Optimal designs for $K$-factor two-level models with first-order interactions on a symmetrically restricted design region

Fritjof Freise
TU Dortmund University, Department of Statistics, Vogelpothsweg 87, 44227 Dortmund, Germany, e-mail: fritjof.freise@tu-dortmund.de

Rainer Schwabe
University of Magdeburg, Institute for Mathematical Stochastics, Universitätsplatz 2, 39106 Magdeburg, Germany, e-mail: rainer.schwabe@ovgu.de

Abstract

We develop $D$-optimal designs for linear models with first-order interactions on a subset of the $2^K$ full factorial design region, when both the number of factors set to the higher level and the number of factors set to the lower level are simultaneously bounded by the same threshold. It turns out that in the case of narrow margins the optimal design is concentrated only on those design points, for which either the threshold is attained or the numbers of high and low levels are as equal as possible. In the case of wider 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.

1 Introduction

In the situation of item calibration for psychological tests the goal is to estimate the difficulty of new items or of the effect of certain attributes of an item. In the rule based approach for item generation the difficulty of an item can be split into several components corresponding to different rules, which may or may not be applied. Conceptually this results in a linear predictor for the difficulty based on the active rules. Typically an item will become more difficult, if more rules are used in its construction. To avoid so called ceiling or bottom effects, i.e. an item is answered correctly or wrong, respectively, by all the participants, items should not be too difficult nor too easy. Moreover, the assumed model may become inappropriate if too extreme items, i.e. items with too many or items with too few rules, are used. All this may cause the necessity to restrict the number of rules used from below and above. In this scenario standard designs like full or standard fractional factorials are no longer applicable.

The application, which motivated this research, was in the latter regime. Here the total number of rules was six and items with two up to four active rules were to be used. This lead directly to the question in which cases fully efficient designs exist, i.e. designs which are as efficient as the full factorial design. These results, which will be presented in Theorem 1, can also be the basis for the search for and construction of irregular fractions.

For the case of a linear predictor which contains only main effects, optimal designs have been characterized in Freise, Holling and Schwabe (2018). We will follow the lines indicated there to extend the results to situations where first-order (two-factor) interactions have to be incorporated. The approach used for characterizing optimal designs is based on invariance and equivariance considerations with respect

\footnote{corresponding author}
to natural symmetries in both the model and the design region. This approach has successfully been applied also in other settings like spring balance weighing (see Filová, Harman and Klein [2011]), and the findings obtained here may be transferred to other situations, where there are natural constraints on the simultaneous occurrence of high or of low levels, respectively. To keep notations simple and to reduce technicalities, we will confine ourselves to the case of symmetric constraints.

The manuscript is organized as follows. After a brief description of the model and basic concepts of design and invariance in Section 2, the general structure of the information matrix is presented in Section 3. In Section 4 we specialize to the symmetric case and present characterizations of optimal designs in Section 5. The manuscript concludes with a brief discussion on potential extensions in Section 6 and is augmented by tables of optimal designs for up to 22 rules. All proofs are deferred to an appendix.

2 Model Description, Information and Invariance

We consider an experiment in which \( N \) items are presented and \( K \) rules may be used to construct an item. Then an item can be characterized by its settings (design points) \( x = (x_1, \ldots, x_K)^\top \in \{-1, +1\}^K \), where \( x_k = +1 \), if the \( k \)-th rule is used in the construction of the item, and \( x_k = -1 \), if the \( k \)-th rule is absent.

Even though using 0 and 1 for inactive and active rules would seem to be more natural in our application, the present parametrization was chosen out of convenience. Especially the information matrices have a more intuitive representation. Note also, that for the \( D \)-criterion, which is primarily of interest here, reparametrization has no influence on the optimal design.

We assume an underlying analysis of variance model with first-order (two-factor) interactions for the observations, i.e. for the item scores, \( Y_1, \ldots, Y_N \) obtained for \( N \) items described by their settings \( x_1, \ldots, x_N \). This model can be written as

\[
Y_i = f(x_i)^\top \beta + \varepsilon_i, \\
i = 1, \ldots, N,
\]

where the regression function \( f \) is specified by

\[
f(x) = \begin{pmatrix} 1 & x^\top \tilde{x}^\top \end{pmatrix}^\top
\]

and \( \tilde{x} = (x_1 x_2, \ldots, x_{K-1} x_K)^\top \) collects the interactions. The difficulties of the items are, hence, specified by the \( p \)-dimensional parameter vector \( \beta \), which includes a constant term, \( K \) parameters corresponding to the main effects and \( \binom{K}{2} = K(K - 1)/2 \) parameters for the first-order (two-factor) interactions. Thus the total number of parameters amounts to \( p = 1 + K(K + 1)/2 \). The error terms \( \varepsilon_1, \ldots, \varepsilon_N \) are assumed to be centered, uncorrelated and homoscedastic, with \( \text{Var}(\varepsilon_i) = \sigma^2 \).

Note, that in the calibration example several items may be solved by the same person and, hence, the assumption of uncorrelated observations may be violated. Nonetheless, uncorrelatedness of the observations will be assumed here, to keep the results simple.

The quality of an experiment may be measured in terms of the information matrix

\[
M(x_1, \ldots, x_N) = \sum_{i=1}^{N} f(x_i)f(x_i)^\top.
\]

It is well-known that in the case of full rank the variance-covariance matrix of the least squares estimator is proportional to the inverse of the information matrix. Thus the aim of an optimal design is to find optimal settings \( x_1, \ldots, x_N \), which minimize
the variance-covariance matrix or, equivalently, maximize the information matrix in a suitable sense. As a uniform optimization of the matrices in the Loewner ordering of nonnegative definiteness is impossible, one has to choose some real-valued information functional on the matrices. Here we will adopt the most popular criterion of D-optimality, which aims at maximizing the determinant of the information matrix. This can be interpreted as minimizing the volume of the confidence ellipsoid for the whole parameter vector under the additional assumption of Gaussian error terms. However, the results obtained may be generalized also to other criteria which share the invariance properties described below. Examples include A- and E-optimality (see also Filová et al., 2011).

To facilitate the search for optimal designs we will make use of the concepts of approximate designs and the corresponding well-developed theory (see for example Silvey, 1980): An approximate design

\[
\xi = \left\{ x_1 \ldots x_n \right\} \left\{ w_1 \ldots w_n \right\}
\]

is defined by \( n \) mutually different settings \( x_1, \ldots, x_n \) with associated weights \( w_i \geq 0 \) satisfying \( \sum_{i=1}^{n} w_i = 1 \). The settings \( x_i \) in the approximate design \( \xi \) correspond to the mutually different settings occurring in the exact design \( (x_1, \ldots, x_N) \) of sample size \( N \) specified before, and the weights represent the corresponding frequencies \( w_i = N_i / N \) of occurrence, where \( N_i \) is the number of replications of \( x_i \). However, in general, for an approximate design the condition on the weights being multiples of \( 1/N \) is relaxed.

The weighted (per observation) information matrix of an approximate design \( \xi \) is then defined by

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

For an exact design of sample size \( N \) this definition coincides with the standardized information matrix \( 1/N \cdot M(x_1, \ldots, x_N) \).

