Optimal Designs for Second-Order Interactions in Paired Comparison Experiments with Binary Attributes

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Abstract
In paired comparison experiments respondents usually evaluate pairs of competing options. For this situation we introduce an appropriate model and derive optimal designs in the presence of second-order interactions when all attributes are dichotomous.

Keywords: Attributes; Full profile; Interactions; Optimal design; Paired comparison experiments

1 Introduction
Paired comparisons are closely related to experiments with choice sets of size two. For this situation optimal designs are usually derived under the indifference assumption of equal choice probabilities where the information matrix of a paired comparison experiment in a linear paired comparison model is equivalent to the information matrix of a discrete choice experiment in a multinomial logit model. Such experiments have received considerable attention during the last few years in many fields of applications like psychology, health economics, transport and marketing for learning consumer preferences towards new products or services. Typical with paired comparisons, judges evaluate pairs of competing alternatives in a hypothetical setting which are generated by an experimental design, and are characterized by a number of attribute levels. A comprehensive introduction to the general area can be found in the monographs of Louviere et al. (2000) and Train (2003) (see also Großmann and Schwabe, 2015).

The aim of this paper is to introduce an appropriate model and derive optimal designs in the presence of interactions. In this paper we treat the case when the components of the alternatives are characterized by two-level attributes. This factorial $2^K$ setting has been investigated by both van Berkum (1987a,b) and Street and Burgess (2004) in the case of full profiles in a main effects and first-order (two factor) interactions situation, and by Schwabe et al. (2003) for
partial profiles. Corresponding results have been presented by Graßhoff et al. (2003) in the general level case in a first-order interactions setup for both full and partial profiles. Here, we treat the case of second-order (three factor) interactions and provide detailed proofs.

The remainder of the paper is organized as follows. In Section 2 a general model is introduced for paired comparisons which is related to a block (choice set) of size two. The second-order interactions model for full profiles is presented in Section 3. Optimal designs are characterized in Section 4 and the final Section 5 offers some conclusions. The proof of the major results is deferred to the Appendix.

2 General setting

The outcome of any experimental situation depends on some factors $K$ of influence which are normally referred to as attributes in the paired comparison experiment literature. This dependence is best described by a functional relationship $f$ which quantifies the effect of the alternative $i$ of the attributes of influence. Hence, we formalize the experimental situation by a general linear model

$$
\tilde{Y}_{na}(i) = \mu_n + f(i)\top \beta + \tilde{\varepsilon}_{na},
$$

for the value (utility) $\tilde{Y}_{na}(i)$ of a single alternative $i$ within a pair of alternatives ($a = 1, 2$) subject to a random error $\tilde{\varepsilon}_{na}$. The index $n$ denotes the nth presentation in which $i$ is chosen from a set $I$ of possible realizations for the alternative. In general, each alternative is characterized by a number of distinct attributes (components) of influence such that $i = (i_1, \ldots, i_K)$ for $k = 1, \ldots, K$. In this setting $f = (f_1, \ldots, f_p)\top$ is a vector of known regression functions which describe the form of the functional relationship between the alternative $i$ and the corresponding mean response $E(\tilde{Y}_{na}(i)) = f(i)\top \beta$, and $\beta = (\beta_1, \ldots, \beta_p)\top$ is the unknown parameter vector of interest. Usually in order to make statistical inference on the unknown parameters more than one observation is presented to get rid of the influence of the presentation effect $\mu_n$ due to a variety of unobservable influences.

However, unlike standard design problems, in paired comparison experiments the utilities for the alternatives are usually not directly observed. Only observations $Y_n(i, j) = \tilde{Y}_{n1}(i) - \tilde{Y}_{n2}(j)$ of the amount of preference are available for comparing pairs $(i, j)$ of alternatives $i$ and $j$ which are chosen from the design region $X = I \times I$. In that case the utilities for the alternatives are properly described by the linear paired comparison model

$$
Y_n(i, j) = (f(i) - f(j))\top \beta + \varepsilon_n,
$$

where $f(i) - f(j)$ is the derived regression function and the random errors $\varepsilon_n(i, j) = \tilde{\varepsilon}_{n1}(i) - \tilde{\varepsilon}_{n2}(j)$ associated with the different pairs $(i, j)$ are assumed to be uncorrelated with constant variance. Here, the pair effects $\mu_n$ become immaterial. Moreover, we note that the linear difference model considered here can be realized as a linearization of the binary response model by Bradley and Terry (1952) under the assumption $\beta = 0$ (see e.g. Großmann et al. 2002).
under this indifference assumption of equal choice probabilities, the Bradley-Terry type choice experiments in which the probability of choosing \(i\) from the pair \((i, j)\) given by \(\exp(f(i)^\top \beta)/(\exp(f(i)^\top \beta) + \exp(f(j)^\top \beta))\) as in the work of [Street and Burgess (2007)] can be derived by considering the linear paired comparison model.

The quality of a design is measured by its information matrix

\[
M((i_1, j_1), \ldots, (i_N, j_N)) = \sum_{n=1}^N M((i_n, j_n))
\]

where \(M((i, j)) = (f(i) - f(j))(f(i) - f(j))^\top\) is the information of a single pair \((i, j)\). The performance of the statistical analysis based on a paired comparison experiment depends on the pairs (alternatives) in the choice sets that are presented. The choice of such pairs \((i_1, j_1), \ldots, (i_N, j_N)\) is called a design.

