.2842	0	0
d_1	5.0995	4.9649	15.8724	18.1602	20.1190	20.9524
d_2	5.0995	4.8575	15.8724	11.7319	14.3873	14.6758
d_3		5.2447				
d_4	5.0264	5.0126	15.6607	16.5709	17.4248	18.5088
$\mathring{G}$-efficiency	98.0	95.3	88.2	77.1	69.6	66.8
D-efficiency	99.0	99.9	98.9	92.7	91.3	88.6

1) Between brackets the number of pairs is given.

Table 5.5.5
Constants determining exact designs as given in section 5.5.3

$n = 4$					
Choice of n_1, n_2, n_3, n_4 and q_4 1)	$q_4 = 1$ $n_1 = 2; n_2 = 0;$ $n_3 = 2; n_4 = 0; (112)$		$q_4 = 1$ $n_1 = 1; n_2 = 0; n_3 = 1; n_4 = 0; (56)$, or $n_1 = 2; n_2 = 0; n_3 = 2; n_4 = 0; (112)$		
Restrictions					
$\delta + 4\xi = 0$	1	0	0	0	-
$w_2 = w_3$	0	0	1	1	-
$w_1 = w_2 = w_3$	0	0	0	0	-
Criterion	$\dot{G}$	D	$\dot{G}$	D	-
w_1	-	-	-	-	-
w_2	0.5073	−0.3276	−0.3623	−0.1544	0
w_3	−0.3808	−0.1062			0
w_4	-	-	-	-	-
α	2.7424	1.9775	2.3186	1.8365	1.75
δ	0.6341	0.6963	0.7361	0.7067	0.7
γ	0.5852	0.6122	0.5215	0.6178	0.7
ξ	−0.1586	−0.0873	0	0	0
d_1	14.8267	16.0387	15.9496	16.2490	16.8
d_2	14.8264	13.4595	15.9496	14.3546	14.4049
d_3					
d_4	14.8261	15.0663	15.1337	15.1786	15.75
$\dot{G}$-efficiency	94.4	87.3	87.8	86.2	83.3
D-efficiency	94.4	97.8	94.2	97.7	95.9

1) Between brackets the number of pairs is given.

Table 5.5.5
Constants determining exact designs as given in section 5.5.3

$n = 4$					
Choice of n_1, n_2, n_3, n_4 and q_4 1)	$q_4 = 1$ $n_1 = 1; n_2 = 0; n_3 = 2; n_4 = 2; (184)$,				
Restrictions					
$\delta + 4\xi = 0$	1	0	0	1	-
$w_2 = w_3$	0	0	1	1	-
$w_1 = w_2 = w_3$	0	0	0	0	-
Criterion	$\overset{*}{G}$	D	$\overset{*}{G}$	D	-
w_1	-	-	-	-	-
w_2	—0.4105	—0.2044	—0.0936	—0.1157	0
w_3	—0.0612	—0.0930			0
w_4	0.4311	0.0757	0.106	0.0771	0
α	2.6528	2.1765	2.1519	2.1392	2.0909
δ	0.6167	0.6702	0.6612	0.6718	0.6765
γ	0.5515	0.5395	0.5525	0.5410	0.5610
ξ	—0.1542	—0.0268	0	0	0
d_1	14.2783	15.0393	14.9983	15.0764	15.3113
d_2	14.2784	14.6810	14.9983	14.9560	14.8904
d_3					
d_4	14.2468	14.3883	14.4036	14.4077	14.5893
$\overset{*}{G}$-efficiency	98.1	93.1	93.3	92.9	91.4
D-efficiency	98.1	99.3	99.2	99.3	98.6

1) Between brackets the number of pairs is given.

5.6. Robustness of the designs

As in section 4.5 we will give some lower bounds for the D-efficiencies of the discrete D-optimal designs which are given in section 5.2 when the condition (1.8.6) is not satisfied. The arguments given in section 4.5 also hold in the case of a hypercube as experimentel region. Lemma 4.5.1 is used to compute the lower bounds for some values of δ. The results are similar to the ones given in section 4.5 for $n = 2, 3, 4$. No lower bounds have been computed for $n = 5$.

