Optimal designs for two-level main effects models on a restricted design region

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Abstract

We develop $D$-optimal designs for linear main effects models on a subset of the $2^K$ full factorial design region, when the number of factors set to the higher level is bounded. It turns out that in the case of narrow margins only those settings of the design points are admitted, where the number of high levels is equal to the upper or lower bounds, while in the case of wide margins the settings are more spread and the resulting optimal designs are as efficient as a full factorial design. These findings also apply to other optimality criteria.

Keywords: $D$-optimality, Restricted design region, Invariant design criterion, Two-level factorial designs

1 Introduction

The motivation for this work comes from the problem of calibration of items in educational and psychological tests. These items are constructed using a number of rules which may be either applied or not. In calibration experiments items are presented to a large number of individuals with essentially known ability. The item parameters describe the influence of each rule on the mean score of the individuals and are to be estimated by the responses in the calibration experiment.

A restriction arising in this scenario is, that items become more difficult, if the number of active rules is increased. Hence, from a practical point of view it would not make much sense to use only one rule or no rule at all, because

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the item would be too easy. On the other hand the item would become too difficult, if the number of active rules is too large. For those items with too few or too many rules it would be doubtful that a linear model assumed is valid. This matter imposes a restriction on the design region, which allows only such items with a bounded number of active rules. For example, in an experiment with six different rules it would be meaningful to restrict to items with at least two and at most four active rules. In particular, under these constraints neither the full factorial nor regular fractional factorial designs can be used any more.

In the present paper we will consider a linear model providing the fundamentals of the so-called classical test theory (e.g. McDonald, 1999) which are still mostly used for the development and calibration of educational and psychological tests.

We will start in Section 2 by briefly outlining rule based item generation. Then, in Section 3 the model and its information matrix are presented, which is the basis for the comparison of designs. After a short introduction to optimal design and invariance, the special structure of the information matrix is discussed in Section 4. This is followed in the subsequent section by the main results, which constitute conditions on designs for $D$-optimality. Proofs and exemplary tables of designs are deferred to appendices.

Our results are related to work in spring balance weighing and chemical balance weighing designs. In contrast to the model considered here these usually do not incorporate constants. For $D$- and $A$-optimal designs with restrictions on the number of objects used in each weighing see Huda and Mukerjee (1988). Optimality for spring balance designs without restrictions but including a constant in the model is considered in Filová, Harman and Klein (2011).

2 Rule-based item generation

Items of educational and psychological tests should neither be too easy nor too difficult. Otherwise, ceiling or bottom effects may occur, i.e. the number of correctly solved items of several respondents reach the maximal or minimal value. The information of such items may be severely impaired. Furthermore, according to a well-known result of classical test theory mean item difficulties are desirable since they foster high item discriminations, i.e. high correlations between item scores and the total scores.

For rule-based item generation (e.g. Arendasy and Sommer, 2007), an efficient method for item development, this objective can be best achieved by items with an appropriate number of rules. The rules are usually represented by particular demands on cognitive processing and determine the item parameters, mostly item difficulty. Such item generation will be briefly illustrated by items measuring mental speed for numerical operations.
Each item may consist of a comparable set of 20 numbers with 4 digits, such as 3412, 5364, 2774, ..., 8732. These numbers are nowadays often generated on the fly and displayed on a computer screen for a certain amount of time. For items with only one rule respondents with high ability will mark most numbers correctly if not all. On the other hand, difficult items characterised by 6 or more rules will lead to low scores especially for respondents with low abilities.

Another example for rule-based generated items which measure human memory are represented by sets of stimuli which are defined by binary characteristics (rules) and generated according to a full factorial design. Two basic elements, e.g., circles and triangles are furthermore characterised by a set of binary attributes, for example, colour, size, or shading. Again, the difficulty of these items is mainly determined by the number of the attributes (rules). These items will be displayed to the respondents for a certain period of time and have to be recognised by the respondents some time later.

In general, when a set of rule-based items will be presented to a sample of respondents, items with a too small or a too large number of rules should not be used in order to avoid ceiling and bottom effects. Furthermore, many respondents will not obtain item scores near to the mean score. Hence, to estimate the influence of the rules on the difficulty of the items by linear models the design region has to be restricted.

3 Model, Information and Design Invariance

We consider an experiment in which \( N \) items are presented and responses \( Y_1, \ldots, Y_N \) are observed. The number of rules, which are used to construct the items, is \( K \). Then the items can be characterised by the corresponding design points \( x_i = (x_{i1}, \ldots, x_{iK})^\top \in \{-1, +1\}^K \), where the entries \( x_{ij} \) are equal to +1, if the \( j \)-th rule is used in the construction of the \( i \)-th item, and \( x_{ij} = -1 \), if the rule is not used. We assume that only main effects occur and that there are no interactions between the rules. Then the difficulties of the items are specified by the parameter vector \( \beta = (\beta_0, \beta_1, \ldots, \beta_K)^\top \in \mathbb{R}^p \), where the number of parameters equals \( p = K + 1 \), and which includes a constant term \( \beta_0 \) besides \( K \) parameters \( \beta_j \), \( j = 1, \ldots, K \), corresponding to the main effects of the \( K \) rules. The model can be written in a general linear model equation as

\[
Y_i = f(x_i)^\top \beta + \varepsilon_i,
\]

\( i = 1, \ldots, N \), with regression function \( f(x) = (1, x^\top)^\top = (1, x_1, \ldots, x_K)^\top \).