In the present paper we restrict our attention to approximate or continuous designs \(\xi\) as detailed in [Kiefer (1959)], which are defined as discrete probability measures on the design region \(X\) of all pairs \((i, j)\). Moreover, every approximate design \(\xi\) which assigns only rational weights \(\xi(i, j)\) to all pairs \((i, j)\) in its support points can be realized as an exact design \(\xi_N = ((i_1, j_1), \ldots, (i_N, j_N))\) for some sample size \(N\).

The standardized (per observation) information matrix of an approximate design \(\xi\) in the linear paired comparison model (2) is defined by

\[
M(\xi) = \sum_{(i,j)\in X} \xi(i,j)M((i,j)).
\]

Note that for an exact design \(\xi_N = ((i_1, j_1), \ldots, (i_N, j_N))\) the relation \(M(\xi_N) = \frac{1}{N} M((i_1, j_1), \ldots, (i_N, j_N))\) holds.

Optimality criteria for approximate designs \(\xi\) are functionals of \(M(\xi)\). As in a majority of works about optimal designs for paired comparison experiments, here we confine ourselves to the \(D\)-optimality criterion which aims at maximizing the determinant of the information matrix. For instance, an approximate design \(\xi^*\) is \(D\)-optimal if it maximizes the determinant of the information matrix, that is, if \(\det M(\xi^*) \geq \det M(\xi)\) for every approximate design \(\xi\).

**Example 1.** One-way layout (two levels)

For illustrative purposes we first consider the situation of just one attribute \((K = 1)\) which may vary only over two levels \((i, j = 1, 2)\), and we adopt the standard parameterization of effect-coding (see [Graßhoff et al. (2004)]). In this setting, the effects of each single level \(i = 1, 2\) has parameters \(\alpha_i\) satisfying the identifiability condition \(\alpha_1 + \alpha_2 = 0\). Hence,

\[
\tilde{Y}_{na}(i) = \mu_n + \alpha_i + \tilde{\epsilon}_{na}
\]

with \(i \in I = \{1, 2\}\), where \(\mu_n\) denotes the block effects, \(n = 1, \ldots, N\), and \(\tilde{\epsilon}_{na}\) the random error is assumed to be uncorrelated with constant variance and zero mean. For effect-coding the regression function \(f = g\) is given by \(g(1) = 1\) and \(g(2) = -1\), respectively. This ensures the usual identifiability condition \(\alpha_2 = -\alpha_1\) such that

\[
\tilde{Y}_{na}(i) = \mu_n + g(i)\beta + \tilde{\epsilon}_{na},
\]
where $\beta = \alpha_1 = -\alpha_2$.

Then for paired comparisons an observation of the effects $\alpha_i - \alpha_j$ of level $i$ compared to level $j$ can be characterized by the response

$$Y_n(i, j) = (g(i) - g(j))\beta + \varepsilon_n = \alpha_i - \alpha_j + \varepsilon_n.$$  \hfill (7)

Note that $M((i, j)) = (\pm 2)^2 = 4$ for $i \neq j$, while $M((i, i)) = 0$. From this it is obvious that only pairs with different levels should be used and that, in particular, the design $\xi$ which assigns equal weight $1/2$ to each of the two pairs $(1, 2)$ and $(2, 1)$ is optimal with resulting information

$$M(\xi) = 4.$$  \hfill (8)

This design $\xi$ will serve as a brick for constructing optimal designs in situations with more than one attribute later on.

### 3 Model with second-order interactions

For the setting of binary attributes the results for main effects and first-order interactions have been derived by van Berkum (1987b) and have been extended to more than two levels by Graßhoff et al. (2003). Here, we focus on second-order interaction effects for binary attributes.

In what follows, we take into consideration $k = 1, \ldots, K$ attributes having two levels each that are assumed to derive the preferences for the alternatives in a paired comparison experiment. In paired comparison experiments the alternatives are represented by combinations of attribute levels. For alternatives in a choice set, we denote by $i = (i_1, \ldots, i_K)$ the first alternative and the second alternative by $j = (j_1, \ldots, j_K)$ which are both elements of the set $\mathcal{I} = \{1, 2\}^K$ where the numbers 1 and 2 represent the first and second level of each attribute. The choice set $(i, j)$ is an ordered pair of alternatives $i$ and $j$ which is chosen from the design region $\bar{X} = \mathcal{I} \times \mathcal{I}$. For each attribute (component) $k$ the corresponding marginal model coincides with that of the one-way layout with regression functions $f_k = g$ as defined in Example 1.

More formally, for the case of direct response $\tilde{Y}_{na}$ at alternative $i = (i_1, \ldots, i_K)$, we consider the second-order interactions model

$$\tilde{Y}_{na}(i) = \mu_n + \sum_{k=1}^{K} a_{k}^{(k)} + \sum_{k < \ell} a_{k, \ell}^{(k, \ell)} + \sum_{k < \ell < m} a_{k, \ell, m}^{(k, \ell, m)} + \varepsilon_{na},$$  \hfill (9)

where $a_{k}^{(k)}$ is the main effect of the $k$-th attribute when the corresponding level is $i_k$, $a_{k, \ell}^{(k, \ell)}$ is the first-order interactions effect of the $k$-th and $\ell$-th attribute when the corresponding levels are $i_k$ and $i_\ell$, respectively, and $a_{k, \ell, m}^{(k, \ell, m)}$ is the second-order interactions effect of the $k$-th, $\ell$-th and $m$-th attribute when the corresponding levels are $i_k$, $i_\ell$ and $i_m$, respectively.