The settings \( x_i \) may be chosen from a design region \( X \) of possible settings, for which the model equation holds. In the present situation we assume that the design region \( X \subset \{-1,+1\}^K \) is restricted by the possible combinations of rules, i.e. by the number of rules simultaneously applied. Denote by \( d(x) = (\sum_{k=1}^{K} x_k + K)/2 \) the number of active rules, i.e. the number of entries equal to +1 in a design point \( x \) and let \( L \) and \( U \) be the minimal and maximal number, respectively, of active rules allowed. Then the design region is defined as

\[
X_{L,U} = \{ x \in \{-1,+1\}^K; \ L \leq d(x) \leq U \}.
\]

The condition on \( d(x) \) can be rewritten as \( 2L - K \leq \sum_{k=1}^{K} x_k \leq 2U - K \).

One of the major results in the context of approximate design theory is the equivalence theorem of Kiefer and Wolfowitz (1960). It states that a design \( \xi^\ast \) is D-optimal if and only if

\[
f(x)^\top M(\xi^\ast)^{-1} f(x) \leq p
\]

for all design points \( x \) in the design region \( X \). The left-hand side is the so called sensitivity function and will be denoted by \( \psi(x) \).

We will make use of invariance properties to reduce the complexity of the optimization problem. See for example Pukelsheim (1993) and Schwabe (1996) for details and further references. The design problem on the vertices of the hypercube \( \{-1,+1\}^K \) is invariant under permutation of entries in the design point, i.e. the permutation of rules. These permutations constitute a transformation group on the full
2^K hypercube as well as on the restricted design region \( \mathcal{X}_{L,U} \). On the full hypercube there are \( K + 1 \) orbits under the permutation, denoted \( \mathcal{O}_0, \ldots, \mathcal{O}_K \). Each orbit \( \mathcal{O}_k \) consists of all items with \( k \) active rules or, equivalently, of the design points with \( d(\mathbf{x}) = k \) entries equal to +1, \( k = 0, 1, \ldots, K \). Moreover, the regression function is linearly equivariant with respect to these permutations, i.e. for each permutation \( g \) there is a matrix \( Q_g \) such that \( f(g(\mathbf{x})) = Q_g f(\mathbf{x}) \) for all \( \mathbf{x} \). Since the D-criterion is invariant under these conditions, there exists a D-optimal design uniform on the orbits, i.e. all settings within one orbit get the same weight. Such designs will also be called invariant with respect to permutations, since they remain unchanged, if the support is transformed.

Denote the uniform design on the orbit \( \mathcal{O}_k \) with \( k \) active rules by \( \tilde{\xi}_k \). The corresponding information matrix \( M(\tilde{\xi}_k) \) measuring the information of the orbit \( \mathcal{O}_k \) is given by

\[
M(\tilde{\xi}_k) = C(K,k)^{-1} \sum_{\mathbf{x} \in \mathcal{O}_k} f(\mathbf{x})f(\mathbf{x})^\top,
\]

where here and later on we use the notation \( C(K,k) \) for the binomial coefficient \( \binom{K}{k} \), when this is more convenient.

Any invariant design \( \tilde{\xi} \) is a convex combination of these single orbit designs:

\[
\tilde{\xi} = \sum_{k=0}^{K} \tilde{w}_k \tilde{\xi}_k
\]

with weights \( \tilde{w}_k \geq 0 \), \( \sum_{k=0}^{K} \tilde{w}_k = 1 \). Thus the information matrix of an invariant design \( \tilde{\xi} \) becomes

\[
M(\tilde{\xi}) = \sum_{k=0}^{K} \tilde{w}_k M(\tilde{\xi}_k).
\]

Hence, the optimization can be confined to finding optimal weights \( \tilde{w}_k \) on the orbits. Note that the restricted design region \( \mathcal{X}_{L,U} \) just imposes the side conditions \( \tilde{w}_k = 0 \) for \( k < L \) or \( k > U \).

In the following we further consider the special case of design regions of the form \( \mathcal{X}_{L,K-L} \), i.e. symmetric thresholds \( U = K - L \), which bound both the number \( d(\mathbf{x}) \) of active rules and the number \( K - d(\mathbf{x}) \) of inactive rules by the same threshold \( U \) form above. Under this condition we may utilize a further symmetry with respect to simultaneous sign change of all entries in the vector \( \mathbf{x} \) representing the design point, i.e. \( d(\mathbf{x}) \) active rules are changed to become inactive and vice versa. The corresponding transformation matches orbits \( \mathcal{O}_k \) and \( \mathcal{O}_{K-k} \) for \( 0 \leq k \leq K/2 \). Then, under the full group of permutations and symmetry, there are \( K/2 + 1 \) or \( (K+1)/2 \) orbits, if \( K \) is even or odd, respectively, which consist of all items with \( k \) or \( K - k \) active rules. It follows, that for the invariant optimal design \( \tilde{w}_k = \tilde{w}_{K-k} \) can be chosen.

### 3 General Structure of the Information Matrix

As usual under the current parametrization the entries of the information matrix \( M(\xi) \) can be considered as moments

\[
\sum_{i=1}^{n} w_i x_i^r x_i^s x_i^t x_i^u, \quad j, k, \ell, m \in \{1, \ldots, K\}, \quad r, s, t, u \in \{0, 1, 2\},
\]
with respect to the design $\xi$, where the $x_{ik}$ denote the entries in $x_i$. The diagonal entries of the information matrix are given by

$$
\sum_{i=1}^{n} w_i = \sum_{i=1}^{n} w_i x_{ik}^2 = \sum_{i=1}^{n} w_i x_{ij} x_{ik} = 1, \quad j, k \in \{1, \ldots, K\}, j \neq k.
$$

Moreover, for designs invariant with respect to permutations there are only four further potentially different entries for the off-diagonal elements. In the first row and first column the first moments for the main effects are

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

while the first moments for the interactions as well as the mixed moments for the main effects become

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

For the mixed main effect/interaction moments we obtain $m_3(\bar{\xi})$, when the main effect factor is involved in the interaction, and

$$m_3(\bar{\xi}) = \sum_{i=1}^{n} w_i x_{ij} x_{ik} x_{il}, \quad 1 \leq j < k < l \leq K,$$

otherwise. For the mixed interaction moments we get $m_4(\bar{\xi})$, when there is a common factor in both interactions, and

$$m_4(\bar{\xi}) = \sum_{i=1}^{n} w_i x_{ij} x_{ik} x_{il} x_{im}, \quad 1 \leq j < k < l < m \leq K,$$

if all factors are different.