As usual in linear models it is assumed that the errors \( \varepsilon_1, \ldots, \varepsilon_N \) are uncorrelated and homoscedastic with mean \( \text{E}(\varepsilon_i) = 0 \) and variance \( \text{Var}(\varepsilon_i) = \sigma^2 \).

By letting \( Y = (Y_1, \ldots, Y_N)^\top \) and \( \varepsilon = (\varepsilon_1, \ldots, \varepsilon_N)^\top \) the vector of observations and errors, respectively, and \( F = (f(x_1), \ldots, f(x_N))^\top \) the design
matrix, the model can be written in vector notation

\[ Y = F\beta + \varepsilon. \]

In what follows we consider the situation that the design region \( \mathcal{X} \subseteq \{-1,+1\}^K \) is restricted by the possible number of active rules, i.e. the number of factor levels +1 in a design point \( \mathbf{x} \), which is given by \( d(\mathbf{x}) = (K + \sum_{j=1}^{K} x_j)/2 \). We denote the minimal and maximal number of active rules by \( L \) and \( U \), respectively, and assume \( L < U \). This excludes the case \( L = U \), in which the design matrix \( F \) would not have full column rank and hence \( \beta \) could not be estimated. The design region is then specified by

\[ \mathcal{X} = \{ \mathbf{x} \in \{-1,+1\}^K \mid L \leq d(\mathbf{x}) \leq U \} = \{ \mathbf{x} \mid 2L - K \leq \sum_{j=1}^{K} x_j \leq 2U - K \}. \]

The (unrestricted) full factorial design region would be given by \( L = 0 \) and \( U = K \).

It is well-known (see e.g. [Searle, 1971, p. 90, or Rao, 1973, p. 226]), that for \( F \) with full column rank \( \beta \) is estimable and the variance of the least squares estimator is proportional to the inverse of the information matrix

\[ F^\top F = \sum_{i=1}^{N} f(x_i) f(x_i)^\top. \]

To facilitate the search for optimal designs we will make use of approximate design theory (see for example [Silvey, 1980]). In this context an approximate design \( \xi \) is defined by

\[ \xi = \begin{bmatrix} x_1 & \ldots & x_n \\ w_1 & \ldots & w_n \end{bmatrix}, \]

where \( x_1, \ldots, x_n \in \mathcal{X} \) are mutually distinct settings with weights \( w_i \geq 0 \), \( i = 1, \ldots, n \), \( \sum_{i=1}^{n} w_i = 1 \). Here the weights \( w_i \) represent the proportions \( \xi(x_i) \) of observations, which should be spent at \( \mathbf{x} \).

The corresponding (weighted) information matrix is defined as

\[ \mathbf{M}(\xi) = \sum_{i=1}^{n} w_i f(x_i) f(x_i)^\top, \]

which is the average information per observation. In the case of an exact design \( (x_1, \ldots, x_N) \) for \( N \) observation the weights \( w_i \) equal \( N_i/N \), where \( N_i \) is the number of replications at \( x_i \), and the weighted information matrix equals \( N^{-1}F^\top F \).

A design \( \xi^* \) on \( \mathcal{X} \) is \( D \)-optimal if and only if it maximises the determinant of the information matrix, i.e.

\[ \det(\mathbf{M}(\xi^*)) \geq \det(\mathbf{M}(\xi)). \]
for all designs $\xi$ on $X$. Under the $D$-criterion the volume of the confidence ellipsoid for $\beta$ is minimised.

We will use invariance properties to reduce the complexity of the optimisation problem. See for example Pukelsheim (1993) and Schwabe (1996) for details and further references. This approach is also used in Filová et al. (2011) to derive results on $E$-optimal spring balance weighing designs. In this context the design region consists of the vertices of the $K$ dimensional unit cube $\{0, 1\}^K$ and no restriction on the number of active levels 1 is considered.

The design region $X$, considered as a subset of the vertices of the hypercube $\{-1, +1\}^K$, is invariant under permutations of the entries in the design points, i.e. permutations of rules, which result in appropriate rotations of the hypercube. Under the group of these permutations there are $U - L + 1$ orbits, which will be denoted by $O_k$, $k = L, \ldots, U$. The orbit $O_k = \{x|d(x) = k\}$ consists of all items with $k$ active rules or, equivalently, of the design points with $k$ entries equal to $+1$, i.e.

$$O_k = \{x \in X | \sum_{j=1}^{K} x_j = 2k - K\}.$$  

Note, that the orbits yield a partition of the design region $X$, i.e. they are mutually disjoint and $X = \bigcup_{k=L}^{U} O_k$. The present main effects model is linearly equivariant with respect to permutations, i.e. for each permutation $P$ exists a matrix $Q$ such that $f(Px) = Qf(x)$ uniformly in $x$. A design $\xi$, which remains unchanged, if the support is transformed, here by permutation of rules, is called invariant. From the equivariance of the model and the invariance of the design region follows that there exists an invariant $D$-optimal design.