Moreover, by the common identifiability conditions of effect-coding the following equalities hold: $a_{1}^{(1)} = \beta_{1}$ and $a_{2}^{(1)} = -\beta_{1}$, $a_{1, 1}^{(1, 1)} = \alpha_{2, 2} = \beta_{1}$ and $a_{1, 1}^{(k, \ell)} = \alpha_{2, 2}^{(k, \ell)} = a_{1, 1}^{(k, \ell)} = \alpha_{1, 1}^{(k, \ell)} = \beta_{1}$, $\alpha_{1, 1}^{(1, 1)} = \beta_{1}$, $\alpha_{1, 1}^{(k, \ell)} = \alpha_{1, 1}^{(k, \ell, m)} = \alpha_{1, 1}^{(k, \ell, m)} = \alpha_{1, 1}^{(k, \ell, m)} = \beta_{k, \ell, m}$ and $\alpha_{1, 1}^{(k, \ell, m)} = \alpha_{1, 1}^{(k, \ell, m)} = \alpha_{1, 1}^{(k, \ell, m)} = \alpha_{1, 1}^{(k, \ell, m)} = -\beta_{k, \ell, m}$. Then

$$\beta = (\beta_1, \ldots, \beta_K, \beta_{1, 2}, \ldots, \beta_{K-1}, \beta_{1, 2, 3}, \ldots, \beta_{K-2, K-1})^T$$
is a minimal vector of parameters, where \((\beta_1, \ldots, \beta_K)^\top\) is the vector of main effects of dimension \(p_1 = K\), \((\beta_{1,2}, \ldots, \beta_{K-1,K})^\top\) is the vector of first-order interactions of dimension \(p_2 = \binom{K}{2}\), and \((\beta_{1,2,3}, \ldots, \beta_{K-2,K-1,K})^\top\) is the vector of second-order interactions of dimension \(p_3 = \binom{K}{3}\). Hence, \(\beta\) is a vector of dimension \(p = p_1 + p_2 + p_3 = K(K^2 + 5)/6\).

With the above notation the model can be rewritten as

\[
\hat{Y}_{na}(i) = \mu_n + \sum_{k=1}^{K} \beta_k f_k(i_k) + \sum_{k<\ell} \beta_{k,\ell} f_k(i_k)f_\ell(i_\ell) + \sum_{k<\ell<m} \beta_{k,\ell,m} f_k(i_k)f_\ell(i_\ell)f_m(i_m) + \varepsilon_{na},
\]

with the vector

\[
f(i) = (f_1(i_1), \ldots, f_K(i_K), f_1(i_1)f_2(i_2), \ldots, f_{K-1}(i_{K-1})f_K(i_K), f_1(i_1)f_2(i_2)f_3(i_3), \ldots, f_{K-2}(i_{K-2})f_{K-1}(i_{K-1})f_K(i_K))^\top
\]

of regression functions of dimension \(p\). Also here, the first \(K\) entries \(f_1(i_1), \ldots, f_K(i_K)\) of \(f(i)\) are associated with the main effects. Moreover, the second set of entries \(f_1(i_1)f_2(i_2), \ldots, f_{K-1}(i_{K-1})f_K(i_K)\) of \(f(i)\) are associated with the first-order interactions and has dimension \(p_2 = K(K-1)/2\), and the remaining entries \(f_1(i_1)f_2(i_2)f_3(i_3), \ldots, f_{K-2}(i_{K-2})f_{K-1}(i_{K-1})f_K(i_K)\) of \(f(i)\) are associated with the second-order interactions and has dimension \(p_3 = K(K-1)(K-2)/6\).

Note that \(f_k = g\) from Example 1 for all \(k = 1, \ldots, K\). Finally, the resulting paired comparison model is given by

\[
Y_{n}(i,j) = \sum_{k=1}^{K} (g(i_k) - g(j_k))\delta_k + \sum_{k<\ell} (g(i_k)g(i_\ell) - g(j_k)g(j_\ell))\delta_{k,\ell} + \sum_{k<\ell<m} (g(i_k)g(i_\ell)g(i_m) - g(j_k)g(j_\ell)g(j_m))\delta_{k,\ell,m} + \varepsilon_n,
\]

where the corresponding regression functions may only attain the values \(-2\), 0 or +2.

4 Optimal designs

We consider the second-order interactions paired comparison model \((12)\) with corresponding regression functions \(f(i)\) given by \((11)\). For what follows, we introduce the comparison depth \(d\) as in \cite{GrBh2003} which describes the number of attributes in which the two alternatives differ. These sets are very essential for optimal designs construction. The design region \(\mathcal{X}\) can be partitioned into disjoint sets such that the pairs in each set differ only in a fixed number \(d\) of the attributes. More precisely, for a comparison depth \(d = 0, \ldots, K\), let \(\mathcal{X}_d = \{(i,j) \in \mathcal{X} : \{k : i_k \neq j_k\} = d\}\) be the set of all pairs of alternatives which differ in exactly \(d\) attributes. These sets constitute the orbits with respect to permutations of both the levels \(i_k = 1, 2\) within the attributes as well as among attributes \(k = 1, \ldots, K\) themselves. Note that the \(D\)-criterion is
invariant with respect to those permutations (see Schwabe, 1996). As a result, it is sufficient to look for optimality in the class of invariant designs which are uniform on the orbits of fixed comparison depth.

