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REGULAR ARTICLE

Optimal 2^K paired comparison designs for third-order interactions

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Abstract
In psychological research often paired comparisons are used in which either full or partial profiles of the alternatives described by a common set of two-level attributes are presented. For this situation the problem of finding optimal designs is considered in the presence of third-order interactions.

Keywords Comparison depth · Full profile · Interactions · Optimal design · Paired comparisons · Partial profile · Profile strength

Mathematics Subject Classification 62K05 · 62J15 · 62K15

1 Introduction

Paired comparison experiments have received considerable attention in many fields of applications like psychology, health economics, transportation economics and marketing to study people's preferences for goods or services where behaviors of interest involve either qualitative (so-called discrete choice experiments) or quantitative responses (so-called conjoint analysis). A comprehensive introduction to this general area of paired comparison experiments can be found in Großmann and Schwabe (2015), van Berkum (1987b) and Louviere et al. (2000).

Typically with paired comparisons, respondents usually evaluate pairs of competing options (alternatives) in a hypothetical (occasionally real) setting which are generated by an experimental design and are represented by a combination of the levels of several attributes (factors). However, in applications, situations may arise in which one may be interested in special relations between the attributes (interactions). For example, Elrod et al. (1992) considered a study on student preferences for rental apartments in which

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four attribute interactions were of special interest. The corresponding result is well summarized in Table 2 of their paper. A full factorial experiment where four attribute interactions were of interest can also be found in Collins et al. 2009, p. 17). As was pointed out by Collins et al. (2009), there are few areas in the social and behavioral sciences in which theory makes specific predictions about higher-order interactions (four attribute interactions, for example), and it appears that to date there has been relatively little empirical investigation of such interactions. This paper is motivated by the situation where the designs enable identification of main effects and two and three and four attribute interactions, which may not be of primary application interest but theoretically worthwhile (e.g., see El-Helbawy and Ahmed 1984; Quenouille and John 1971; Lewis and Tuck 1985).

In applications the preference (or choice task) imposes cognitive burden when the alternatives presented are specified by too many attributes. This has a detrimental effect on the validity of the estimated parameters. In this situation, a way to simplify the choice task is to specify only a few components (attributes) of the alternatives known as partial profiles (e.g., see Graßhoff et al. 2003; Chrzan 2010; Großmann 2018). The number of attributes that are presented in this restricted setting is called the profile strength (Graßhoff et al. 2003). It should be noted that for full profiles, the alternatives are represented by level combinations in which all attributes are involved.

The aim of this paper is to introduce an appropriate model for the situation of full and partial profiles and to derive optimal designs in the presence of interactions. We consider the case when the alternatives are specified by a common set of two-level attributes. Work on determining the structure of the optimal designs in this two-level situation has been carried out by van Berkum (1987a, b) and Street et al. (2001) in the case of full profiles in a main effects and first-order interactions setup, and by Schwabe et al. (2003) for partial profiles. Corresponding results when the common number of the attribute levels is larger than two have been obtained by Graßhoff et al. (2003) and Nyarko (2019) in a first- and second-order interactions setup, respectively, for both full and partial profiles. The two-level situation for the corresponding second-order interactions setup has been investigated by Nyarko and Schwabe (2019). Here we treat the case of third-order interactions and provide detailed proofs.

The remainder of the paper is organized as follows. In Sect. 2 a general model is introduced for paired comparison experiments. Section 3 provides the third-order interactions model for both full and partial profiles. Optimal designs are characterized in Sect. 4 and the final Sect. 5 offers some conclusions. All major proofs are deferred to the Appendix.

2 General setting

2.1 Model considerations

We consider the context in which K attributes (or factors) are of influence. In many contexts we would obtain at least one direct observation under some, if not all, of the combinations of these K factors. However in the context of paired comparison experiments, we only obtain (comparative) observations under some, if not all, pairs of these combinations.