These invariant designs have uniform weights on each orbit, i.e. for all $x_1, x_2 \in O_k$ follows $\xi(x_1) = \xi(x_2)$. Denote the uniform design on the orbit $O_k$ with $k$ rules by $\xi_k$. These are called vertex designs in Filová et al. (2011). For the invariant design $\xi_k$ on $O_k$ the weights $\xi_k(x) = 1/\binom{K}{k}$ are determined as the reciprocal of the number $\binom{K}{k}$ of design points in the orbit, and the information matrix is given by

$$M(\xi_k) = \binom{K}{k}^{-1} \sum_{x \in O_k} f(x)f(x)\top.$$  

Every invariant design $\xi$ can be written as a weighted sum of vertex designs, $\xi = \sum_{k=L}^{U} \bar{w}_k \xi_k$ with weights $\bar{w}_k \geq 0$, $\sum_{k=L}^{U} \bar{w}_k = 1$, for the orbits. Then the information matrix of an invariant design $\xi$ on $X$ equals

$$M(\xi) = \sum_{k=L}^{U} \bar{w}_k M(\xi_k).$$
Hence the optimisation can be confined to finding the optimal weights \( \bar{w}_k \). Each invariant design can be characterised by the orbits \( O_k \) and their corresponding weights \( \bar{w}_k \). Due to this fact we can use the notation

\[
\bar{\xi} = \begin{pmatrix} k_1 & \cdots & k_n \\ \bar{w}_1 & \cdots & \bar{w}_n \end{pmatrix}
\]

\( k_i \in \{ L, \ldots, U \}, i = 1, \ldots, n \), whenever an invariant design on \( n \) orbits is given explicitly, where only orbits with non-zero weights \( \bar{w}_k \) are specified.

In the particular case that the constraints are symmetric, \( L + U = K \), i.e. whenever items with \( k \) active rules are allowed then so are those with \( K - k \) active rules, then invariance additionally is present with respect to the sign change of the whole vector of the design point, i.e. switching from \( k \) active rules to \( k \) inactive rules. Consequently it follows in this case, that there is an invariant \( D \)-optimal design with \( \bar{w}_k = \bar{w}_{K-k} \).

4 Structure of the Information Matrix

The entries of the weighted information matrix are moments with respect to the design \( \bar{\xi} \), with the general form

\[
\sum_{i=1}^{n} w_i x_{ik}^u x_{i\ell}^v, \quad k, \ell \in \{1, \ldots, K\}, u, v \in \{0, 1\}.
\]

For an invariant design \( \bar{\xi} \) the moments reduce to only three different values. The diagonal, with the constant \( (u = v = 0) \) and second moments \( (k = \ell, u = v = 1) \), is given by

\[
\sum_{i=1}^{n} w_i = 1 \quad \text{and} \quad \sum_{i=1}^{n} w_i x_{ik}^2 = 1, \quad k = 1, \ldots, K.
\]

The off-diagonal entries in the first row and first column, i.e. the first moments \( (u = 0, v = 1 \text{ or vice versa}) \), are identical

\[
m_1(\bar{\xi}) = \sum_{i=1}^{n} w_i x_{ik}, \quad k = 1, \ldots, K,
\]

while all other off-diagonal entries, i.e. the mixed moments \( (k \neq \ell, u = v = 1) \), also coincide

\[
m_2(\bar{\xi}) = \sum_{i=1}^{n} w_i x_{ik} x_{i\ell}, \quad 1 \leq k < \ell \leq K.
\]

Denoting the \( K \)-dimensional vector of ones by \( 1_K \) and the \( K \times K \) identity matrix by \( I_K \), the information matrix becomes

\[
M(\bar{\xi}) = \begin{pmatrix} 1 \\ m_1(\bar{\xi})1_K^{\top} & M_{22}(\bar{\xi}) \end{pmatrix} \quad (1)
\]
with the submatrix
\[
M_{22}(\bar{\xi}) = (1 - m_2(\bar{\xi}))I_K + m_2(\bar{\xi})1_K1_K^T.
\]

Even though \(m_1(\bar{\xi}), m_2(\bar{\xi})\) and hence \(M_{22}(\bar{\xi})\) depend on the design \(\bar{\xi}\), we will omit the argument for the sake of brevity, where it does not lead to confusions.

As we have seen before, the information matrix of an invariant design can be written as a weighted sum of the information matrices of the orbits. These matrices \(M(\bar{\xi}_k)\) have the same structure as in (1), with the moments replaced by the moments of the \(k\)-th orbit,

\[
m_1(\bar{\xi}_k) = \frac{2k - K}{K}, \tag{2}
\]

and

\[
m_2(\bar{\xi}_k) = \frac{(2k - K)^2 - K}{K(K - 1)}, \tag{3}
\]

which can be calculated by counting the number of summands equal to \(+1\) or \(-1\). Some properties following from counting the number of summands equal to \(+1\) or \(-1\). Some properties following from (2) and (3) we will need later are

\[
m_1(\bar{\xi}_k) \leq 0 \text{ if and only if } k \leq \frac{K}{2}, \tag{4}
\]

and

\[
m_2(\bar{\xi}_k) \leq 0 \text{ if and only if } \frac{K - \sqrt{K}}{2} \leq k \leq \frac{K + \sqrt{K}}{2}. \tag{5}
\]

Equality holds on the left-hand side of (4) if and only if equality holds on the right-hand side. Analogously \(m_2(\bar{\xi}_k) = 0\) in (5) if and only if equality holds for one of the relations on the right-hand side of the condition. Note, that due to symmetry

\[
m_1(\bar{\xi}_k) = -m_1(\bar{\xi}_{K-k}) \quad \text{and} \quad m_2(\bar{\xi}_k) = m_2(\bar{\xi}_{K-k}). \tag{6}
\]

For further calculations also note that

\[
m_1 = \sum_{k=L}^{U} \bar{w}_k m_1(\bar{\xi}_k) P \quad \text{and} \quad m_2 = \sum_{k=L}^{U} \bar{w}_k m_2(\bar{\xi}_k). \tag{7}
\]

For designs, which are also invariant with respect to sign change, it follows that \(\bar{w}_k = \bar{w}_{K-k}\) and hence \(m_1 = 0\). This can be easily seen from (7) and (6).