Denote by \( N_d = 2^K \binom{K}{d} \) the number of different (ordered) pairs in \( \mathcal{X}_d \) which vary in exactly \( d \) attributes and by \( \xi_d \) the uniform approximate design which assigns equal weights \( \xi_d(i,j) = 1/N_d \) to each pair \((i,j)\) in \( \mathcal{X}_d \) and weight zero to all remaining pairs in \( \mathcal{X} \). We next obtain the information matrix for these invariant designs.

**Lemma 1.** Let \( d \) be a fixed comparison depth. The uniform design \( \xi_d \) on the set \( \mathcal{X}_d \) of comparison depth \( d \) has a diagonal information matrix

\[
M(\xi_d) = \begin{pmatrix}
h_1(d) \text{Id}_K & 0 & 0 \\
0 & h_2(d) \text{Id}_{(K)} & 0 \\
0 & 0 & h_3(d) \text{Id}_{(K)}
\end{pmatrix},
\]

where \( h_1(d) = \frac{4d}{K} \), \( h_2(d) = \frac{8d(K-d)}{K(K-1)} \) and \( h_3(d) = \frac{4d(3K^2-6dK+4d^2-3K+2)}{K(K-1)(K-2)} \).

Here, \( \text{Id}_m \) denotes the identity matrix of order \( m \). The proof of Lemma 1 is given in the Appendix.

Note that for \( d = 0 \) all pairs have identical attributes \((i = j)\), \( h_r(0) = 0 \) for \( r = 1, 2, 3 \), and the information is zero. Hence, the comparison depth \( d = 0 \) can be neglected. Moreover, every invariant design \( \xi \) can be written as a convex combination \( \xi = \sum_{d=1}^{K} w_d \xi_d \) of uniform designs on the comparison depths \( d \) with corresponding weights \( w_d \geq 0 \), \( \sum_{d=1}^{K} w_d = 1 \). Consequently, every invariant design has also diagonal information matrix.

**Lemma 2.** Let \( \bar{\xi} \) be an invariant design on \( \mathcal{X} \), i.e. \( \bar{\xi} = \sum_{d=1}^{K} w_d \bar{\xi}_d \), then \( \bar{\xi} \) has diagonal information matrix

\[
M(\bar{\xi}) = \begin{pmatrix}
h_1(\bar{\xi}) \text{Id}_K & 0 & 0 \\
0 & h_2(\bar{\xi}) \text{Id}_{(K)} & 0 \\
0 & 0 & h_3(\bar{\xi}) \text{Id}_{(K)}
\end{pmatrix},
\]

where \( h_r(\bar{\xi}) = \sum_{d=1}^{K} w_d h_r(d) \), \( r = 1, 2, 3 \).

Next, we consider optimal designs for the main effects, the first-order interaction and the second-order interaction terms separately by maximizing the corresponding entries \( h_1(d), h_2(d) \) and \( h_3(d) \), respectively, in the information matrix. The resulting designs are optimal with respect to any invariant criterion including \( D_A \)-optimality for the corresponding subset of the parameter vector.

**Theorem 1.** Let \( d^*_1 = K \). Then the uniform design \( \xi_{d^*_1} = \xi_K \) on the largest possible comparison depth \( K \) is universally optimal for the main effects \((\beta_1, \ldots, \beta_K)^\top\).

This means that for the main effects only those pairs of alternatives should be used which differ in all attributes. The proof of Theorem 1 follows directly from \( h_1(d) = 4d/K \) which attains its maximum at \( d^*_1 = K \).

**Theorem 2.** Let \( d^* = K/2 \) for \( K \) even and \( d^* = (K-1)/2 \) or \( d^* = (K+1)/2 \) for \( K \) odd, respectively. Then the uniform design \( \xi_{d^*_2} \) is universally optimal for the first-order interaction effects \((\beta_1, 2, \ldots, \beta_{K-1}, K)^\top\).
This means that for the first-order interactions only those pairs of alternatives should be used which differ in about half of the attributes. For the proof of Theorem 2 note that \( h_2(0) = h_2(K) = 0 \) and \( h_2 \) is a quadratic polynomial in \( d \) with negative leading coefficient. Then \( h_2 \) attains its maximum at the middle point \( K/2 \) which is integer for \( K \) even. For \( K \) odd the maximum occurs at both of the symmetrical adjacent integers \((K - 1)/2\) and \((K + 1)/2\).

It is worth-while mentioning that \( h_1(d) \) and \( h_2(d) \) are identical to the corresponding values in the first-order interactions model considered in Graßhoff et al. (2003) and, hence, the optimal designs of Theorem 1 and 2 are the same as in the first-order interactions model. However, for the second-order interactions the following result is new.

**Theorem 3.** Let \( d_3^1 = 1 \) or \( d_3^3 = 3 \) for \( K = 3 \) and \( d_3^2 = K \) for \( K \geq 4 \), respectively. Then the uniform design \( \xi_{d_3} \) is universally optimal for the second-order interaction effects \((\beta_1, 2, 3, \ldots, \beta_{K - 2, K - 1, K})^\top\).