Let $\mathbf{i} = (i_1, i_2, \ldots, i_K)$ and $\mathbf{j} = (j_1, j_2, \ldots, j_K)$ denote two factor combinations or sets of attributes, defining a pair $(\mathbf{i}, \mathbf{j})$, under which we obtain an nth observation. So i_k and j_k denote levels of the kth attribute of influence, $k = 1, 2, \ldots, K$. Also $(\mathbf{i}, \mathbf{j})$ define a pair of alternatives, which we label 1, 2 (for 1st and 2nd) respectively and we let $a = (1, 2)$. Denote this observation by $Y_n(\mathbf{i}, \mathbf{j})$. So n indexes both Y and $\mathbf{i}, \mathbf{j}$. To motivate a model for $Y_n(\mathbf{i}, \mathbf{j})$, it is useful to imagine what models we might consider for observations under each of $\mathbf{i}$ ($a = 1$) and $\mathbf{j}$ ($a = 2$) separately. Denote these observations by $Y_{n1}(\mathbf{i})$ and $Y_{n2}(\mathbf{j})$. Potential general linear models for these are:

$$\begin{aligned} Y_{n1}(\mathbf{i}) &= \mu_n + \mathbf{f}(\mathbf{i})^\top \boldsymbol{\beta} + \varepsilon_{n1}(\mathbf{i}) \\ Y_{n2}(\mathbf{j}) &= \mu_n + \mathbf{f}(\mathbf{j})^\top \boldsymbol{\beta} + \varepsilon_{n2}(\mathbf{j}). \end{aligned} \tag{1}$$

Here $\boldsymbol{\beta}$ is the vector of parameters of interest, while the term μ_n is the block or pair effect. Its dependence on n would normally create an identifiability problem. However it is removed from our model for $Y_n(\mathbf{i}, \mathbf{j})$ under the assumption that the preferences between alternatives $(\mathbf{i}, \mathbf{j})$ is defined as the difference

$$Y_n(\mathbf{i}, \mathbf{j}) = Y_{n1}(\mathbf{i}) - Y_{n2}(\mathbf{j}).$$

This can be viewed as a difference between utilities of the two options. So a model for $Y_n(\mathbf{i}, \mathbf{j})$ is:

$$Y_n(\mathbf{i}, \mathbf{j}) = [\mathbf{f}(\mathbf{i}) - \mathbf{f}(\mathbf{j})]^\top \boldsymbol{\beta} + \varepsilon_n(\mathbf{i}, \mathbf{j}). \tag{2}$$

Here $[\mathbf{f}(\mathbf{i}) - \mathbf{f}(\mathbf{j})]$ is the derived regression function and the random errors $\varepsilon_n(\mathbf{i}, \mathbf{j}) = \varepsilon_{n1}(\mathbf{i}) - \varepsilon_{n2}(\mathbf{j})$, associated with the different pairs, are assumed to be uncorrelated, and with constant variance.

2.2 Design considerations

Further the settings $\mathbf{x} = (\mathbf{i}, \mathbf{j})$ are chosen from the design region $\mathcal{X} = \mathcal{I} \times \mathcal{I}$ of possible pairs of alternatives.

The quality of the statistical analysis based on a paired comparison experiment depends on the set of pairs (alternatives) in the choice sets which are presented. The choice of such pairs $(\mathbf{i}_1, \mathbf{j}_1), \ldots, (\mathbf{i}_N, \mathbf{j}_N)$ is called a design ξ_N of size N. The performance of the design ξ_N is measured by its information matrix

$$\mathbf{M}(\xi_N) = \sum_{n=1}^{N} (\mathbf{f}(\mathbf{i}_n) - \mathbf{f}(\mathbf{j}_n))(\mathbf{f}(\mathbf{i}_n) - \mathbf{f}(\mathbf{j}_n))^\top. \tag{3}$$

To enhance efficient comparison of designs with different sample sizes we have to make use of the standardized (per observation) information matrices

$$\mathbf{M}(\xi) = \frac{1}{N}\mathbf{M}(\xi_N) \tag{4}$$

which are related to the concept of generalized (approximate) designs (e.g., see Kiefer 1959), which are defined as discrete probability measures ξ on the design region $\mathcal{X}$.