In fact \(m_1 = 0\) holds for all symmetric invariant designs, i.e. \(\bar{w}_k = \bar{w}_{K-k}\), for all \(k = L, \ldots, U\). In an invariant design with at least two orbits a necessary condition for \(m_1 = 0\) is, that there are \(k, \ell \in \{L, \ldots, U\}\), with \(\bar{w}_k > 0\) and
\( \bar{w}_\ell > 0 \), such that \( k < K/2 < \ell \). This follows from (4). Analogously follows from (5) that \( m_2 = 0 \) only if either

\[
k \in \left( \frac{K - \sqrt{K}}{2}, \frac{K + \sqrt{K}}{2} \right) \quad \text{and} \quad \ell \notin \left( \frac{K - \sqrt{K}}{2}, \frac{K + \sqrt{K}}{2} \right)
\]

or, if the boundaries of the given interval are integers, the design consists of the two orbits corresponding to \( (K - \sqrt{K})/2 \) and \( (K + \sqrt{K})/2 \) only.

5 Invariant \( D \)-optimal Designs

As stated in the previous section, we can confine the optimisation on finding optimal weights \( \bar{w}_L, \bar{w}_{L+1}, \ldots, \bar{w}_U \). The determinant of the information matrix can be calculated using some standard results on determinants:

\[
\det(\mathbf{M}(\xi)) = \det \left( \mathbf{M}_{22} - m_1^2 \mathbf{1}_K \mathbf{1}_K^T \right) \\
= \det \left( (1 - m_2)\mathbf{I}_K + (m_2 - m_1^2) \mathbf{1}_K \mathbf{1}_K^T \right) \\
= (1 - m_2)^{K-1} (1 + (K - 1)m_2 - Km_1^2) . \quad (8)
\]

As a direct consequence conditions for the regularity of the information matrix follow:

Lemma 1. For an invariant design \( \bar{\xi} \) the information matrix \( \mathbf{M}(\bar{\xi}) \) is regular if and only if there exist \( k, \ell \in \{L, \ldots, U\}, k \neq \ell \), such that \( \bar{w}_k > 0 \) and \( \bar{w}_\ell > 0 \), and, for \( K \geq 2 \), either \( k \) or \( \ell \) is strictly between 0 and \( K \).

As we will see shortly, there are two different cases for optimal invariant designs: Either \( m_1 = m_2 = 0 \) or its complement. The first case holds if and only if \( (K - 2L)(2U - K) \geq K \). The corresponding information matrix is the identity matrix and hence the designs are as efficient as the \( 2^K \) full factorial design. Even for the unrestricted design region \( \{-1, +1\}^K \). Theorem 2 shows the corresponding result.

If on the other hand \( (K - 2L)(2U - K) < K \), invariant designs on the boundary orbits \( \mathcal{O}_L \) and \( \mathcal{O}_U \) are optimal. In fact \( D \)-optimal designs have to be concentrated on these two orbits. This can happen if the interval \([L, U]\) is too narrow or does not include \( K/2 \). In those cases it follows that \( m_1 \neq 0 \) or \( m_2 \neq 0 \) from (4) and (5). (See Lemma 3 in the Appendix)

The weight \( \bar{w}_L^* \) in the following Theorem maximises the determinant of the information matrix for invariant designs with \( \bar{w}_U = 1 - \bar{w}_L \).
Theorem 1. Let \( \bar{w}^*_L = 1/2 \) if \( L + U = K \) and
\[
\bar{w}^*_L = \frac{(U - L)(L + U - K)K - 2U(K - U)}{2(U - L)(L + U - K)(K + 1)} + \frac{\sqrt{(U - L)^2(L + U - K)^2K^2 + 4L(K - L)U(K - U)}}{2(U - L)(L + U - K)(K + 1)}
\]
otherwise.

In the case
\[
(K - 2L)(2U - K) < K
\]
the invariant design on the orbits \( \mathcal{O}_L \) and \( \mathcal{O}_U \) with weights \( \bar{w}^*_L \) and \( \bar{w}^*_U = 1 - \bar{w}^*_L \) is \( D \)-optimal.

The weight \( \bar{w}^*_L \) simplifies considerably for \( L = 0 \) and does not depend on \( U \). In this case \( \bar{w}^*_L = 1/(K + 1) \). This is exemplified in Table 1. Because of symmetry follows \( \bar{w}^*_L = K/(K + 1) \), if \( U = K \).

Another property of the weight \( \bar{w}^*_L \) as a function of \( U \), which is visible in the table, is the symmetry around \( K/2 \). For fixed \( L, K \) and some constant \( c > 0 \) the weight for \( U = K/2 + c \) is the same as for \( U = K/2 - c \). Taking into account that for optimality \( 10 \) and \( L < U \) must be satisfied, this is especially relevant for \( U \) close to \( K/2 \), e.g. for \( K \) odd and \( U = (K \pm 1)/2 \).

For symmetric constraints the following result is immediate.

Corollary 1. Let \( L + U = K \). If
\[
\frac{K - \sqrt{K}}{2} < L
\]
then the invariant design with \( \bar{w}_L = \bar{w}_U = 1/2 \) is \( D \)-optimal.

The next result is concerned with designs on a sufficiently wide range of orbits.

Theorem 2. In the case
\[
(K - 2L)(2U - K) \geq K.
\]
an invariant design is \( D \)-optimal if and only if \( m_1 = m_2 = 0 \).