Even though $m_1$ through $m_4$ depend on the design $\bar{\xi}$, we will omit the argument for the sake of brevity, when this does not cause confusion. With this notation the information matrix becomes

$$
\mathbf{M}(\bar{\xi}) = \begin{pmatrix}
1 & m_1 \mathbf{1}_K^\top & m_3 \mathbf{1}_C(K,2)^\top \\
m_3 \mathbf{1}_K & \mathbf{M}_{11} & \mathbf{M}_{12} \\
m_3 \mathbf{1}_C(K,2) & \mathbf{M}_{12} & \mathbf{M}_{22}
\end{pmatrix},
$$

where $\mathbf{1}_\ell$ denotes a $\ell$-dimensional vector with all entries equal to 1. The block $\mathbf{M}_{11}$ corresponding to the main effects has the form

$$\mathbf{M}_{11} = (1 - m_2) \mathbf{I}_K + m_2 \mathbf{J}_K,$$

where $\mathbf{I}_\ell$ and $\mathbf{J}_\ell$ denote the $\ell \times \ell$ identity matrix and the $\ell \times \ell$ matrix with all entries equal to 1, respectively. The blocks involving interactions are given by

$$\mathbf{M}_{12} = (m_1 - m_3) \mathbf{S}_K^\top + m_3 \mathbf{1}_K \mathbf{1}_C(K,2)^\top,$$

and

$$\mathbf{M}_{22} = (1 - 2m_2 + m_4) \mathbf{I}_C(K,2) + (m_2 - m_4) \mathbf{S}_K \mathbf{S}_K^\top + m_4 \mathbf{J}_C(K,2).$$
where the $C(K,2) \times K$-matrix $S_K$ contains only entries equal to 1 or 0 indicating whether the corresponding main effect is involved in the associated interaction – or not. For illustrative purposes we exhibit this matrix in the case $K = 6$:

$$S_6^T = \begin{pmatrix}
1 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 & 1 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 1 & 0 & 1 & 1 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 1 & 0 & 1 
\end{pmatrix}.$$ 

Because the matrix $S_K$ has 2 entries equal to one in each row and $K - 1$ in each column, we get

$$S_K 1_K = 2 \cdot 1_{C(K,2)} \quad \text{and} \quad S_K^T 1_{C(K,2)} = (K - 1) 1_K$$

and, furthermore,

$$S_K^T S_K = (K - 2) I_K + J_K.$$ 

For further use we note that the vector $1_K$ is an eigenvector of $S_K^T S_K$ with corresponding eigenvalue $2(K - 1)$, and the remaining $K - 1$ eigenvalues of $S_K^T S_K$ are all equal to $K - 2$ with corresponding eigenvectors, which are orthogonal to $1_K$. As a consequence, these values are also the non-zero eigenvalues of $S_K S_K^T$, where the eigenvalue $2(K - 1)$ corresponds to the eigenvector $1_{C(K,2)}$. By this observation, the eigenvalues of the diagonal block $M_{22}$ of the information matrix associated with the interactions can be determined as $1 - 2m_2 + m_4 + 2(K - 1)(m_2 - m_4) + C(K,2)m_4 = 1 + 2(K - 2)m_2 + (K - 2)(K - 3)m_4/2$ with multiplicity one, corresponding to the eigenvector $1_{C(K,2)}$. $1 - 2m_2 + m_4 + (K - 2)(m_2 - m_4) = 1 + (K - 4)m_2 - (K - 3)m_4$ with multiplicity $K - 1$, corresponding to the remaining eigenvectors of $S_K S_K^T$, and $1 - 2m_2 + m_4$ with multiplicity $C(K,2) - K = K(K - 3)/2$, corresponding to the eigenvectors orthogonal to the previous ones.

As has been seen before, the information matrix of an invariant design can be written as a weighted sum of the information matrices of the orbits. For the information matrices of the orbits the entries can be calculated combinatorially by counting the number of terms in the sums which are equal to +1 and −1, respectively. While the diagonal entries in the information matrices are all equal to 1, the off-diagonal entries are determined by the moments, which, in general, can be derived as

$$m_j(\xi_k) = C(K,k)^{-1} \sum_{i=0}^{j} (-1)^{i+j} C(j,i) C(K-j,k-i).$$ \hfill (2)

In particular, we obtain

$$m_1(\xi_k) = \frac{2k - K}{K},$$ \hfill (3)

$$m_2(\xi_k) = \frac{(2k - K)^2 - K}{K(K - 1)},$$ \hfill (4)

$$m_3(\xi_k) = \frac{(2k - K)^3 - (3K - 2)(2k - K)}{K(K - 1)(K - 2)}, \quad \text{and}$$

$$m_4(\xi_k) = \frac{(2k - K)^4 - (6K - 8)(2k - K)^2 + 3K(K - 2)}{K(K - 1)(K - 2)(K - 3)}$$ \hfill (6)

for $j \leq K$, and $m_j(\xi_k) = 0$ otherwise. Obviously, for $j \leq K$, the moments $m_j(\xi_k)$ are polynomials in $k$ of degree $j$ with positive leading terms, which are symmetric with respect to $K/2$. 

6
4 Symmetric case

First note that $m_j(\tilde{\xi}_{K-k}) = -m_j(\tilde{\xi}_k)$ for $j$ odd and $m_j(\tilde{\xi}_{K-k}) = m_j(\tilde{\xi}_k)$ for $j$ even, respectively.

Additionally in the case of symmetric constraints ($L + U = K$) we have equal weights $\tilde{w}_{K-k} = \tilde{w}_k$ for symmetric invariant designs. For these designs follows immediately that their odd moments vanish ($m_1 = m_3 = 0$) and hence we have $M_{12} = 0$ for the off-diagonal block in the information matrix. Thus the information matrix can be obtained as

$$M(\tilde{\xi}) = \begin{pmatrix}
1 & 0 & m_21^\top_{C(K,2)} \\
0 & M_{11} & 0 \\
m_21_{C(K,2)} & 0 & M_{22}
\end{pmatrix},$$

(7)

where $\mathbf{0}$ denotes a vector or a matrix of appropriate size with all entries equal to 0.

The determinant of this matrix can be calculated by using standard formulae as

$$\det(M(\tilde{\xi})) = \det(M_{11}) \det(M_{22} - m_2^2 J_{C(K,2)}).$$

For the first determinant on the right-hand side we have

$$\det(M_{11}) = (1 + (K - 1)m_2)(1 - m_2)^{K-1}.$$ 

For the second determinant observe that the eigenvalue of the matrix $M_{22} - m_2^2 J_{C(K,2)}$ associated with the eigenvector $1_{C(K,2)}$ equals that of $M_{22}$ reduced by $m_2^2 C(K,2)$, while the remaining eigenvalues stay the same. As a consequence the determinant can be obtained as

$$\det(M_{22} - m_2^2 J_{C(K,2)}) = (1 + 2(K - 2)m_2 + \frac{1}{2}(K - 2)(K - 3)m_4 - \frac{1}{2}K(K - 1)m_2^2)$$

$$\times (1 + (K - 4)m_2 - (K - 3)m_4)^{K-1}$$

$$\times (1 - 2m_2 + m_4)^{K(K-3)/2}.$$

The occurring eigenvalues are all nonnegative because the information matrix is nonnegative definite. For estimability of all parameters it has to be shown that these eigenvalues are all positive.

The following lemma establishes necessary and sufficient conditions for the information matrix of an invariant symmetric design to be nonsingular. For this we denote by $\tilde{\xi}_k = (\tilde{\xi}_k + \tilde{\xi}_{K-k})/2$ the uniform design on the symmetric orbit $\tilde{O}_k = \tilde{O}_k \cup \tilde{O}_{K-k}$.

Note that for $K$ even the symmetric orbit for $k = K/2$ is degenerate, $\tilde{O}_{K/2} = \tilde{O}_{K/2}$.

**Lemma 1.** Let $K \geq 2$. For a symmetric invariant design $\tilde{\xi}$ the information matrix $M(\tilde{\xi})$ is nonsingular if only if $\tilde{\xi}$ is supported on, at least, two distinct symmetric orbits $\tilde{O}_k$ and $\tilde{O}_\ell$, $0 \leq k < \ell \leq K/2$, where either $K \leq 3$, $k > 0$ or $2 \leq \ell < K/2$.