As a performance measure in a majority of works about optimal designs for paired comparison experiments, we confine ourselves to the D-optimality criterion which aims at maximizing the determinant of the information matrix $\mathbf{M}(\xi)$. Any design that is proposed for estimating the model parameters can be compared to these designs. In general, the D-efficiency of the approximate design ξ is given by $(\det\mathbf{M}(\xi)/\det\mathbf{M}(\xi^*))^{1/p}$ where ξ^* is D-optimal and p is the number of parameters that have to be estimated in the model.

2.3 Related contributions

It is worthwhile mentioning 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 of indifference, $\boldsymbol{\beta} = \mathbf{0}$ (e.g., see Großmann et al. 2002). Specifically, under this indifference assumption of equal choice probabilities, the Bradley-Terry type choice experiments in which the probability of choosing $\mathbf{i}$ from the pair $(\mathbf{i}, \mathbf{j})$ [given by $\exp[\mathbf{f}(\mathbf{i})^\top\boldsymbol{\beta}]/(\exp[\mathbf{f}(\mathbf{i})^\top\boldsymbol{\beta}] + \exp[\mathbf{f}(\mathbf{j})^\top\boldsymbol{\beta}])$], and the probability of choosing $\mathbf{j}$ from the pair $(\mathbf{i}, \mathbf{j})$ [given by $1 - \exp[\mathbf{f}(\mathbf{i})^\top\boldsymbol{\beta}]/(\exp[\mathbf{f}(\mathbf{i})^\top\boldsymbol{\beta}] + \exp[\mathbf{f}(\mathbf{j})^\top\boldsymbol{\beta}])$ as in the work of Street and Burgess (2007), amongst others] can be derived by considering the linear paired comparison model. In particular, this assumption simplifies the information matrix of the binary logit model which coincides with the information matrix of the linear paired comparison model. This is the approach taken by others (see Graßhoff et al. 2003, 2004; Großmann and Schwabe 2015).

3 Third-order interactions model

Usually, in paired comparison experiments one may be interested in both the main effects and interactions of the attributes. For that setting optimal designs have been derived (see van Berkum 1987b; Graßhoff et al. 2003; Nyarko and Schwabe 2019) in a first- and second-order interactions setup. In this paper we derive optimal designs for the third-order interactions model.

In what follows, we commence with the situation of full profiles where two options (alternatives) are considered simultaneously. As was already pointed out, in this case the alternatives are represented by level combinations in which all attributes are involved. The first alternative is denote by $\mathbf{i} = (i_1, i_2, \ldots, i_K)$ and the second alternative by $\mathbf{j} = (j_1, j_2, \ldots, j_K)$, which are both elements of the set $\mathcal{I} = \{-1, 1\}^K$ where 1 and -1 represent the first and second level of each attribute, respectively. Specifically, the choice set $(\mathbf{i}, \mathbf{j})$ is an ordered pair of alternatives $\mathbf{i}$ and $\mathbf{j}$ which is chosen from the design region $\mathcal{X} = \mathcal{I} \times \mathcal{I}$. Note that for each attribute (component) k the corresponding regression functions f_k is just the identiy, $f_k(i_k) = i_k$ for alternatives $i_k \in \mathcal{I} = \{-1, 1\}$ (see e.g., Nyarko and Schwabe 2019).

In the presence of up to third-order interactions we consider the model

$$Y_{na}(\mathbf{i}) = \mu_n + \sum_{k=1}^{K} \beta_k i_k + \sum_{k<\ell} \beta_{k\ell} i_k i_\ell + \sum_{k<\ell<m} \beta_{k\ell m} i_k i_\ell i_m + \sum_{k<\ell<m<r} \beta_{k,\ell,m,r} i_k i_\ell i_m i_r + \varepsilon_{na}(\mathbf{i}) \tag{5}$$