For symmetric regions the result again simplifies:

Corollary 2. Let \( L + U = K \). If
\[
L \leq \frac{K - \sqrt{K}}{2}
\]
then an invariant design is \( D \)-optimal if and only if \( m_2 = 0 \).
In the situation of Theorem 2 and Corollary 2 the information matrix of the optimal design is the \( p \times p \) identity matrix and coincides with the information matrix of the \( 2^K \) factorial on the unrestricted design region.

In the proof of Theorem 2 given in the appendix we show that exemplary designs \( \xi^* \) of the form

\[
\xi^* = \begin{pmatrix}
L & \ell & U \\
\bar{w}_L^* & 1 - \bar{w}_L^* - \bar{w}_U^* & \bar{w}_U^*
\end{pmatrix}
\]

(13)

fulfil the conditions of the theorem. If \( K \) is even \( \ell = K/2 \) may be chosen for the interior orbit. If \( K \) is odd the choice depends on \( L \) and \( U \), too. If \( L < (K - \sqrt{K})/2 \) choose \( \ell = (K - 1)/2 \). If \( U > (K + \sqrt{K})/2 \) choose \( \ell = (K + 1)/2 \). If both conditions are met, we can choose any of the two given values. These choices ensure, that \( L < \ell < U \).

On the boundary orbits the weights are

\[
\bar{w}_L^* = \frac{K + (2\ell - K)(2U - K)}{4(\ell - L)(U - L)} \quad \text{and} \quad \bar{w}_U^* = \frac{K + (2L - K)(2\ell - K)}{4(U - \ell)(U - L)}. \quad (14)
\]

Condition (11) guarantees, that the weight of the interior orbit is non-negative. If equality holds in (11), then the middle weight is 0, and a two orbit design on \( O_L \) and \( O_U \) with weights

\[
\bar{w}_L^* = \frac{2U - K}{2(U - L)} \quad \text{and} \quad \bar{w}_U^* = \frac{K - 2L}{2(U - L)}
\]

is optimal. Examples for these designs are given in Table 2.

Note that under the conditions of Theorem 2 the optimal design is not necessarily unique. The weights for a general optimal three orbit design with orbits \( O_L, O_\ell \) and \( O_U \), \( L \leq \ell < \bar{U} \leq U \) can be calculated by substituting \( L \) and \( U \) with \( \bar{L} \) and \( \bar{U} \), respectively, in (14). Condition (11) of Theorem 2 is replaced by

\[
(K - 2\bar{L})(2\bar{U} - K) \geq K \\
(2\bar{\ell} - K)(2\bar{U} - K) \geq -K \\
(2\bar{L} - K)(2\bar{\ell} - K) \geq -K.
\]

Again these conditions ensure, that the weights are non-negative.

An example for a symmetric optimal design, still under the conditions of Theorem 2 is given by

\[
\begin{pmatrix}
K_1^* & K_2^* & K - k_2^* & K - k_1^* \\
\bar{w}_1^* & \bar{w}_2^* & \bar{w}_2^* & \bar{w}_1^*
\end{pmatrix}
\]

with weights

\[
\bar{w}_1^* = \frac{K - (K - 2k_2^*)^2}{8(k_2^* - k_1^*)(K - k_1^* - k_2^*)} \quad \text{and} \quad \bar{w}_2^* = \frac{1 - 2\bar{w}_1^*}{2}
\]
for any $k_1^*, k_2^*$ satisfying
\[
L \leq k_1^* < \frac{K - \sqrt{K}}{2} \leq k_2^* \leq \frac{K}{2} \quad \text{and} \quad K - k_1^* \leq U.
\]
If $k_2^* = (K - \sqrt{K})/2$ the weight $\bar{w}_1^* = 0$ and the design reduces to a symmetric design on two orbits $\mathcal{O}_{k_2}$ and $\mathcal{O}_{K-k_2}$ with $\bar{w}_2^* = 1/2$. For $k_2^* = K/2$ it becomes a symmetric three-orbit design.

Note especially, that designs with symmetric orbits can be optimal in the case of asymmetric restrictions on the design region and vice versa. See for example Table 3.

6 Concluding Remarks

It is noteworthy, that the above mentioned three and four orbit designs have rational weights and hence can be implemented in practice quite easily. For the two orbit designs from Theorem 1 this is not always the case. An affirmative example for $K = 6$ rules and bounds $L = 2$, $U = 4$ with 30 observations is given in Table 4.

The optimal designs in Theorem 2 result in an information matrix equal to the identity and are, hence, as efficient as the full factorial design. Therefore they are also optimal for other optimality criteria like the A-criterion for minimising the average variance of the parameter estimates, the $E$-criterion of maximising the smallest eigenvalue of the information matrix, or the general class of Kiefer’s $\Phi_q$-criteria based on the eigenvalues of the information matrix (see e.g. Pukelsheim, 1993).

In some particular cases of wide margins the optimal designs turn out to be regular fractional factorial designs. Consider for example $K = 4$, $L = 1$ and $U = 3$. An optimal design is given by the orbits $\mathcal{O}_1$ and $\mathcal{O}_3$ with $\bar{w}_1 = 1/2$ which form an $2^3-1$ fractional factorial design. In general orthogonal arrays can occur. The symmetric four orbit design in the case $K = 5$ with $k_1^* = 1$ and $k_2^* = 2$ is given by the first columns of an $OA(40, 2^{20})$ (Sloan, 2018). While orthogonal arrays appear naturally in these cases, further studies are necessary to explore the specific relationship. Further work has also to be done to generalise the present results to models incorporating interactions between the rules.