Table 5.6.1
Lower bounds for the D-efficiency of some designs

$n=2$					smallest	
β_0					value	lower
β_1	β_2	β_{11}	β_{12}	β_{12}	of $\pi_{l.ij}$	bound
0.05	0.05	0.05	0.05	0.05	0.435	0.996
−0.05	0.05	0.05	0.05	0.05	0.450	0.996
0.05	0.05	−0.05	0.05	0.05	0.438	0.996
0.1	0.1	0.1	0.1	0.1	0.372	0.984
−0.1	0.1	0.1	0.1	0.1	0.401	0.984
0.1	0.1	−0.1	0.1	0.1	0.378	0.984
0.2	0.2	0.2	0.2	0.2	0.270	0.939
−0.2	0.2	0.2	0.2	0.2	0.310	0.937
0.2	0.2	−0.2	0.2	0.2	0.270	0.941
0.3	0.3	0.3	0.3	0.3	0.172	0.877
−0.3	0.3	0.3	0.3	0.3	0.232	0.868
0.3	0.3	−0.3	0.3	0.3	0.183	0.877
0.5	0.5	0.5	0.5	0.5	0.068	0.737
−0.5	0.5	0.5	0.5	0.5	0.119	0.699
0.5	0.5	−0.5	0.5	0.5	0.076	0.727
1	1	1	1	1	0.005	0.485
−1	1	1	1	1	0.018	0.359
1	1	−1	1	1	0.007	0.418
0.1	0	0	0	0	0.450	0.995
0.3	0	0	0	0	0.354	0.956
0.5	0	0	0	0	0.269	0.887
1	0	0	0	0	0.119	0.657
0	0	0.1	0	0	0.475	0.999
0	0	0.3	0	0	0.427	0.987
0	0	0.5	0	0	0.379	0.965
0	0	1	0	0	0.272	0.874
0	0	0	0	0.1	0.450	0.997
0	0	0	0	0.3	0.354	0.971
0	0	0	0	0.5	0.269	0.923
0	0	0	0	1	0.119	0.748

$n=3$									smallest	
β_0									value	lower
β_1	β_2	β_3	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}	of $\pi_{i,ij}$	bound
0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.386	0.992
0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.283	0.971
−0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.310	0.970
−0.1	−0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.310	0.970
0.2	0.2	0.2	0.2	0.2	0.2	0.2	0.2	0.2	0.135	0.901
−0.2	0.2	0.2	−0.2	0.2	0.2	0.2	0.2	0.2	0.256	0.895
−0.2	0.2	0.2	−0.2	0.2	0.2	−0.2	0.2	0.2	0.168	0.895
0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.058	0.820
−0.3	−0.3	0.3	−0.3	−0.3	0.3	−0.3	0.3	0.3	0.083	0.821
0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.009	0.682
0.5	0.5	0.5							0.119	0.746
0.5									0.269	0.890
0.5			0.5						0.259	0.869
0.5			0.5			0.5			0.176	0.805
1.0									0.119	0.668

The entries that are not given in this table are zero.

$n = 4$			
β_0 non zero parameters	value of the non zero parameters	smallest value of $\pi_{I.IJ}$	lower bound
β_1	0.1	0.4502	0.9955
	1	0.1192	0.7034
β_{11}	0.1	0.4750	0.9990
β_{12}	0.1	0.4502	0.9959
β_i ,$1 \leqslant i \leqslant 4$	0.1	0.3780	0.9823
	0.2	0.2697	0.9341
	0.5	0.0765	0.7174
	1	0.0068	0.4540
β_{ii} ,$1 \leqslant i \leqslant 4$	0.1	0.4024	0.9951
	0.2	0.3120	0.9811
β_{ij} ,$1 \leqslant i < j \leqslant 4$	0.1	0.3100	0.9764
	0.2	0.1680	0.9197
β_i ,β_{ij} ,$1 \leqslant i \leqslant j \leqslant 4$	0.1	0.1929	0.9573
	0.2	0.0540	0.8690
	0.3	0.0135	0.7787
	0.5	0.0008	0.6292
	1	0.0000	0.4169
$\beta_1, \beta_{11}, \beta_{12}$	0.2	0.3100	0.9631
$\beta_1, \beta_3, \beta_{12}$	0.2	0.2315	0.9510

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Samenvatting

In experimenten met paarsgewijze vergelijkingen worden waarnemingen gedaan door telkens twee objecten met elkaar te vergelijken. Paarsgewijze vergelijkingen worden veel gebruikt in situaties waar de beoordeling van de te onderzoeken variabele subjectief is, bijvoorbeeld bij het beoordelen van etenswaar. Aan een aantal proefpersonen wordt dan gevraagd een voorkeur uit te spreken voor één van een tweetal aangeboden producten. In dit proefschrift worden proefopzetten ontwikkeld voor dergelijke situaties.