for the direct response $Y_{na}(\mathbf{i})$ at the corresponding alternative $\mathbf{i} = (i_1, i_2 \ldots, i_K)$ of full profiles. Here β_k denotes the main effect of the kth attribute, $\beta_{k\ell}$ is the first-order interaction of the kth and ℓth attribute, $\beta_{k\ell m}$ is the second-order interaction of the kth, ℓth and mth attribute and $\beta_{k\ell mr}$ is the third-order interaction of the kth, ℓth, mth and rth attribute. The vectors $(\beta_k)_{1\le k\le K}$ of main effects, $(\beta_{k\ell})_{1\le k<\ell\le K}$ of first-order interactions, $(\beta_{k\ell m})_{1\le k<\ell<m\le K}$ of second-order interactions and $(\beta_{k\ell mr})_{1\le k<\ell<m<r\le K}$ of third-order interactions have dimensions $p_1 = K$, $p_2 = K(K-1)/2$, $p_3 = K(K-1)(K-2)/6$ and $p_4 = (1/24)K(K-1)(K-2)(K-3)$, respectively. Hence, the complete parameter vector $\boldsymbol{\beta} = (\beta_1, \ldots, \beta_K, (\beta_{k\ell})_{k<\ell}^\top, (\beta_{k\ell m})_{k<\ell<m}^\top, (\beta_{k\ell mr})_{k<\ell<m<r}^\top)^\top$ has dimension $p = p_1 + p_2 + p_3 + p_4$. Here the regression functions are given by

$$\mathbf{f}(\mathbf{i}) = (i_1, \ldots, i_K, (i_k i_\ell)_{k<\ell}^\top, (i_k i_\ell i_m)_{k<\ell<m}^\top, (i_k i_\ell i_m i_r)_{k<\ell<m<r}^\top)^\top \tag{6}$$

of dimension p, where, in $\mathbf{f}(\mathbf{i})$, the first $p_1 = K$ components $i_1, \ldots, i_K$ are associated with the main effects, the second set of p_2 components $i_k i_\ell$, $1 \le k < \ell \le K$, are associated with the first-order interactions, the third set of p_3 components $i_k i_\ell i_m$, $1 \le k < \ell < m \le K$, are associated with the second-order interactions, and the remaining p_4 components $i_k i_\ell i_m i_r$, $1 \le k < \ell < m < r \le K$, are associated with the third-order interactions.

Due to the cognitive burden associated with alternatives involving a large number of attributes and its detrimental effect on the validity of the estimated model parameters, it has become common practice in the literature to hold the levels of some of the attributes constant in the alternatives that are presented within a single paired comparison. These constant attributes are usually set to zero, i.e. $i_k = 0$ in the preference task (presented scenarios) and the remaining attributes constitute the resulting preference task. The profiles in such a preference task are known as partial profiles, and the number of attributes that are allowed in the partial profiles is called the profile strength, denoted as S (see Graßhoff et al. 2003; Kessels et al. 2011). Here the remaining $K-S$ attributes are not shown and remain thus unspecified.

Now, for partial profiles, a direct observation may be described by model (5) when summation is taken only over those S attributes contained in the describing subset. Note that a profile strength $S \ge 4$ is required to ensure identifiability of the interactions. As already pointed out, we introduce an additional level 0 for each attribute indicating that the corresponding attribute is not present in the partial profile. In this setting a direct observation can be described by (5) even when one considers a partial profile $\mathbf{i}$

from the set

$$\mathcal{I}^{(S)} = \{\mathbf{i};\; i_k \in \{-1, 1\} \text{ for } S \text{ components and} \\ i_k = 0 \text{ for } K - S \text{ components}\}, \tag{7}$$

of alternatives with profile strength S. In particular, $\mathcal{I}^{(K)} = \mathcal{I}^{(S)}$ in the case of full profiles $S = K$. For general profile strength S the vector of regression functions $\mathbf{f}$ and the interpretation of the parameter vector $\boldsymbol{\beta}$ remain unchanged.