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Appendix A: Proofs

Proof of Lemma 1. The information matrix is regular if and only if its determinant is positive. Since the factors of the determinant in (8) are non-negative, this is equivalent to both of the factors being positive. Consider

\[ 1 + (K - 1)m_2 - Km_1^2 = \frac{4}{K} \sum_{k=L}^U \bar{w}_k \left( k - \left( \sum_{\ell=L}^U \bar{w}_\ell \right) \right)^2 \geq 0, \]

which is 0 if and only if \( \bar{w}_k = 1 \) for some \( k \in \{L, \ldots, U\} \). Hence there have to be at least two orbits with positive weight.

For \( K \geq 2 \) note that

\[ 1 - m_2 = \frac{4}{K(K - 1)} \sum_{k=L}^U \bar{w}_k(K - k) \geq 0. \]

This expression is equal to 0 if and only if \( \bar{w}_k = 0 \) for all \( k \in \{1, \ldots, K - 1\} \cap \{L, \ldots, U\} \). Hence the Lemma follows.

Before we give the proof for Theorem 1 we introduce the following auxiliary result:

Lemma 2. Let \( \bar{\xi} \) be an invariant design. Then the sensitivity function \( \psi(x) = f(x)^\top M(\bar{\xi})^{-1} f(x) \) is constant on the orbits, \( \psi(x) = \tilde{\psi}(k) \) for \( x \in O_k \), say, and the function \( \tilde{\psi} \) is a polynomial in \( k \) of degree at most 2.

Proof of Lemma 2. In our case the sensitivity \( \psi \) is given by

\[ \psi(x) = a_0 + a_1 (1_k^\top x) + a_2 (1_k^\top x)^2 \]

with the following coefficients:

\[ a_0 = \frac{1 + (K - 1)m_2}{1 + (K - 1)m_2 - Km_1^2} + \frac{K}{1 - m_2}, \quad a_1 = -\frac{2m_1}{1 + (K - 1)m_2 - Km_1^2}, \]

\[ a_2 = \frac{m_1^2 - m_2}{(1 - m_2)(1 + (K - 1)m_2 - Km_1^2)}. \]

Since \( 1_k^\top x = 2k - K \) for \( x \in O_k \), the sensitivity function \( \psi \) is constant on the orbits and \( \tilde{\psi}(k) = a_0 + a_1(2k - K) + a_2(2k - K)^2 \), for \( x \in O_k \), is a polynomial of degree at most 2.

Lemma 3. Let \( (K - 2L)(2U - K) < K \), then \( m_1 \neq 0 \) or \( m_2 \neq 0 \) for every invariant design \( \bar{\xi} \).
Proof of Lemma 3. We prove the lemma by contradiction. Let \( m_1 = m_2 = 0 \), then \( \sum_{k=L}^{U} \bar{w}_k(2k - K) = 0 \) and

\[
\sum_{k=L}^{U} \bar{w}_k(2k - K)^2 = K. \tag{16}
\]

These sums can be seen as the mean and variance of a discrete zero-mean random variable taking values in \( \{2L-K, \ldots, 2U-K\} \). Using the inequality in Bhatia and Davis (2000) the variance is bounded above:

\[
\sum_{k=L}^{U} \bar{w}_k(2k - K)^2 \leq (K - 2L)(2U - K).
\]

Since \( (K - 2L)(2U - K) < K \) this is a contradiction to equation (16).

Proof of Theorem 1. We will show first, that the optimal design has to be concentrated on the two boundary orbits.

For an optimal design \( \xi^* \) the equivalence theorem [Kiefer and Wolfowitz, 1960] yields

\[
\psi(x) = f(x)^\top M(\bar{\xi}^*)^{-1} f(x) \leq p \tag{17}
\]

for all \( x \in \mathcal{X} \). For an optimal invariant design this can be written equivalently as \( \bar{\psi}(k) \leq p \) for all \( k \in \{L, \ldots, U\} \). Consider the leading coefficient \( a_2 \) of \( \psi \).

Let \( a_2 \leq 0 \), then, following from the equivalence theorem, either \( \bar{\psi}(k) = p \) for exactly one \( k \in \{L, \ldots, U\} \) or \( \bar{\psi}(k) = \bar{\psi}(k+1) = p \) for some \( k \in \{L, \ldots, U-1\} \).

In the latter case \( \bar{\psi}(k) \leq p \) for all \( k \in \{0, \ldots, K\} \) and thus the design would be optimal not only on the design region \( \mathcal{X} \) but on the whole set \( \{-1,+1\}^K \). It follows, that the information matrix is the identity matrix. But this contradicts, that by Lemma 3 either \( m_1 \neq 0 \) or \( m_2 \neq 0 \).

In the first case the optimal design would be concentrated on the orbit \( \mathcal{O}_k \), which leads to a singular information matrix and consequently to a contradiction.

Hence, \( a_2 > 0 \) and \( \bar{\psi} \) attains its maximum (equal to \( p \)) on the boundary, i.e. the optimal design is concentrated on the orbits \( \mathcal{O}_L \) and \( \mathcal{O}_U \).

In order to obtain the optimal design, it remains to find the optimal weight \( w^*_L \) on \( \mathcal{O}_L \) (and consequently \( w^*_U = 1 - w^*_L \) on \( \mathcal{O}_U \)). Optimizing the determinant then yields the optimal weight \( w^*_L \) specified in the theorem.