This means that also for the second-order interactions only those pairs of alternatives should be used which differ in all attributes.

**Proof of Theorem 3.** For \( K = 3 \) we get \( h_3(1) = h_3(3) = 4 \) and \( h_3(2) = 0 \) which establishes the result in this case.

For \( K \geq 4 \) note that the function \( h_3 \) is a cubic polynomial in the comparison depth \( d \) with positive leading coefficient. Extended to a function on the real line \( h_3 \) is point symmetric with respect to \((K/2, h_3(K)/2)\) and attains its local maximum and local minimum at \( d_{3, \text{max}} = K/2 - \sqrt{3K - 3} / 6 \) and \( d_{3, \text{min}} = K/2 + \sqrt{3K - 3}/6 \), respectively. Now, the numerator of \( h_3(d_{3, \text{min}}) \) is proportional to \( d_{3, \text{min}}^3(3K - 4d_{3, \text{min}}) \). Inserting the solution for \( d_{3, \text{min}} \) into the last factor yields \( 3K - 4d_{3, \text{min}} = K - 2 \sqrt{K - 2}/3 \) which is equal to 0.349 for \( K = 4 \) and increasing in \( K \geq 3 \). Hence, \( h_3(d_{3, \text{min}}) > 0 \) for \( K \leq 4 \) and, by symmetry, \( h_3(d_{3, \text{max}}) < h_3(K) \) which proves the result.

It is worth-while mentioning that a single comparison depth \( d \) may be sufficient for non-singularity of the information matrix \( M(\xi_j) \), i.e. for the identifiability of all parameters. This can be easily seen by observing \( h_i(1) > 0, r = 1, 2, 3, \) for \( d = 1 \). But this is not true for all comparison depths as \( h_2(K) = 0 \). Moreover, in view of Theorems 1, 2 and 3 no design exists which is universally optimal for the whole parameter vector. As a consequence, we confine ourselves to the \( D \)-criterion to derive optimal design for the whole parameter vector.

Define by \( v((i, j), \xi) = (f(i) - f(j))^\top M(\xi)^{-1} (f(i) - f(j)) \) the variance function for the design \( \xi \) which plays an important role for the \( D \)-criterion. According to the Kiefer-Wolfowitz equivalence theorem (Kiefer and Wolfowitz 1960) a design \( \xi^* \) is \( D \)-optimal if the associated variance function is bounded by the number of parameters, \( v((f(i), f(j)), \xi^*) \leq p \). Now, for invariant designs \( \xi \) the variance function \( v((i, j), \xi) \) is also invariant with respect to permutations of levels and attributes and is, hence, constant on the orbits \( \mathcal{X}_d \) of fixed comparison depth \( d \). Hence, the value of the variance function for an invariant design \( \xi \) evaluated at comparison depth \( d \) may be denoted by \( v(d, \xi) \), say, where \( v(d, \xi) = v((i, j), \xi) \) on \( \mathcal{X}_d \). The following results provide formulae for calculating the variance function.
Theorem 4. For every invariant design $\xi$ the variance function $v(d, \xi)$ is given by

$$v(d, \xi) = 4d \left( \frac{1}{h_1(\xi)} + \frac{K - d}{h_2(\xi)} + \frac{3K^2 - 6dK + 4d^2 - 3K + 2}{6h_3(\xi)} \right)$$

The proof is given in the Appendix. If the invariant design $\xi$ is concentrated on a single comparison depth, then this representation simplifies.

Corollary 1. For a uniform design $\bar{\xi}_{d'}$ on a single comparison depth $d'$ the variance function is given by

$$v(d, \bar{\xi}_{d'}) = \frac{d}{d'} \left( p_1 + p_2 \frac{K - d}{K - d'} + p_3 \frac{3K^2 - 6dK + 4d^2 - 3K + 2}{3K^2 - 6d'K + 4d'^2 - 3K + 2} \right).$$

As a consequence, for $d = d'$, we immediately obtain $v(d, \bar{\xi}_{d}) = p_1 + p_2 + p_3 = p$ which recovers the $D$-optimality of $\xi_{d}$ on $X_d$ in view of the Kiefer-Wolfowitz equivalence theorem. The following result gives an upper bound on the number of comparison depths required for a $D$-optimal design.

Theorem 5. In the second-order interactions model the $D$-optimal design $\xi^*$ is supported on, at most, three different comparison depths $K$, $d^*$ and $d^* + 1$, say, i.e., $\xi^* = w_{d^*}^K \xi_K + w_{d^*}^d \xi_d + (1 - w_{d^*}^K - w_{d^*}^d) \xi_{d^*+1}$.

Proof. According to a corollary of the Kiefer-Wolfowitz equivalence theorem for the $D$-optimal design $\xi^*$ the variance function $v(d, \xi^*)$ is equal to the number of parameters $p$ for all $d$ such that $w_{d^*}^d > 0$. By Theorem 4 the variance function is a cubic polynomial in the comparison depth $d$ with positive leading coefficient. According to the fundamental theorem of algebra the variance function $v(d, \xi^*)$ may thus be equal to $p$ for, at most, three different values $d_1 < d_2 < d_3$ of $d$, say. Now, by the Kiefer-Wolfowitz equivalence theorem itself $v(d, \xi^*) \leq p$ for all $d = 0, 1, \ldots, K$. Hence, by the shape of the variance function we obtain that in the case of three different comparison depths $d_3 = K$ and $d_2 = d_1$ must hold. For two comparison depths either $d_2 = K$ or two adjacent comparison depths $d_1$ and $d_2 = d_1 + 1$ are included.