The corresponding paired comparison model is thus given by

$$Y_n(\mathbf{i}, \mathbf{j}) = \sum_{k=1}^{K}(i_k - j_k)\beta_k + \sum_{k<\ell}(i_k i_\ell - j_k j_\ell)\beta_{k\ell} + \sum_{k<\ell<m}(i_k i_\ell i_m - j_k j_\ell j_m)\beta_{k\ell m} \\ + \sum_{k<\ell<m<r}(i_k i_\ell i_m i_r - j_k j_\ell j_m j_r)\beta_{k\ell mr} + \varepsilon_n(\mathbf{i}, \mathbf{j}) \tag{8}$$

as before. However, caution is necessary for the specification of the design region in the case of partial profiles. Then it has to be taken into account that the same S attributes are used in both alternatives. To accommodate this restriction, the design region can be specified as

$$\mathcal{X}^{(S)} = \{(\mathbf{i}, \mathbf{j});\; i_k, j_k \in \{-1, 1\} \text{ for } S \text{ components and} \\ i_k = j_k = 0 \text{ for } K - S \text{ components}\} \tag{9}$$

for the set of partial profiles with profile strength S.

4 Optimal designs

In the present setting, we derive optimal designs for the paired comparison model (8) with corresponding regression functions $\mathbf{f}(\mathbf{i})$ defined by (6). Without loss of generality, we define d as the comparison depth which describes the number of attributes presented in which the two alternatives differ satisfying $1 \leq d \leq S \leq K$ (see Graßhoff et al. 2003).

Following Nyarko and Schwabe (2019), for profile strength S the design region $\mathcal{X}^{(S)}$ can be partitioned into disjoint sets as

$$\mathcal{X}^{(S)} = \bigcup_{d=1}^{S} \mathcal{X}_d^{(S)}, \tag{10}$$

where $(\mathbf{i}, \mathbf{j}) \in \mathcal{X}_d^{(S)}$: $\mathbf{i}$ and $\mathbf{j}$ differ by exactly d components. These sets constitute the orbits with respect to both permutations of the levels $i_k, j_k = -1, 1$ for each attribute and to permutations of the attributes $k = 1, \ldots, K$, themselves.

The D-criterion is invariant with respect to those permutations (see Schwabe 1996, p. 17), which induce a linear reparameterization. Hence, it suffices to find optimal designs within the class of invariant designs.

Let $N_d = 2^S \binom{K}{S}\binom{S}{d}$ be the number of paired comparisons in $\mathcal{X}_d^{(S)}$ with comparison depth d and denote by $\bar{\xi}_d$ the uniform approximate design which assigns equal weights $\bar{\xi}_d(\mathbf{i}, \mathbf{j}) = 1/N_d$ to each pair $(\mathbf{i}, \mathbf{j})$ in $\mathcal{X}_d^{(S)}$ and weight zero to all remaining pairs in $\mathcal{X}^{(S)}$. The information matrix for $\bar{\xi}_d$ is given in the following. We mention that the three functions $h_1(d)$, $h_2(d)$ and $h_3(d)$ are identical to the terms for the second-order interaction models considered by Nyarko and Schwabe (2019), and $\mathbf{Id}_m$ denotes the identity matrix of order m for every m.

Lemma 1 *Let $d \in \{0, \dots, S\}$. The uniform design $\bar{\xi}_d$ on the set $\mathcal{X}_d^{(S)}$ of comparison depth d has block diagonal information matrix*

$$\mathbf{M}(\bar{\xi}_d) = \begin{pmatrix} h_1(d)\mathbf{Id}_K & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & h_2(d)\mathbf{Id}_{\binom{K}{2}} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & h_3(d)\mathbf{Id}_{\binom{K}{3}} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & h_4(d)\mathbf{Id}_{\binom{K}{4}} \end{pmatrix},$$

where $h_1(d) = \dfrac{4d}{K}$, $h_2(d) = \dfrac{8d(S-d)}{K(K-1)}$, $h_3(d) = \dfrac{4d(3S^2 - 6Sd + 4d^2 - 3S + 2)}{K(K-1)(K-2)}$ *and* $h_4(d) = \dfrac{16d(S-d)(2d^2 - 2Sd + S^2 - 3S + 4)}{K(K-1)(K-2)(K-3)}$.