Proof of Theorem 2. Since any invariant design \( \bar{\xi} \) on \( \mathcal{X} \) with \( m_1 = m_2 = 0 \) is optimal on the unrestricted design region \( \{-1,+1\}^K \), by majorization, these designs are also optimal on the design region \( \mathcal{X} \).
For $K = 1$ there is nothing to show. For $K \geq 2$ we will show that the design in (13) yields $m_1 = m_2 = 0$ and hence is optimal.

It follows from condition (11) of the theorem, that

$$L < \frac{K - \sqrt{K}}{2} \quad \text{or} \quad U > \frac{K + \sqrt{K}}{2}$$

and, that $L < K/2 < U$. Hence we can choose the interior orbit $O_\ell$ as described after (13). The weights are non-negative by the choice of $\ell$, since $L < \ell < U$. For the first moment $m_1$ it follows that

$$m_1 = \frac{2(L - \ell)}{K} \bar{w}_L + \frac{2\ell - K}{K} \bar{w}_U = \frac{(2\ell - K)(-2U + K + 2U - 2L + 2L - K)}{2K(U - L)} = 0.$$ 

The second quantity $m_2$ can be written as

$$m_2 = \frac{4(\ell - L)(K - L - \ell)}{K(K - 1)} \bar{w}_L + \frac{(2\ell - K)^2 - K}{K(K - 1)} \bar{w}_U + \frac{4(U - \ell)(U + \ell - K)}{K(K - 1)} \bar{w}_U.$$ 

Substituting the weights yields

$$m_2 = \frac{(K - L - \ell)(K + (2\ell - K)(2U - K)) + ((2\ell - K)^2 - K)(U - L)}{K(K - 1)(U - L)} + \frac{(U + \ell - K)(K + (2\ell - K)(2L - K))}{K(K - 1)(U - L)} = 0.$$ 

Hence $m_1 = m_2 = 0$ and the given design is $D$-optimal, which concludes the proof.

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### Table 1: Examples for optimal invariant two orbit designs from Theorem 1 and their efficiency with respect to the full factorial design

| $K$ | $K - \sqrt{K}$ | $K + \sqrt{K}$ | $L$ | $\tilde{U}$ | $\tilde{U}_i$ | Efficiency |
|-----|----------------|----------------|-----|------------|-------------|------------|
| 2   | 0.29           | 1.71           | 0   | 1          | 0.3333      | 0.6667     | 0.8399     |
|     | 1              | 2              | 0.5000 | 0.5000   | 0.8774     |
| 3   | 0.63           | 2.37           | 0   | 1          | 0.2500      | 0.7500     | 0.7071     |
|     | 1              | 2              | 0.2000 | 0.2000   | 0.6063     |
|     | 0              | 2              | 0.2000 | 0.8000   | 0.9507     |
|     | 1              | 2              | 0.2000 | 0.6000   | 0.8386     |
| 4   | 1.00           | 3.00           | 0   | 1          | 0.1667      | 0.8333     | 0.5291     |
|     | 0              | 2              | 0.1667 | 0.8333   | 0.8736     |
|     | 1              | 2              | 0.3333 | 0.6667   | 0.7828     |
|     | 1              | 3              | 0.3333 | 0.6667   | 0.9863     |
|     | 2              | 3              | 0.5000 | 0.5000   | 0.8636     |
| 5   | 1.38           | 3.62           | 0   | 1          | 0.1429      | 0.8571     | 0.4688     |
|     | 0              | 2              | 0.1429 | 0.8571   | 0.7994     |
|     | 0              | 3              | 0.1429 | 0.8571   | 0.9764     |
|     | 1              | 2              | 0.2857 | 0.7143   | 0.7263     |
|     | 1              | 3              | 0.2590 | 0.7410   | 0.9486     |
|     | 2              | 3              | 0.4286 | 0.5714   | 0.8491     |
|     | 2              | 4              | 0.5000 | 0.5000   | 0.9882     |
| 6   | 1.78           | 4.22           | 0   | 1          | 0.1000      | 0.9000     | 0.3482     |
|     | 0              | 2              | 0.1000 | 0.9000   | 0.6259     |
|     | 0              | 3              | 0.1000 | 0.9000   | 0.8299     |
|     | 0              | 4              | 0.1000 | 0.9000   | 0.9564     |
|     | 1              | 2              | 0.2000 | 0.8000   | 0.5844     |
|     | 1              | 3              | 0.1643 | 0.8357   | 0.8045     |
|     | 1              | 4              | 0.1545 | 0.8455   | 0.9432     |
|     | 1              | 5              | 0.1545 | 0.8455   | 0.9991     |
|     | 2              | 3              | 0.3000 | 0.7000   | 0.7465     |
|     | 2              | 4              | 0.2539 | 0.7461   | 0.9158     |
|     | 2              | 5              | 0.2539 | 0.7461   | 0.9932     |
|     | 3              | 4              | 0.4000 | 0.6000   | 0.8418     |
|     | 3              | 5              | 0.4000 | 0.6000   | 0.9670     |
|     | 4              | 5              | 0.5000 | 0.5000   | 0.8733     |
Table 2: Optimal invariant three orbit designs from Theorem 2