In hoofdstuk 1 wordt een aantal modellen gegeven die met betrekking tot paarsgewijze vergelijkingen geformuleerd zijn. Met name het Bradley-Terry model komt aan de orde. Dit model postuleert het bestaan van een parameter (of evaluatiewaarde) horend bij het object. De preferentiekansen kunnen in deze parameters worden uitgedrukt en met behulp van de waarnemingen kunnen de parameters geschat worden. De covariantiematrix van de schatters van de parameters wordt besproken. Deze is van belang omdat veel criteria voor het ontwikkelen van proefopzetten afhangen van de covariantiematrix. In dit proefschrift wordt het D-criterium en een voor paarsgewijze vergelijkingen aangepast G-criterium gebruikt om proefopzetten te ontwikkelen. Het D-criterium minimaliseert de determinant van de covariantiematrix; het G-criterium minimaliseert het maximum van de variantie van de responsfunctie.

In hoofdstuk 2 wordt een methode gegeven om proefopzetten te construeren. Deze methode is geschikt voor het geval dat er een lineair model geformuleerd kan worden voor de evaluatiewaarde. Dat wil zeggen dat de evaluatiewaarde een functie is van een aantal verklarende variabelen. De covariantiematrix hangt echter af van de onbekende parameters. Daarom is het bij het construeren van proefopzetten nodig een veronderstelling te maken met betrekking tot de parameters. De gebruikelijke veronderstelling is dat alle parameters gelijk zijn. Bij het construeren van proefopzetten is het nuttig om gebruik te maken van (gestandaardiseerde) discrete proefopzetten. Discreet staat in tegenstelling tot exact, waarbij in ieder paar één (of meerdere) waarnemingen worden gedaan. Bij discrete proefopzetten is sprake van een wegingscoëfficiënt per paar. De wegingscoëfficiënt kan iedere positieve waarde aannemen. Gestandaardiseerd wil zeggen dat de som van de wegingscoëfficiënten gelijk is aan één. Bij gestandaardiseerde exacte proefopzetten zijn alle wegingscoëfficiënten gelijk aan (een veelvoud van) de reciproke waarde van het totaal aantal waarnemingen.

In hoofdstuk 3, 4 en 5 worden toepassingen gegeven. Hoofdstuk 3 behandelt het geval van een factorieel model met hoofdeffecten en interacties van twee factoren. Exacte D-optimale proefopzetten worden gegeven, zowel voor de situatie dat het experimentele gebied een hyperkubus is, als voor de situatie dat het een hyperbol is. Sommige van deze proefopzetten zijn bekend in de literatuur. Hoofdstuk 4 en 5 behandelen een volledig tweedegraads model, waaarbij het experimentele gebied in hoofdstuk 4 een hyperbol is en in hoofdstuk 5 een hyperkubus. In beide hoofdstukken worden discrete D-optimale proefopzetten

geconstrueerd. Bij sommige van deze proefopzetten is het aantal paren groot. Daarom worden proefopzetten ontwikkeld waarbij het aantal paren kleiner is. Met behulp van deze discrete proefopzetten worden exacte proefopzetten geconstrueerd die een goede efficiëntie hebben en waarvan het aantal paren niet al te groot is. De robuustheid van de optimale discrete proefopzetten wordt onderzocht; dat wil zeggen: er wordt besproken wat de efficiëntie van de proefopzetten is als niet voldaan is aan de aanname dat er geen verschillen zijn in de objecten.