Generally, invariant designs $\bar{\xi}$ can be written as a convex combination $\bar{\xi} = \sum_{d=1}^{S} w_d \bar{\xi}_d$ of uniform designs $\bar{\xi}_d$ on the comparison depths d (which describes the number of attributes presented in which the two alternatives differ) with corresponding weights $w_d \geq 0$, $\sum_{d=1}^{S} w_d = 1$. Consequently, for every invariant design the information matrix can be obtained as the corresponding convex combination of the information matrices for the uniform designs on fixed comparison depths.

Lemma 2 *Every invariant design $\bar{\xi} = \sum_{d=1}^{S} w_d \bar{\xi}_d$ on the set $\mathcal{X}^{(S)}$ has block diagonal information matrix*

$$\mathbf{M}(\bar{\xi}) = \begin{pmatrix} h_1(\bar{\xi})\mathbf{Id}_K & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & h_2(\bar{\xi})\mathbf{Id}_{\binom{K}{2}} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & h_3(\bar{\xi})\mathbf{Id}_{\binom{K}{3}} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & h_4(\bar{\xi})\mathbf{Id}_{\binom{K}{4}} \end{pmatrix},$$

where $h_r(\bar{\xi}) = \sum_{d=1}^{S} w_d h_r(d)$, $r = 1, 2, 3, 4$.

First we consider optimal designs for the main effects, the first-order interaction, the second-order interaction and the third-order interaction terms separately by maximizing the corresponding entries $h_1(d)$, $h_2(d)$, $h_3(d)$ and $h_4(d)$, respectively, in the information matrix. The resulting designs are optimal with respect to any invariant criterion for the corresponding subset of the full parameter vector $\boldsymbol{\beta} = (\beta_1, \ldots, \beta_K, (\beta_{k\ell})^\top_{k<\ell}, (\beta_{k\ell m})^\top_{k<\ell<m}, (\beta_{k\ell mr})^\top_{k<\ell<m<r})^\top$. To start with, we mention that the three following results (Result 1, Result 2 and Result 3) paraphrase theorems given in Graßhoff et al. (2003) and Nyarko and Schwabe (2019) for both first and second-order interaction models.

Result 1 *The uniform design $\bar{\xi}_S$ on the largest possible comparison depth S is optimal for the vector of 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 presented, subject to the profile strength S.

Result 2 (a) *For S even the uniform design $\bar{\xi}_{S/2}$ is optimal for the vector of first-order interaction effects $(\beta_{k\ell})^\top_{k<\ell}$.*
(b) *For S odd the uniform designs $\bar{\xi}_{(S-1)/2}$ and $\bar{\xi}_{(S+1)/2}$ are both optimal for the vector of first-order interaction effects $(\beta_{k\ell})^\top_{k<\ell}$.*

This means that, for first-order interactions those pairs of alternatives should be used which differ in about half of the attributes presented, subject to the profile strength S.

Result 3 (a) *For $S = 3$ the uniform designs $\bar{\xi}_1$ and $\bar{\xi}_3$ are both optimal for the vector of second-order interaction effects $(\beta_{k\ell m})^\top_{k<\ell<m}$.*
(b) *For $S \geq 4$ the uniform design $\bar{\xi}_S$ is optimal for the vector of second-order interaction effects $(\beta_{k\ell m})^\top_{k<\ell<m}$.*

This also means that, for the second-order interactions only, those pairs of alternatives should be used, which differ in all attributes presented, subject to the profile strength S.

The optimal designs of Results 1, 2 and 3 are the same as in the first- and second-order interactions models (see Graßhoff et al. 2003; Nyarko and Schwabe 2019). However, for the present setting of third-order interactions, we obtain the following result.