For $K = 3$ the $D$-optimal design can be given explicitly.

Theorem 6. For $K = 3$ the uniform design $\xi^* = \frac{3}{7} \xi_1 + \frac{3}{7} \xi_2 + \frac{1}{7} \xi_3$ on all pairs with non-zero comparison depth is $D$-optimal in the second-order interactions model.

Proof. For $K = 3$ the second-order interactions model is a full interactions model. Hence, the results follows directly from Theorem 4 in Grahlhoff et al. (2003).

Alternatively, we may compute the variance function by first computing $h_r(\xi^*) = 16/7$, $r = 1, 2, 3$, and then deriving $v(d, \xi^*) = 7d(d^2 - 6d + 11)/6$ which results in $v(d, \xi^*) = 7$ for $d = 1, 2, 3$. Because $p = 7$ for $K = 3$ the $D$-optimality of $\xi^*$ follows from the Kiefer-Wolfowitz equivalence theorem.

Hence, for $K = 3$ all three comparison depths are needed for $D$-optimality. For $K \geq 4$ numerical computations indicate that only two different comparison depths $K$ and $d^*$ are required. In Table I numerical solutions are presented for numbers $K$ of attributes between 4 and 10.
Table 1: Optimal comparison depths and optimal weights for $K$ binary attributes

| $K$ | 4   | 5   | 6   | 7   | 8   | 9   | 10  |
|-----|-----|-----|-----|-----|-----|-----|-----|
| $w_{K}^*$ | 0.143 | 0.167 | 0.268 | 0.303 | 0.356 | 0.423 | 0.462 |
| $d^*$ | 2   | 2   | 3   | 3   | 3   | 4   | 4   |
| $w_{d^*}^*$ | 0.857 | 0.833 | 0.732 | 0.697 | 0.644 | 0.577 | 0.538 |

For fixed number $K$ of attributes and intermediate comparison depth $d$ the optimal weights $w_{K}^*$ and $w_{d^*}^* = 1 - w_{K}^*$ have been determined analytically by direct maximization of $\ln(\det(M(w_K \xi_K + (1 - w_K)\xi_d)))$. In particular, for $K = 5, 7$ and $9$ we obtain the optimal intermediate comparison depth $d^* = (K - 1)/2$ and corresponding optimal weights

$$w_{K}^* = \frac{2K^3 - 6K^2 + 7K - K\sqrt{K^6 - 12K^3 - 64K^2 + 448K - 636K + 369} + 15}{-K^3 + 2K^2 - 2K^2 + 10K + 15}$$

and $w_{d^*}^* = 1 - w_{K}^*$. For $K = 4$ and $6$ we get the optimal intermediate comparison depth $d^* = K/2$ and corresponding optimal weights

$$w_{K}^* = \frac{K^2 - 6K + 11}{K^2 + 5}$$

and $w_{d^*}^* = 1 - w_{K}^*$, respectively, while for $K = 8$ and $10$ the optimal intermediate comparison depth is $d^* = (K/2) - 1$ with corresponding optimal weights

$$w_{K}^* = \frac{K^3 + 5K + (K - K^2)\sqrt{K^4 - 10K^4 + 37K^2 - 60K + 180} + 30}{-K^4 + K^2 + K^2 + 3K + 30}$$

and $w_{d^*}^* = 1 - w_{K}^*$, respectively. The analytical results were computed using the Maple (version 2017) software (Maple Inc., 1981-2017). The optimality of these designs has been checked numerically by virtue of the Kiefer-Wolfowitz equivalence theorem. The corresponding values of the normalized variance function $v(d, \xi^*)/p$ are recorded in Table 2 in the Appendix, where maximal values less or equal to 1 establish optimality.

Based on numerical findings for larger $K$ up to 100 we conjecture that for all numbers $K \geq 4$ of attributes only one intermediate comparison depth $d^*$ is required for $D$-optimality which is equal to $(K - 1)/2$ for $K$ odd and $(K/2) - 1$ for $K \geq 8$ even, respectively.

5 Discussion

For paired comparisons in an additive (main effects only) model optimal designs require that the components of the alternatives in the choice sets show distinct levels in all attributes (see [Graßhoff et al., 2004]). In a first-order interactions model we have to consider pairs for an optimal design in which approximately one half of the attributes are distinct and one half of the attributes coincide (see [Graßhoff et al., 2003]). Here, it is shown that in a second-order interactions model we have to consider both types of pairs in which either all attributes have distinct levels or approximately one half of the attributes are distinct and one
half of the attributes coincide to obtain a $D$-optimal design for the whole parameter vector. The invariance considerations used here can be readily extended to partial profiles, to higher-order interaction models and to larger numbers of levels for each attribute.