Note that it follows from Lemma [1] that for $K = 2$ and $K = 3$ the full $2^K$ factorial would be required for estimability of the parameters, and that for a symmetric invariant design with more than two different symmetric orbits estimability of all parameters is always ensured.

If the information matrix $M(\tilde{\xi})$ is nonsingular, its inverse has the same chess-board structure,

$$M(\tilde{\xi})^{-1} = \begin{pmatrix}
c_0 & 0 & -c_21^\top_{C(K,2)} \\
0 & M_{11}^{-1} & 0 \\
-c_21_{C(K,2)} & 0 & C_{22}
\end{pmatrix},$$

(8)
where

\[ c_2 = \frac{2m_2}{2 + 4(K - 2)m_2 + (K - 2)(K - 3)m_4 - K(K - 1)m_2^2} \]

\[ c_0 = 1 + c_2C(K, 2)m_2 \]

\[ M_{11}^{-1} = \frac{1}{1 - m_2}\left( I_K - \frac{m_2}{1 + (K - 1)m_2}J_K \right) \]

and

\[ C_{22} = \frac{1}{1 - 2m_2 + m_4}\left( I_{C(K, 2)} - \delta_S S K S K^{-1} - \delta_J J_{C(K, 2)} \right) \]

The coefficients \( \delta_S \) and \( \delta_J \) are given by

\[ \delta_S = \frac{m_2 - m_4}{1 + (K - 4)m_2 - (K - 3)m_4} \]

and

\[ \delta_J = \frac{2m_4 - 4\delta_S((K - 3)m_4 + 2m_2) - 2c_2m_2(1 - 2m_2 + m_4)}{2 + 4(K - 2)m_2 + (K - 2)(K - 3)m_4} \]

That the matrix in \( S \) indeed is the inverse of the information matrix, can be verified by straightforward multiplication of the matrices.

5 Optimal Designs

Without constraints on the design region the full factorial design, which assigns equal weights \( 2^{-K} \) to each of the \( 2^K \) vertices, may be used. The information matrix of the full factorial design is equal to the identity matrix \( I_p \), and the full factorial is well-known to be optimal with respect to a variety of criteria including \( D \)-optimality. Hence, any design \( \xi \) satisfying \( M(\xi) = I_p \) will be optimal on the unrestricted design region and, by a majorization argument, also optimal on a restricted design region as long as the support of \( \xi \) is included in that design region. Thus for finding an optimal design \( \xi^* \) on \( X \) it would be sufficient to show that \( M(\xi^*) = I_p \) or, equivalently, for a symmetric invariant design \( \xi^* \) that \( m_2(\xi^*) = 0 \) and \( m_4(\xi^*) = 0 \).

In particular, if \( K \geq 6 \) is even and \( L = 1 \) we may take the regular half fraction \( \tilde{\xi} = 2^{-(K - 1)}\sum_{j=1}^{K/2} C(K, 2j - 1)\xi_{2j-1} \) which is uniform on all settings belonging to the odd orbits \( \mathcal{O}_1, \mathcal{O}_3, \ldots, \mathcal{O}_{K-1} \). This half fraction \( \tilde{\xi} \) has an information matrix equal to the identity and is thus optimal on the restricted design region \( X_{1,K-1} \).

In general, for larger \( L \) the search for such designs may be more complicated. If \( L \) becomes too large, then the constraints may become so severe that the condition \( M(\xi) = I_p \) cannot be met by any design on \( X_{L,K-L} \), and optimal designs have to be characterized in another way.

Moreover, it would be desirable to reduce the number of support points, i.e. the number of orbits for a symmetric invariant optimal design. Therefore, we first establish a result which provides optimal designs supported on, at most, three symmetric orbits for small to moderate thresholds \( L \). Then for \( L \) up to a suitable threshold the following results shows that there exist optimal designs on \( X_{L,K-L} \) which are equally good as the full factorial design. We start with the situation where \( L \) is equal to the threshold. There symmetric invariant designs turn out to be optimal which are supported on the two symmetric orbits with minimal and maximal number of active rules or with (nearly) half of the rules active, respectively.
Lemma 2. Let either

(a.) $K$ be even, $L = (K - \sqrt{3K - 2})/2$, $\bar{w}_L = K/(2(3K - 2))$, and $\xi = \bar{w}_L \xi_L + (1 - 2\bar{w}_L)\xi_{K/2} + \bar{w}_L \xi_{K-L}$, or

(b.) $K$ be odd, $L = (K - \sqrt{3K})/2$, $\bar{w}_L = (K - 1)/(2(3K - 1))$, and $\xi = \bar{w}_L \xi_L + (1/2 - \bar{w}_L)\xi_{(K-1)/2} + (1/2 - \bar{w}_L)\xi_{(K+1)/2} + \bar{w}_L \xi_{K-L}$.

Then the information matrix $M(\xi)$ is equal to the identity $I_p$.

The proof follows by straightforward calculation of $m_2(\xi) = m_4(\xi) = 0$, which establishes $M(\xi) = I_p$.

The conditions of Lemma 2 are met only in rare cases. For $K = 3$ we recover the $2^3$ full factorial, and for $K = 6$ the given design is the $2^{6-1}$ fractional factorial on the odd orbits mentioned above. For $K = 22$ we obtain an optimal design concentrated on three orbits with 7, 11, and 15 active rules, but with unequal weights on the individual settings. Similarly, for $K = 27$ the optimal design is supported on four orbits with 9, 13, 14, and 18 active rules, where also the weights differ between the settings of the outer and inner orbits.

For notational convenience we introduce the abbreviation $B_K$ for the threshold occurring in Lemma 2

$$B_K = \begin{cases} \frac{K - \sqrt{3K - 2}}{2}, & K \text{ even} \\ \frac{K - \sqrt{3K}}{2}, & K \text{ odd} \end{cases}$$

When $L$ is less or equal to the threshold $B_K$, then, in general, at least three symmetric orbits are required.

Theorem 1. Let $L \leq B_K$, then there exist symmetric invariant designs $\tilde{\xi}^*$ with $M(\tilde{\xi}^*) = I_p$ which are supported on, at most, three symmetric orbits in $\tilde{\xi}_{L,K-L}$.

In the corresponding proof in the appendix particular designs will be constructed which include the outmost and the central symmetric orbits $\tilde{\mathcal{O}}_L$ and $\tilde{\mathcal{O}}_{K/2}$ or $\tilde{\mathcal{O}}_{(K-1)/2}$, respectively. For $K$ up to 22 a list of such designs is provided in Table 1. Note that there the index $c$ stands for a central orbit with $c = K/2$ or $c = (K - 1)/2$, respectively.

All these designs are optimal because their information matrices coincide with that of a full factorial design, which is known to be optimal on the unrestricted design region $\{-1, +1\}^K$. By a majorization argument we may thus state the following result.

Corollary 1. The designs specified in Theorem 1 are $D$-optimal.

However, the designs in Theorem 1 and Corollary 1 typically need not be unique. For example, if $L \leq B_K - 1$, then the outmost orbit $\tilde{\mathcal{O}}_L$ can be replaced by a less extreme one, i.e. $\tilde{\mathcal{O}}_k$ with $L < k \leq B_K$, more orbits can be included by mixing different optimal designs, and even the central orbit may be replaced as in half fractions on odd orbits when $K$ is a multiple of four.