Curriculum vitae

De schrijver van dit proefschrift werd op 20 februari 1955 geboren te 's–Gravenhage. In 1973 behaalde hij het diploma Gymnasium–β aan het St–Bernardinuscollege te Heerlen. Vervolgens studeerde hij wiskunde aan de Technische Hogeschool Eindhoven. Het kandidaatsexamen werd afgelegd in februari 1977 en in augustus 1981 werd het diploma wiskundig ingenieur behaald, na afstudeerwerk onder leiding van prof.dr. R. Doornbos. Van oktober 1981 tot september 1985 was de schrijver werkzaam als wetenschappelijk assistent aan de onderafdeling der Wiskunde en Informatica van de Technische Hogeschool Eindhoven, onder toezicht van prof.dr. R. Doornbos. In deze periode is dit proefschrift tot stand gekomen. Vanaf september 1985 is de schrijver werkzaam als universitair docent bij de vakgroep Informatica van bovengenoemde onderafdeling en hogeschool.

Stellingen

I

Een proefopzet heet roteerbaar als de variantiefunctie alleen afhangt van de afstand tot het centrum van het experimentele gebied. Deze naamgeving is verwarrend, want roteerbaarheid wil in het algemeen niet zeggen dat de punten van de proefopzet over een gelijke hoek ten opzichte van het centrum geroteerd kunnen worden zonder dat deze eigenschap verloren gaat.

II

Indien bij een proefopzet als experimenteel gebied niet een (hyper-)bol wordt gekozen, is het minder zinvol te eisen dat de proefopzet roteerbaar is.

III

De principes van statistische proefopzetten kunnen soms met vrucht worden toegepast om het globale optimum te vinden van een deterministische responsefunctie.

P.J.J. Maas, Onderzoek naar de geometrie van een grote-terts klok. Afstudeerverslag Afdeling Werktuigbouwkunde THE, mei 1985.

IV

Nu robuuste schattingsmethoden de laatste tijd veel navolging vinden, bestaat het gevaar dat de klassieke methoden ondergewaardeerd worden. Zij blijven echter voor veel experimenten geschikt, mits men 'gezond verstand' gebruikt, bijvoorbeeld voor het vinden van uitschieters.

V

Het bewijs van theorema 3 van hoofdstuk 11 van Athreya and Ney (1972) is onvolledig. Er wordt afgeleid dat

$$\lim_{n \to \infty} \frac{f_n^i(s) - q^i}{\gamma^n} = Q(s)\, i\, q^{i-1} ,$$

met

$$f_n^i(s) = \sum_{j=0}^{\infty} P_n(i,j)\, s_j ,$$

en

$$Q(s) = \sum_{j=0}^{\infty} \nu_j\, s^j .$$

Nu wordt gesteld dat
"Comparing coefficients on both sides implies:

$$\lim_{n \to \infty} \frac{P_n(i,j)}{\gamma^n} = i\, q^{i-1} \nu_j \text{ ."}$$

Dit is niet correct. Een juist argument kan gevonden worden in Karlin and McGregor (1966). Daarin wordt gebruikt dat

$$Q_n(s) = \frac{f_n(s) - q}{\gamma^n} \text{ en } Q(s)$$

analytisch zijn en dat $Q_n(s)$ uniform convergeert naar $Q(s)$.

Athreya, K.B. and Ney, P.E. (1972). *Branching Processes*. Springer-Verlag, Berlin.

Karlin, S. and McGregor, J. (1966). Spectral theory of branching processes. I. The case of a discrete spectrum. *ZW* 5, 6–33.

VI

Het personeelsbeleid aan universiteiten en hogescholen dient meer dan nu het geval is gericht te zijn op het aanstellen van wetenschappelijk personeel met interesse voor het geven van onderwijs en met didactische kwaliteiten.

VII

Bij atletiek is een verrassend goede vuistregel ter bepaling van de gemiddelde snelheid die men kan lopen op een afstand als functie van de snelheid op een andere afstand de volgende

$$v_2 = v_1 - {}^2\log\left(\frac{x_2}{x_1}\right),$$

waar x_i afstanden en v_i de bijbehorende snelheden in km/uur zijn ($i = 1,2$). Dat wil zeggen: als de afstand verdubbelt verliest men 1 km/uur aan snelheid. De omstandigheden moeten enigszins vergelijkbaar zijn.