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APPENDIX

Proof of Lemma 1. First we note that for the function \( g \) defined in Example 1 we have \( g(i)^2 = 1, g(i)g(j) = -1, (g(i) - g(j))^2 = 4 \) for \( i \neq j \). Given a fixed comparison depth \( d \) we obtain for the regression functions \( f_k = g \) associated with the \( k \)-th main effect

\[
\sum_{(i,j) \in X_d} (f_k(i_k) - f_k(j_k))^2 = \left( \frac{K-1}{d-1} \right) 2^K \cdot 4 = \left( \frac{K-1}{d-1} \right) 2^{K+2}
\]

because there are \( \left( \frac{K-1}{d-1} \right) 2^K \) pairs in \( X_d \) for which \( i_k \) and \( j_k \) differ. Since the number \( N_d \) of paired comparisons in \( X_d \) equals \( N_d = \left( \frac{K}{d} \right) 2^K \), the corresponding diagonal entries \( h_1(d) \) in the information matrix are given by

\[
h_1(d) = \frac{1}{N_d} \sum_{(i,j) \in X_d} (f_k(i_k) - f_k(j_k))^2 = \frac{4d}{K}
\]

(compare Graßhoff et al. 2003, where a slightly different normalization is used).

For first-order interactions, we consider attributes \( k \) and \( \ell \), say, and distinguish between pairs in which both attributes are distinct and pairs in which only one of these attributes has distinct levels in the alternatives while the same level is presented in both alternatives for the other attribute.

In the case \( i_k \neq j_k \) and \( i_\ell \neq j_\ell \) we have \( g(i_k)g(i_\ell) = g(j_k)g(j_\ell) \), while for \( i_k = j_k \) and \( i_\ell = j_\ell \) we get \( g(i_k)g(i_\ell) = -g(j_k)g(j_\ell) \). Hence

\[
(g(i_k)g(i_\ell) - g(j_k)g(j_\ell))^2 = 0 \quad \text{for} \quad i_k \neq j_k \quad \text{and} \quad i_\ell \neq j_\ell
\]

and

\[
(g(i_k)g(i_\ell) - g(j_k)g(j_\ell))^2 = 4 \quad \text{for} \quad i_k \neq j_k \quad \text{and} \quad i_\ell = j_\ell,
\]

respectively, where (in the latter case) the roles of the attributes \( k \) and \( \ell \) may be interchanged.

For given attributes \( k \) and \( \ell \) pairs with distinct levels in both attributes occur \( \left( \frac{K-2}{d-2} \right) 2^K \) times in \( X_d \), while those which differ only in one attribute occur \( \left( \frac{1}{d-1} \right) \left( \frac{K-2}{d-1} \right) 2^K \) times. As a result, for the first-order interactions the diagonal elements \( h_2(d) \) in the information matrix are given by

\[
h_2(d) = \frac{1}{N_d} \sum_{(i,j) \in X_d} (f_k(i_k) - f_k(j_k))^2 = \frac{8d(K-d)}{K(K-1)}
\]
Accordingly, for second-order interactions, we consider attributes \( k, \ell \) and \( m \), say, and distinguish between pairs in which all three attributes are distinct, pairs in which two of these attributes are distinct, pairs in which none of the attributes are distinct and, finally, pairs in which only one of the attributes, say, \( k \), has distinct levels in the alternatives while the same level is presented in both alternatives for the remaining attribute and, finally, pairs in which only one of the attributes, say, \( k \), has distinct levels in the alternatives while the same level is presented in both alternatives for the two remaining attributes. Then \( g(i_k)g(i_\ell)g(i_m) = -g(j_k)g(j_\ell)g(j_m) \) in the first and third case, while \( g(i_k)g(i_\ell)g(i_m) = g(j_k)g(j_\ell)g(j_m) \) in the second case. Hence,

\[
(g(i_k)g(i_\ell)g(i_m) - g(j_k)g(j_\ell)g(j_m))^2 = 4 \quad \text{for} \quad i_k \neq j_k, \ i_\ell \neq j_\ell \quad \text{and} \quad i_m \neq j_m,
\]

\[
(g(i_k)g(i_\ell)g(i_m) - g(j_k)g(j_\ell)g(j_m))^2 = 0 \quad \text{for} \quad i_k \neq j_k, \ i_\ell \neq j_\ell \quad \text{and} \quad i_m = j_m
\]

and

\[
(g(i_k)g(i_\ell)g(i_m) - g(j_k)g(j_\ell)g(j_m))^2 = 4 \quad \text{for} \quad i_k \neq j_k, \ i_\ell = j_\ell \quad \text{and} \quad i_m = j_m,
\]

respectively, where again the roles of the attributes \( k, \ell \) and \( m \) may be interchanged.

For given attributes \( k, \ell \) and \( m \) the pairs with distinct levels in the three attributes occur \( \binom{K-3}{d-3} 2^K \) times in \( \mathcal{X}_d \) while those which differ in two attributes occur \( \binom{K-3}{d-2} 2^K \) times in \( \mathcal{X}_d \), and those which differ only in one attribute occur \( \binom{K-3}{d-1} 2^K \) times. As a result, for the second-order interactions the diagonal elements \( h_3(d) \) in the information matrix are given by

\[
h_3(d) = \frac{1}{N_d} \left( \binom{K-3}{d-3} 2^K \cdot 4 + 3 \binom{K-3}{d-1} 2^K \cdot 4 \right)
= \frac{4d(d-1)(d-2) + 3(K-d)(K-d-1)}{K(K-1)(K-2)}
= \frac{4d(3K^2 - 6dK + 4d^2 - 3K + 2)}{K(K-1)(K-2)}.
\]