For $K = 6$ we get $B_K = 1$ for the threshold. Therefore the results cannot be applied to the example with $L = 2$. But as was mentioned before the $2^{6-1}$ fractional factorial design on the odd orbits is optimal for $L \leq 1$.

For narrower constraints ($L > B_K$) the full information can no longer be retained, and the $D$-optimal designs will result in an information matrix different from the identity, i.e. $m_2 \neq 0$ and/or $m_4 \neq 0$. 

9
Theorem 2. Let $B_K < L < K/2$. Then the symmetric invariant design $\tilde{\xi} = \tilde{\omega}_L^* \bar{\xi}_L + (1 - 2\tilde{\omega}_L^*)\xi_{K/2} + \tilde{\omega}_L^* \bar{\xi}_{K-L}$ in the case $K$ even and $\tilde{\xi} = \tilde{\omega}_L^* \bar{\xi}_L + (1/2 - \tilde{\omega}_L^*)\xi_{(K-1)/2} + (1/2 + \tilde{\omega}_L^*)\xi_{(K+1)/2} + \tilde{\omega}_L^* \bar{\xi}_{K-L}$ in the case $K$ odd with optimized weight $\tilde{\omega}_L^*$ is $D$-optimal.

From the proof given in the appendix it can be seen that the optimal design specified in Theorem 2 is unique within the class of symmetric invariant designs.

The weights $\tilde{\omega}_L^*$ can be expressed as roots of polynomials of degree three for $K$ even or five for $K$ odd, which arise from setting the derivative of the criterion function $\log \det(M(\xi))$ with respect to the weight equal to zero. In general these roots are not rational numbers, and the optimal designs from Theorem 2 cannot be directly realized as exact designs. However, they may well serve as benchmarks for realistic candidates.

For the introductory example of $K = 6$, in which $L = 2$ up to $K-L = 4$ rules can be active, the symmetric invariant optimal design is supported by all possible orbits $O_2$, $O_3$ and $O_4$ of $X_{2,4}$ with weights $\tilde{\omega}_2^* = \tilde{\omega}_4^* = (45 - 6 \cdot \sqrt{37})/22 \approx 0.3865$ and $\tilde{\omega}_3^* = 1 - 2\tilde{\omega}_2^* \approx 0.2270$. The efficiency of this design with respect to the full factorial design is $\det(M(\xi^*))^{(1/p)} \approx 0.8854$. The weights for individual design points are $\tilde{\xi}^*(x) \approx 0.0258$ for $x \in O_2 \cup O_4$ and $\tilde{\xi}^*(x) \approx 0.0113$ for $x \in O_3$.

Numerical values for optimal weights $\tilde{\omega}_L^*$ are given in Table 2. Note that also there the index $c$ stands for a central orbit. The values in the tables were computed in R (R Core Team, 2018). For Table 1 the weights of the designs given in the proof of Theorem 1 were implemented. In the other case, for Table 2 the weights are roots of polynomials, as was mentioned above. These were computed using the polynomial package (Venables, Hornik and Maechler, 2013). Optimality of the resulting designs was checked using the equivalence theorem. In all cases condition (11) holds numerically with a maximum error for $\psi(x) - p$ of order $10^{-12}$ or smaller.

For the sake of clarity the results in the tables were rounded to four digits. This concerns especially the values in Table 2. Comparing the $D$-efficiency of the rounded with the original values shows, that the loss is of order $10^{-7}$ and hence negligible.

6 Discussion

In the present paper we developed initial characterizations for $D$-optimal designs in $K$-factorial models with binary predictors, when the number of active factors is symmetrically bounded from below and from above.

For mild to moderate constraints the obtained results have the same information matrix as the full factorial design and have, hence 100% efficiency. This carries over also to other optimality criteria based on the eigenvalues of the information matrix like $A$- and $E$-optimality. Conditions under which a fully efficient design exists, i.e. a design with the information matrix $I_p$, are discussed by Harman (2008) in the context of Schur optimality.

For strong constraints the restriction is so severe that the obtained optimal designs do no longer have the same information matrix as the full factorial. However, the resulting efficiencies, which are listed in Table 2 are still rather high. Also in this situation the results can be extended to other optimality criteria, but different weights have to be determined.

Further research is needed for dealing with asymmetric constraints, in particular, in the case of narrow bounds or when central orbits are excluded. If the bounds are wide enough such that the lower bound is below the threshold $B_K$ and the upper bound is above $K - B_K$, then designs characterized in Theorem 1 can be used, where the bound is chosen as $\max \{L, K-U\}$ by majorization.
Acknowledgment

This work was partly supported under DFG grant SCHW 531/15-4, while the first author was affiliated with the University of Magdeburg.

References

Bhatia, R., and Davis, C. (2000). A Better Bound on the Variance. The American Mathematical Monthly, 107 353–357.

Filová, L., Harman, R., and Klein, T. (2011). Approximate E-optimal designs for the model of spring balance weighing with a constant bias. Journal of Statistical Planning and Inference, 141, 2480–2488.

Freise, F., Holling, H., and Schwabe, R. (2018). Optimal designs for two-level main effects models on a restricted design region. [arXiv:1808.06901] [math.ST].

Harman, R. (2008). Equivalence theorem for Schur optimality of experimental designs. Journal of Statistical Planning and Inference, 138, 1201–1209.

Kiefer, J., and Wolfowitz, J. (1960). The equivalence of two extremum problems. Canadian Journal of Mathematics, 12, 363–366.

Muilwijk, J. (1966). Note on a Theorem of M. N. Murthy and V. K. Sethi Sankhyā: The Indian Journal of Statistics, Series B, 28, 183.

Pukelsheim, F. (1993). Optimal Design of Experiments. Wiley, New York.

R Core Team (2018). R: A Language and Environment for Statistical Computing. https://www.R-project.org/.

Schwabe, R. (1996). Optimum Designs for Multi-factor Models. Springer, New York.

Silvey, S.D. (1980). Optimal Design. Chapman and Hall.

Venables, B., Hornik, K., and Maechler, M. (2016). polynom: A Collection of Functions to Implement a Class for Univariate Polynomial Manipulations. https://CRAN.R-project.org/package=polynom.

Appendix A: Proofs

For the proof of Lemma 1 we need some auxiliary results on the eigenvalues of $M_{22} - m_2^2 J_{C(K,2)}$ for a symmetric invariant design when $K \geq 4$.

Lemma 3. Let

$$\lambda_1 = 1 + 2(K - 2)m_2 + \frac{1}{2}(K - 2)(K - 3)m_4 - \frac{1}{2}K(K - 1)m_2^2$$

be the eigenvalue of $M_{22} - m_2^2 J_{C(K,2)}$ associated with the eigenvector $1_{C(K,2)}$. Then $\lambda_1 > 0$ if and only if the support of $\xi$ includes at least two distinct symmetric orbits.

Proof. First note that for each invariant design $\xi_k$ on a single orbit $O_k$ we get by inserting the moments that the corresponding eigenvalue $\lambda_1(\xi_k)$ is zero. Let $\xi_k$ be the corresponding symmetric invariant design on the symmetric orbit $\tilde{O}_k$. Then $m_2(\xi_k) = m_2(\tilde{\xi}_k)$, $m_4(\xi_k) = m_4(\tilde{\xi}_k)$ and, hence, $\lambda_1(\tilde{\xi}_k) = \lambda_1(\xi_k) = 0$. Consequently at least two distinct symmetric orbits are needed for $\lambda_1 > 0$. 