| $K$ | $L$ | $U$ | $\ell$ | $\bar{w}^*_L$ | $\bar{w}^*_U$ | $\bar{w}^*_\ell$ |
|-----|-----|-----|-------|---------------|---------------|---------------|
| 2   | 0   | 2   | 1     | 0.2500        | 0.2500        | 0.5000        |
| 3   | 0   | 2   | 1     | 0.2500        | 0.7500        | -             |
|     | 0   | 3   | 1     | -             | 0.2500        | 0.7500        |
| 4   | 0   | 3   | 2     | 0.1667        | 0.3333        | 0.5000        |
|     | 0   | 4   | 2     | 0.1250        | 0.1250        | 0.7500        |
|     | 1   | 3   | 2     | 0.5000        | 0.5000        | -             |
| 5   | 0   | 3   | 2     | 0.1667        | 0.8333        | -             |
|     | 0   | 4   | 2     | 0.0625        | 0.3125        | 0.6250        |
|     | 0   | 5   | 2     | -             | 0.1667        | 0.8333        |
|     | 1   | 4   | 2     | 0.1667        | 0.3333        | 0.5000        |
| 6   | 0   | 4   | 3     | 0.1250        | 0.3750        | 0.5000        |
|     | 0   | 5   | 3     | 0.1000        | 0.1500        | 0.7500        |
|     | 0   | 6   | 3     | 0.0833        | 0.0833        | 0.8333        |
|     | 1   | 4   | 3     | 0.2500        | 0.5000        | 0.2500        |
|     | 1   | 5   | 3     | 0.1875        | 0.1875        | 0.6250        |
| 9   | 0   | 5   | 4     | 0.1000        | 0.9000        | -             |
|     | 0   | 6   | 4     | 0.0625        | 0.3750        | 0.5625        |
|     | 0   | 7   | 4     | 0.0357        | 0.2143        | 0.7500        |
|     | 0   | 8   | 4     | 0.0156        | 0.1406        | 0.8438        |
|     | 0   | 9   | 4     | -             | 0.1000        | 0.9000        |
|     | 1   | 6   | 4     | 0.1000        | 0.4000        | 0.5000        |
|     | 1   | 7   | 4     | 0.0556        | 0.2222        | 0.7222        |
|     | 1   | 8   | 4     | 0.0238        | 0.1429        | 0.8333        |
| 2   | 6   | 4     | 0.1875 | 0.4375 | 0.3750 |
| 2   | 7   | 4     | 0.1000 | 0.2333 | 0.6667 |
| 3   | 6   | 4     | 0.5000 | 0.5000 | -     |
Table 3: Optimal symmetric invariant four orbit designs from Theorem 2

| $K$ | $L$ | $U$ | $k_1^*$ | $k_2^*$ | $k_3^*$ | $k_4^*$ | $\bar{w}_1^*$ | $\bar{w}_2^*$ | $\bar{w}_3^*$ | $\bar{w}_4^*$ |
|-----|-----|-----|---------|---------|---------|---------|-------------|-------------|-------------|-------------|
| 3   | 0   | 0   | 3       | 3       | 3       | 3       | 0.1250      | 0.3750      | 0.3750      | 0.1250      |
| 4   | 0   | 4   | 0       | 1       | 2       | 3       | 0.2500      | 0.2500      | 0.2500      | 0.2500      |
| 5   | 0   | 4   | 1       | 2       | 3       | 4       | 0.2500      | 0.2500      | 0.2500      | 0.2500      |
|     | 0   | 5   | 0       | 2       | 3       | 5       | 0.0833      | 0.4167      | 0.4167      | 0.0833      |
|     | 0   | 5   | 1       | 2       | 3       | 4       | 0.2500      | 0.2500      | 0.2500      | 0.2500      |
| 6   | 0   | 5   | 1       | 2       | 4       | 5       | 0.0833      | 0.4167      | 0.4167      | 0.0833      |
|     | 0   | 6   | 0       | 2       | 3       | 5       | 0.0312      | 0.4688      | 0.4688      | 0.0312      |
|     | 0   | 6   | 1       | 2       | 4       | 5       | 0.0833      | 0.4167      | 0.4167      | 0.0833      |
| 7   | 1   | 5   | 1       | 2       | 4       | 5       | 0.0833      | 0.4167      | 0.4167      | 0.0833      |
| 9   | 0   | 7   | 2       | 4       | 5       | 7       | 0.1667      | 0.3333      | 0.3333      | 0.1667      |
|     | 0   | 8   | 1       | 4       | 5       | 8       | 0.0833      | 0.4167      | 0.4167      | 0.0833      |
|     | 0   | 8   | 2       | 4       | 5       | 7       | 0.1667      | 0.3333      | 0.3333      | 0.1667      |
|     | 0   | 9   | 0       | 4       | 5       | 9       | 0.0500      | 0.4500      | 0.4500      | 0.0500      |
|     | 0   | 9   | 1       | 4       | 5       | 8       | 0.0833      | 0.4167      | 0.4167      | 0.0833      |
|     | 0   | 9   | 2       | 4       | 5       | 7       | 0.1667      | 0.3333      | 0.3333      | 0.1667      |
| 1   | 7   | 2   | 4       | 5       | 7       | 0.1667      | 0.3333      | 0.3333      | 0.1667      |
| 1   | 8   | 1   | 4       | 5       | 8       | 0.0833      | 0.4167      | 0.4167      | 0.0833      |
| 1   | 8   | 2   | 4       | 5       | 7       | 0.1667      | 0.3333      | 0.3333      | 0.1667      |
| 2   | 7   | 2   | 4       | 5       | 7       | 0.1667      | 0.3333      | 0.3333      | 0.1667      |
Table 4: Design for the invariant optimal two orbit design for $K = 6$ with $L = 2$ and $U = 4$, $+$ and $-$ denote $+1$ and $-1$, respectively

| + | + | - | - | - |
|---|---|---|---|---|
| + | - | + | - | - |
| - | + | - | - | - |
| + | - | - | + | - |
| - | - | - | + | - |
| - | - | + | - | + |
| - | - | - | + | + |
| + | + | + | - | - |
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