Theorem 1 *There exists a single comparison depth d^* such that subject to the profile strength S, the uniform design $\bar{\xi}_{d^*}$ is D-optimal for the third-order interaction effects $(\beta_{k\ell mr})^\top_{k<\ell<m<r}$.*

This means that also for the third-order interactions only those pairs of alternatives should be used which differ in a portion of the attributes presented subject to the profile strength S. In particular, the corresponding values of d^* from Theorem 1 that are presented in Table 1 were obtained by first calculating the values of $h_4(d)$ and determining the maximum. For the case of full profiles ($S = K = 4$, for example), the pairs of the alternatives which are presented differ in only one, i.e. $d^* = 1$ of all the attributes. Moreover, for the case of partial profiles $S < K$, where, for a total number of attributes $K = 12$, only $S = 8$ are shown; for example, the pairs of the alternatives which are presented differ in only two, i.e. $d^* = 2$ of all the profile strength $S = 8$, while the remaining $K - S = 4$ attributes are not shown (officially set to zero). For a practical approach (a study in health research which is currently being planned) where

Table 1 Values of the optimal comparison depths d^* of the D-optimal uniform designs $\bar{\xi}_{d^*}$ for the third-order interactions with $S \leq K$ binary attributes

	S								
K	4	5	6	7	8	9	10	11	12
4	1								
5	1	1							
6	1	1	1						
7	1	1	1	1					
8	1	1	1	1	2				
9	1	1	1	1	2	2			
10	1	1	1	1	2	2	2		
11	1	1	1	1	2	2	2	3	
12	1	1	1	1	2	2	2	3	3

there are $K = 11$ two-level attributes of which $S = 4$ are shown in each pair and the two alternatives within each pair have different levels for $d^* = 2$ attributes (see Großmann 2018, Example 3).

For results relating to the full parameter vector $\boldsymbol{\beta}$, we note that a single comparison depth d may be sufficient for non-singularity of the information matrix $\mathbf{M}(\bar{\xi}_d)$; i.e. for the identifiability of all parameters. This can easily be seen by observing $h_r(1) > 0$, $r = 1, 2, 3, 4$, for $d = 1$. But this is not true for all comparison depths as for example $h_2(S) = h_4(S) = 0$. In view of Results 1, 2, 3 and Theorem 1 no design exists which simultaneously optimizes the information for the components of the whole parameter vector. Therefore we restrict our attention to the D-criterion for the whole parameter vector.

For later use we mention that a design ξ with nonsingular information matrix $\mathbf{M}(\xi)$ has a variance function of the form $V((\mathbf{i}, \mathbf{j}), \xi) = (\mathbf{f}(\mathbf{i}) - \mathbf{f}(\mathbf{j}))^\top \mathbf{M}(\xi)^{-1}(\mathbf{f}(\mathbf{i}) - \mathbf{f}(\mathbf{j}))$. This variance function plays an important role for the D-criterion. According to the equivalence theorem by Kiefer and Wolfowitz (1960), a design ξ^* is D-optimal if the associated variance function is bounded by the number of parameters p, $V((\mathbf{i}, \mathbf{j}), \xi^*) \leq p$ for all $(\mathbf{i}, \mathbf{j}) \in \mathcal{X}$.

Now, for invariant designs $\bar{\xi}$ the variance function $V((\mathbf{i}, \mathbf{j}), \bar{\xi})$ is also invariant with respect to permutations and, hence constant on the orbits $\mathcal{X}_d^{(S)}$ of fixed comparison depth d. Denote by $V(d, \bar{\xi})$ the value of the variance function for the invariant design $\bar{\xi}$ evaluated at comparison depth d where $V(d, \bar{\xi}) = V((\mathbf{i}, \mathbf{j}), \bar{\xi})$ on $\mathcal{X}_d^{(S)}$. The following result provides a formula for calculating the variance function.