11
Now, let $\xi = \bar{w}_k\xi_k + \bar{w}_\ell\xi_\ell$ be a symmetric invariant design on the symmetric orbits $\bar{O}_k$ and $\bar{O}_\ell$, $k < \ell \leq K/2$, $\bar{w}_k, \bar{w}_\ell > 0$. As $m_2(\xi_k)$ is strictly decreasing in $k$ we have $m_2(\xi_k) \neq m_2(\xi_\ell)$. Thus $m_2(\xi)^2 < \bar{w}_km_2(\xi_k)^2 + \bar{w}_\ell m_2(\xi_\ell)^2$ by the strict concavity of the quadratic function, which implies $\lambda_1 > 0$.

Lemma 4. Let $\lambda_S = 1+ (K-4)m_4-(K-3)m_3$ be the eigenvalue of $M_{22} - m_2^2J_{C(K,2)}$ associated with the remaining eigenvectors of $S_K S_K^\top$ orthogonal to $I_{C(K,2)}$. Then $\lambda_S > 0$ if and only if the support of $\xi$ includes at least one symmetric orbit $\bar{O}_k$ for which $0 < k < K/2$.

Proof. By inserting the moments we get for this eigenvalue
$$\lambda_S(\xi_k) = \frac{(2k-K)^2(K^2 - (2k-K)^2)}{K(K-1)(K-2)}.$$
which is equal to 0 for $k = 0$ or $k = K/2$. Moreover, $\lambda_S(\xi_k)$ is a polynomial in $k$ of degree four, symmetric around $K/2$, and with negative leading term. Hence, there cannot be any other root, and $\lambda_S(\xi_k) > 0$ for all $0 < k < K/2$.

Lemma 5. Let $\lambda_1 = 1 - 2m_2 + m_4$ be the eigenvalue of $M_{22} - m_2^2J_{C(K,2)}$ associated with the remaining eigenvectors orthogonal to those of $S_K S_K^\top$. Then $\lambda_1 > 0$ if and only if the support of $\xi$ includes at least one symmetric orbit $\bar{O}_k$ for which $k > 1$.

Proof. By inserting the moments we see that $\lambda_1(\xi_k)$ is a polynomial in $k$ of degree four, symmetric around $K/2$, and with positive leading term, which is equal to zero for $k = 0$ and $k = 1$. Hence, there cannot be any other root, and $\lambda_1(\xi_k) > 0$ for all $1 < k < K/2$.

Proof of Lemma 4 We note that according to Freise et al. (2018) the matrix $M_{11}$ associated with the main effects is nonsingular when at least two distinct symmetric orbits are involved in the design $\xi$. Hence, the requirement of $M_{11}$ to be nonsingular does not impose any additional condition besides those of Lemmas 3 to 5. Hence, the assertion follows from these lemmas.

Proof of Theorem 5 For $K = 2$ and $K = 3$ we have $B_K < 1$, such that the full factorial design can serve as the asserted symmetric invariant design.

Let $K \geq 4$. If $L = B_K$, then the design of Lemma 3 can be used. Let $L < B_K$ and let $K$ be even. Then choose $\ell$ such that
$$B_K = \frac{K - \sqrt{3K^2 - 2}}{2} \leq \ell \leq \frac{K - \sqrt{K}}{2}.$$
Such $\ell$ always exists (for $K \leq 8$ see Table 4; note that $\sqrt{3K^2 - 2} - \sqrt{K} \geq 2$ for $K \geq 10$).

Let designs $\xi(L)$ and $\xi(\ell)$ be defined as
$$\xi(L) = \bar{w}_L \xi_L + (1 - 2\bar{w}_L) \xi_{K/2} + \bar{w}_L \xi_{K-L} \quad \text{with} \quad \bar{w}_L = \frac{K}{2(2L - K)^2}$$
and
$$\xi(\ell) = \bar{w}_\ell \xi_\ell + (1 - 2\bar{w}_\ell) \xi_{K/2} + \bar{w}_\ell \xi_{K-\ell} \quad \text{with} \quad \bar{w}_\ell = \frac{K}{2(2\ell - K)^2}.$$
According to Freise et al. (2018) the moments $m_2(\xi(L))$ and $m_2(\xi(\ell))$ are equal to 0, because $L, \ell < (K - \sqrt{K})/2$. Next we consider the convex combination
$$\xi^* = \alpha \xi(L) + (1 - \alpha) \xi(\ell) \quad \text{with} \quad \alpha = \frac{3K - 2 - (2\ell - K)^2}{4(\ell - L)(K - L - \ell)}.$$
Also for the symmetric invariant design \( \tilde{\xi}^* \) we have \( m_2(\tilde{\xi}^*) = 0 \). Further we obtain
\[
m_4(\tilde{\xi}^*) = \frac{4\alpha(\ell - L)(K - L - \ell) + (2\ell - K)^2 - (3K - 2)}{(K - 1)(K - 2)(K - 3)} = 0,
\]
which establishes the result for even \( K \).

For \( K \) odd the proof is similar. For \( L < B_K \) choose \( \ell \) as above with the corresponding value for \( B_K \) and the designs
\[
\xi(L) = \bar{w}_L \xi_L + (\frac{1}{2} - \bar{w}_L)\xi(K-1)/2 + (\frac{1}{2} - \bar{w}_L)\xi(K+1)/2 + \bar{w}_L \xi_{K-L}
\]
and
\[
\tilde{\xi}(\ell) = \bar{w}_\ell \tilde{\xi}_\ell + (\frac{1}{2} - \bar{w}_\ell)\tilde{\xi}(K-1)/2 + (\frac{1}{2} - \bar{w}_\ell)\tilde{\xi}(K+1)/2 + \bar{w}_\ell \tilde{\xi}_{K-\ell}
\]
with corresponding weights
\[
\bar{w}_L = \frac{K - 1}{2((2L - K)^2 - 1)} \quad \text{and} \quad \bar{w}_\ell = \frac{K - 1}{2((2\ell - K)^2 - 1)}.
\]
Again such \( \ell \) always exists (for \( K \leq 7 \) see Table 1 for \( K \geq 9 \) note that \( \sqrt{3K - \sqrt{K}} \geq 2 \)) and \( m_2(\tilde{\xi}(L)) = m_2(\tilde{\xi}(\ell)) = 0 \).

Then the convex combination
\[
\tilde{\xi}^* = \alpha \tilde{\xi}(L) + (1 - \alpha) \tilde{\xi}(\ell) \quad \text{with} \quad \alpha = \frac{3K - (2\ell - K)^2}{4(\ell - L)(K - L - \ell)}
\]
yields \( m_4(\tilde{\xi}^*) = 0 \), and the result follows.

For the proof of Theorem 2 we will make use of the celebrated Kiefer-Wolfowitz equivalence theorem [Kiefer and Wolfowitz, 1960]. Therefore we first investigate the sensitivity function (functional derivative).

**Lemma 6.** Let \( \xi \) be a symmetric invariant design. Then the sensitivity function \( \psi(x) = f(x)^\top M(\xi)^{-1} f(x) \) is constant on the orbits, \( \psi(x) = \tilde{\psi}(k) \) for \( x \in O_k \), say, and the function \( \tilde{\psi} \) is a polynomial of degree at most 4, which is symmetric with respect to \( K/2 \) (\( \tilde{\psi}(K - k) = \tilde{\psi}(k) \)).