Finally, it can be noted that all off-diagonal entries in the information matrix vanish because the terms in the corresponding sums add up to zero due to the effect-type coding.

\[\square\]

**Proof of Theorem 4.** First we note that

\[
M(\xi)^{-1} = \begin{pmatrix}
\frac{1}{h_3(\xi)} \text{Id}_K & 0 & 0 \\
0 & \frac{1}{h_2(\xi)} \text{Id}_K & 0 \\
0 & 0 & \frac{1}{h_1(\xi)} \text{Id}_K
\end{pmatrix},
\]

for the inverse of the information matrix of the design \( \xi \). Hence, we obtain for
the variance function

\[ v((i,j), \xi) = (f(i) - f(j))\mathbf{M}^{-1}(f(i) - f(j)) \]

\[ = \frac{1}{h_1(\xi)} \sum_{i=1}^{K} (g(i_k) - g(j_k))^2 \]

\[ + \frac{1}{h_2(\xi)} \sum_{k<\ell} (g(i_k)g(i_\ell) - g(j_k)g(j_\ell))^2 \]

\[ + \frac{1}{h_3(\xi)} \sum_{k<\ell<m} (g(i_k)g(i_\ell)g(i_m) - g(j_k)g(j_\ell)g(j_m))^2. \]

As in the proof of Lemma 11 we note first that for the terms associated with the main effects we have \( (g(i_k) - g(j_k))^2 = 4 \), when \( i_k \neq j_k \), and \( (g(i_k) - g(j_k))^2 = 0 \) otherwise. For a pair \((i,j)\) of comparison depth \(d\) there are exactly \(d\) attributes for which \(i_k\) and \(j_k\) differ. Hence, the first sum on the right hand side of (16) equals \(4d\).

Second, for the terms associated with the first-order interactions we have \( (g(i_k)g(i_\ell) - g(j_k)g(j_\ell))^2 = 4 \), if either \(i_k \neq j_k\) and \(i_\ell = j_\ell\) or \(i_k = j_k\) and \(i_\ell \neq j_\ell\), and \( (g(i_k)g(i_\ell) - g(j_k)g(j_\ell))^2 = 0 \) otherwise. For a pair \((i,j)\) of comparison depth \(d\) there are \(d(K - d)\) first-order interaction terms for which \((i_k, i_\ell)\) and \((j_k, j_\ell)\) differ in exactly one attribute \(k\) or \(\ell\). Hence, the second sum on the right hand side of (16) equals \(4d(K - d)\).

Finally, for the terms associated with the second-order interactions we have \( (g(i_k)g(i_\ell)g(i_m) - g(j_k)g(j_\ell)g(j_m))^2 = 4 \), if \((i_k, i_\ell, i_m)\) and \((j_k, j_\ell, j_m)\) differ in all three attributes \(k, \ell\), and \(m\), or in exactly one of these attributes, and \( (g(i_k)g(i_\ell)g(i_m) - g(j_k)g(j_\ell)g(j_m))^2 = 0 \) otherwise. For a pair \((i,j)\) of comparison depth \(d\) there are \(\binom{d}{2}\) second-order interaction terms for which all three associated attributes differ, and there are \(d\left(\binom{K-d}{2}\right)\) second-order interaction terms for which \((i_k, i_\ell, i_m)\) and \((j_k, j_\ell, j_m)\) differ in exactly one attribute. Hence, there are

\[ \binom{d}{2} + d\left(\binom{K-d}{2}\right) = d(d-1)(d-2)/6 + d(K-d)(K-d-1)/2 \]

\[ = d(3K^2 - 6dK + 4d^2 - 3K + 2)/6 \]

non-zero entries in the third sum on the right hand side of (16), and this sum equals \(4d(3K^2 - 6dK + 4d^2 - 3K + 2)/6\).

By inserting these results into (16) we see that the value of the variance function depends on the pair \((i,j)\) only through its comparison depth \(d\) and obtain the formula proposed.

Proof of Corollary 12. This representation of the variance function follows immediately by inserting the values of \(h_r(\xi_\alpha)\) from Lemma 11 and \(p_r = \binom{K}{r}\), \(r = 1, 2, 3\), into the formula of Theorem 13.
Table 2: Values of the variance function of the $D$-optimal design $\xi^*$ for $K$ binary attributes (boldface 1 corresponds to the optimal comparison depths)

| $K$ | 1  | 2  | 3  | 4  | 5  | 6  | 7  | 8  | 9  | 10 |
|-----|----|----|----|----|----|----|----|----|----|----|
| 4   | 0.875 | 1  | 0.875 | 1  |    |    |    |    |    |    |
| 5   | 0.760 | 1  | 0.960 | 0.880 | 1  |    |    |    |    |    |
| 6   | 0.701 | 0.983 | 1  | 0.906 | 0.855 | 1  |    |    |    |    |
| 7   | 0.615 | 0.917 | 1  | 0.956 | 0.879 | 0.863 | 1  |    |    |    |
| 8   | 0.559 | 0.872 | 1  | 1    | 0.945 | 0.884 | 0.882 | 1  |    |    |
| 9   | 0.504 | 0.811 | 0.962 | 1  | 0.969 | 0.910 | 0.868 | 0.883 | 1  |    |
| 10  | 0.462 | 0.763 | 0.932 | 1  | 0.997 | 0.956 | 0.905 | 0.874 | 0.896 | 1  |