**Proof.** Using the inverse of the information matrix in equation (8) we obtain for the sensitivity function
\[
\psi(x) = c_0 - 2c_2 \tilde{x}^\top \mathbf{1}_{C(K,2)} + x^\top \mathbf{M}_{11}^{-1} x + \tilde{x}^\top \mathbf{C}_{22} \tilde{x}.
\]
Note that \( x^\top x = K \) and \( \tilde{x}^\top \tilde{x} = (K - 1)/2 \). Further, for \( x \in O_k \), we get
\[
x^\top \mathbf{1}_K = 2k - K, \quad \tilde{x}^\top \mathbf{1}_{C(K,2)} = ((2k - K)^2 - K)/2
\]
and
\[
\tilde{x}^\top \mathbf{S}_K \mathbf{S}_K^\top \tilde{x} = (K - 2)(2k - K)^2 + K.
\]
This yields
\[
\psi(x) = a_4(2k - K)^4 + a_2(2k - K)^2 + a_0
\]
with coefficients
\[
a_0 = c_0 + \frac{K}{1 - m_2} + \frac{K(K - 1)}{2(1 - 2m_2 + m_4)} - \frac{\delta_{8K}}{1 - 2m_2 + m_4} - \frac{\delta_{4K^2}}{4(1 - 2m_2 + m_4)}
\]
\[
a_2 = -\left(c_2 + m_2\left(\frac{1}{1 - m_2}(1 + (K - 1)m_2) + \frac{\delta_{8(K - 2)}}{1 - 2m_2 + m_4} - \frac{\delta_{4K}}{2(1 - 2m_2 + m_4)}\right)\right.
\]
\[
a_4 = -\frac{\delta_{4K}}{4(1 - 2m_2 + m_4)}.
\]
Hence, \( \tilde{\psi} \) is a polynomial of degree four in \( k \). The symmetry around \( K/2 \) follows, since only even powers of \( k \) occur.
Lemma 7. Let $B_K < L < K/2$ and $\hat{\xi}^*$ an optimal symmetric invariant design on $X_{L,K}-L$. Then the orbitwise sensitivity function $\hat{\psi}$ has a positive leading term for the fourth order monomial $k^4$.

Proof. We will use the same notation as in Lemma 6 and its proof.

Let $\alpha_4 \leq 0$. Then the function $\hat{\psi}$ as a function in $k$ has either a single maximum at $k = K/2$, two (symmetric) maxima outside $(L, K-L)$ (respectively at $k = L$ and $k = K-L$ for the admitted orbits), two (symmetric) maxima inside $(L, K-L)$, or is constant.

In the first two cases $\hat{\psi}$ is supported on one symmetric orbit only. It follows from Lemma 1 that the information matrix has to be singular. But in this case the function $\hat{\psi}$ would not be defined, which is a contradiction.

In the last case, if the orbitwise sensitivity is constant, we have $\hat{\psi}(k) \leq p$ for all $k \in \{0, \ldots, K\}$ and, consequently, $\hat{\psi}$ is optimal on the unrestricted design region $X_{0,K}$.

In the third case, i.e. two maxima inside of $(L, K-L)$, the optimal invariant design $\hat{\psi}$ has all its weight on either one or two symmetric orbits. If these orbits do not satisfy the conditions in Lemma 1, the information matrix would be singular, which leads to a contradiction. Otherwise the design is optimal on $X_{0,K}$, with the same argument as for the constant case.

Now let $\hat{\psi}$ be optimal on $X_{0,K}$. Then its information matrix is $I_p$. It follows that $m_2 = m_4 = 0$ and thus

$$\sum_{k=L}^{K-L} \hat{w}_k(2k-K)^2 = K \quad \text{and} \quad \sum_{k=L}^{K-L} \hat{w}_k(2k-K)^4 - K^2 = 2K(K-1) . \quad (13)$$

The left-hand sides of these two equations can be interpreted as expectation and variance, respectively, of a discrete random variable taking values $(2k-K)^2$, $k = L, \ldots, K-L$. An upper bound for the variance is given in Muilwijk [1966] (see also Bhatia and Davis, 2000). This yields for the variance

$$\sum_{k=L}^{K-L} \hat{w}_k(2k-K)^4 - K^2 \leq ((2L-K)^2 - K)(K-R_K) ,$$

where $R_K = 0$ for $K$ even and $R_K = 1$ for $K$ odd. Since $B_K < L$ it follows that

$$((2L-K)^2 - K)(K-R_K) < ((2B_K-K)^2 - K)(K-R_K) = 2K(K-1) ,$$

which is in contradiction to (13). Hence $\alpha_4$ and consequently the leading coefficient has to be positive. \hfill \Box

Proof of Theorem 2. Under the assumptions of Theorem 2 the orbitwise sensitivity function $\hat{\psi}$ of the optimal design $\hat{\xi}^*$ is a polynomial of degree four with positive leading term by Lemma 6 and 7. Then, in view of the fundamental theorem of algebra, the equality $\hat{\psi}(k) = p$ can only have at most four distinct roots. Because of the symmetry of the sensitivity function with respect to $K/2$ (cf. Lemma 6) the optimal design has thus to be concentrated on at most two symmetric orbits. In order to fulfill the condition $\hat{\psi}(k) \leq p$ for all $k = L, \ldots, K-L$, imposed by the equivalence theorem on the optimal design $\hat{\xi}^*$, these symmetric orbits can only be the outmost orbit $O_L \cup O_{K-L}$ on the boundaries and the central orbit $O_{K/2}$ for $K$ even and $O_{(K-1)/2} \cup O_{(K+1)/2}$ for $K$ odd, respectively.

On the other hand the nonsingularity condition of Lemma 1 requires that the optimal design $\hat{\xi}^*$ has to be supported by at least two symmetric orbits and, hence, $\hat{\xi}^*$ is of the form specified in the Theorem. Finally only the weights have to be optimized given the two symmetric orbits. \hfill \Box
### Appendix B: Tables

Table 1: Symmetric invariant $D$-optimal designs for wide bounds from Theorem 1

| $K$ | $L$ | $\ell$ | $c$ | $\bar{w}_L^c$ | $\bar{w}_L^B$ | $\bar{w}_C^c$ | $B_K$ |
|-----|-----|-------|----|--------------|--------------|--------------|-------|
| 4   | 0   | 1     | 2  | 0.0625       | 0.2500       | 0.3750       | 0.42  |
| 5   | 0   | 1     | 2  | 0.0312       | 0.1562       | 0.3125       | 0.56  |
| 6   | 0   | 1     | 3  |               | 0.1875       | 0.6250       | 1     |
|     | 1   |       | 3  | 0.1875       |               | 0.6250       | 1     |
| 7   | 0   | 2     | 3  | 0.0187       | 0.2625       | 0.2188       | 1.21  |
|     | 1   | 2     | 3  | 0.0938       | 0.0938       | 0.3125       | 1.21  |
| 8   | 0   | 2     | 4  | 0.0078       | 0.2188       | 0.5469       | 1.65  |
|     | 1   | 2     | 4  | 0.0333       | 0.1750       | 0.5833       | 1.65  |
| 9   | 0   | 2     | 4  | 0.0018       | 0.1607       | 0.3375       | 1.90  |
|     | 0   | 3     | 4  | 0.0125       | 0.3750       | 0.1125       | 1.90  |
|     | 1   | 2     | 4  | 0.0069       | 0.1528       | 0.3403       | 1.90  |
|     | 1   | 3     | 4  | 0.0375       | 0.2750       | 0.1875       | 1.90  |
| 10  | 0   | 3     | 5  | 0.0071       | 0.2679       | 0.4500       | 2.35  |
|     | 1   | 3     | 5  | 0.0195       | 0.2344       | 0.4922       | 2.35  |
|     | 2   | 3     | 5  | 0.0833       | 0.1250       | 0.5833       | 2.35  |
| 11  | 0   | 3     | 5  | 0.0035       | 0.1910       | 0.3056       | 2.63  |
|     | 1   | 3     | 5  | 0.0089       | 0.1786       | 0.3125       | 2.63  |
|     | 2   | 3     | 5  | 0.0347       | 0.1389       | 0.3264       | 2.63  |
| 12  | 0   | 4     | 6  | 0.0059       | 0.3223       | 0.3438       | 3.08  |
|     | 1   | 4     | 6  | 0.0129       | 0.2946       | 0.3850       | 3.08  |
|     | 2   | 4     | 6  | 0.0352       | 0.2344       | 0.4609       | 3.08  |
|     | 3   | 4     | 6  | 0.1500       | 0.0375       | 0.6250       | 3.08  |
| 22  | 0   | 7     | 11 |               | 0.1719       | 0.6562       | 7     |
|     | 0   | 8     | 11 | 0.0014       | 0.2865       | 0.4242       | 7     |
|     | 1   | 7     | 11 |               | 0.1719       | 0.6562       | 7     |
|     | 1   | 8     | 11 | 0.0021       | 0.2821       | 0.4317       | 7     |
|     | 2   | 7     | 11 |               | 0.1719       | 0.6562       | 7     |
|     | 2   | 8     | 11 | 0.0033       | 0.2758       | 0.4417       | 7     |
|     | 3   | 7     | 11 |               | 0.1719       | 0.6562       | 7     |
|     | 3   | 8     | 11 | 0.0055       | 0.2667       | 0.4557       | 7     |
|     | 4   | 7     | 11 |               | 0.1719       | 0.6562       | 7     |
|     | 4   | 8     | 11 | 0.0098       | 0.2521       | 0.4762       | 7     |
|     | 5   | 7     | 11 |               | 0.1719       | 0.6562       | 7     |
|     | 5   | 8     | 11 | 0.0198       | 0.2263       | 0.5077       | 7     |
|     | 6   | 7     | 11 |               | 0.1719       | 0.6562       | 7     |
|     | 6   | 8     | 11 | 0.0481       | 0.1719       | 0.5600       | 7     |
|     | 7   |       | 11 | 0.1719       |               | 0.6562       | 7     |
|     | 7   | 8     | 11 | 0.1719       |               | 0.6562       | 7     |
Table 2: Symmetric invariant $D$-optimal designs for narrow bounds from Theorem 2

| $K$ | $L$ | $c$ | $\tilde{w}_{L}$ | $\tilde{w}_{c}$ | $D$-Efficiency | $B_{K}$ |
|-----|-----|-----|-----------------|-----------------|----------------|--------|
| 4   | 1   | 2   | 0.2993          | 0.4015          | 0.8892         | 0.42   |
| 5   | 1   | 2   | 0.1939          | 0.3061          | 0.9725         | 0.56   |
| 6   | 2   | 3   | 0.3865          | 0.2270          | 0.8854         | 1.00   |
| 7   | 2   | 3   | 0.2798          | 0.2202          | 0.9682         | 1.21   |
| 8   | 2   | 4   | 0.2282          | 0.5435          | 0.9960         | 1.65   |
|     | 3   | 4   | 0.4212          | 0.1576          | 0.8846         | 1.65   |
| 9   | 3   | 4   | 0.3461          | 0.1539          | 0.9660         | 1.90   |
| 10  | 3   | 5   | 0.2744          | 0.4512          | 0.9926         | 2.35   |
|     | 4   | 5   | 0.4397          | 0.1205          | 0.8863         | 2.35   |
| 11  | 3   | 5   | 0.1969          | 0.3031          | 0.9985         | 2.63   |
|     | 4   | 5   | 0.3903          | 0.1097          | 0.9640         | 2.63   |
| 12  | 4   | 6   | 0.3188          | 0.3624          | 0.9905         | 3.08   |
|     | 5   | 6   | 0.4513          | 0.0975          | 0.8892         | 3.08   |
| 13  | 4   | 6   | 0.2313          | 0.2687          | 0.9973         | 3.38   |
|     | 5   | 6   | 0.4178          | 0.0822          | 0.9622         | 3.38   |
| 14  | 4   | 7   | 0.1911          | 0.6177          | 0.9999         | 3.84   |
|     | 5   | 7   | 0.3582          | 0.2836          | 0.9891         | 3.84   |
|     | 6   | 7   | 0.4591          | 0.0818          | 0.8924         | 3.84   |
| 15  | 5   | 7   | 0.2655          | 0.2345          | 0.9965         | 4.15   |
|     | 6   | 7   | 0.4352          | 0.0648          | 0.9607         | 4.15   |
| 16  | 5   | 8   | 0.2146          | 0.5707          | 0.9994         | 4.61   |
|     | 6   | 8   | 0.3904          | 0.2191          | 0.9879         | 4.61   |
|     | 7   | 8   | 0.4648          | 0.0704          | 0.8957         | 4.61   |
| 17  | 6   | 8   | 0.2987          | 0.2013          | 0.9950         | 4.93   |
|     | 7   | 8   | 0.4469          | 0.0531          | 0.9595         | 4.93   |
| 18  | 6   | 9   | 0.2385          | 0.5229          | 0.9990         | 5.39   |
|     | 7   | 9   | 0.4149          | 0.1702          | 0.9868         | 5.39   |
|     | 8   | 9   | 0.4691          | 0.0618          | 0.8990         | 5.39   |
| 19  | 6   | 9   | 0.1842          | 0.3158          | 0.9999         | 5.73   |
|     | 7   | 9   | 0.3301          | 0.1699          | 0.9954         | 5.73   |
|     | 8   | 9   | 0.4551          | 0.0449          | 0.9586         | 5.73   |
| 20  | 7   | 10  | 0.2624          | 0.4751          | 0.9987         | 6.19   |
|     | 8   | 10  | 0.4325          | 0.1349          | 0.9858         | 6.19   |
|     | 9   | 10  | 0.4725          | 0.0550          | 0.9021         | 6.19   |
| 21  | 7   | 10  | 0.2028          | 0.2972          | 0.9997         | 6.53   |
|     | 8   | 10  | 0.3590          | 0.1410          | 0.9950         | 6.53   |
|     | 9   | 10  | 0.4611          | 0.0389          | 0.9580         | 6.53   |
| 22  | 8   | 11  | 0.2861          | 0.4278          | 0.9984         | 7.00   |
|     | 9   | 11  | 0.4451          | 0.1098          | 0.9848         | 7.00   |
|     | 10  | 11  | 0.4752          | 0.0496          | 0.9051         | 7.00   |