Theorem 2 *For every invariant design $\bar{\xi}$ the variance function $V(d, \bar{\xi})$ is given by*

$$V(d, \bar{\xi}) = 4d \left(\frac{1}{h_1(\bar{\xi})} + \frac{S-d}{h_2(\bar{\xi})} + \frac{3S^2-6dS+4d^2-3S+2}{6h_3(\bar{\xi})} + \frac{(S-d)(2d^2-2Sd+S^2-3S+4)}{6h_4(\bar{\xi})} \right).$$

If the invariant design $\bar{\xi}$ 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*

$$V(d, \bar{\xi}_{d'}) = \frac{d}{d'}\left(p_1 + p_2\frac{S-d}{S-d'} + p_3\frac{3S^2-6dS+4d^2-3S+2}{3S^2-6d'S+4d'^2-3S+2} + p_4\frac{(S-d)(2d^2-2Sd+S^2-3S+4)}{(S-d')(2d'^2-2Sd'+S^2-3S+4)}\right).$$

Note that for $d = d'$, $V(d, \bar{\xi}_d) = p_1 + p_2 + p_3 + p_4 = p$ which recovers the D-optimality of $\bar{\xi}_d$ on $\mathcal{X}_d^{(S)}$ in view of the equivalence theorem by Kiefer and Wolfowitz (1960).

The following result gives an upper bound on the number of comparison depths required for a D-optimal design.

Theorem 3 *In the third-order interactions model, the D-optimal design ξ^* is supported on, at most, four different comparison depths d^*, d_1^*, $d^* + 1$ and $d_1^* + 1$, say.*

Further the results for the full parameter vector $\boldsymbol{\beta}$ of the D-optimal design may depend on both the profile strength S and the number K of attributes, as can be seen by the following result and the numerical examples presented in Table 2. In particular, for the case $S = K = 4$ of full profiles, the D-optimal design can be given explicitly. It is worth mentioning that the corresponding situation of $S = K = 4$ of full profiles can also be regarded as complete interactions (see Graßhoff et al. 2003, Theorem 4). Here we show that the corresponding result can be given explicitly.

Theorem 4 *If $S = K = 4$ then the design $\xi^* = \frac{4}{15}\bar{\xi}_1 + \frac{2}{5}\bar{\xi}_2 + \frac{4}{15}\bar{\xi}_3 + \frac{1}{15}\bar{\xi}_4$ which is uniform on all pairs with non-zero comparison depth is D-optimal in the third-order interactions model.*

Note that for $S = K = 4$ all four comparison depths are needed for D-optimality.

For $S \geq 5$, comparison depths d and d_1 with corresponding weights w_d and w_{d_1}, the numerical results presented in Table 2 were obtained by direct maximization of $\ln(\det(\mathbf{M}(w_d\bar{\xi}_d + (1 - w_d)\bar{\xi}_{d_1})))$ for the corresponding optimal comparison depth d^* and optimal weights $w_{d^*}^*$ where $1 - w_{d^*}^* = w_{d_1^*}^*$. In particular, by considering the designs $\xi^* = w_{d^*}^*\bar{\xi}_{d^*} + (1 - w_{d^*}^*)\bar{\xi}_{d_1^*}$, the numerical results show that two different comparison depths d^* and d_1^* may be needed for D-optimality. This is verified by the Kiefer and Wolfowitz (1960) equivalence theorem in Table 4. Specifically, for various choices of profile strengths $S = 5, \ldots, 12$, $S \leq K$ and the optimal comparison depths d^* and d_1^*, the corresponding optimal weights $w_{d^*}^*$ satisfy the condition $w_{d^*}^* = d_1^*/(d^* + d_1^*)$ for $d^* = [(S+1)/3]$ and $d^* + d_1^* = S + 1$.

It is worth mentioning that for $S = K = 4$ the uniform design $\bar{\xi}_{d^*}$ where $d^* = 1$ or 3 has D-efficiency $\mathrm{eff}_D(\bar{\xi}_{d^*}) = 0.909$, while $\bar{\xi}_2$ and $\bar{\xi}_4$ result in singular information matrices. Exhibited in Table 3 are the D-efficiencies for the designs $\bar{\xi}_{d^*}$ with optimal comparison depths d^* for the particular case $S = K = 5, \ldots, 8$. The D-efficiencies are also recorded in the case of full profiles for the designs $\bar{\xi}_1$ as another competitor. The designs $\bar{\xi}_{d^*}$ show quite high efficiencies of at least 90%, while for the competing designs $\bar{\xi}_1$ the efficiencies reduce to about 70% when the number of attributes gets large. We note that the designs for the case $S = K > 8$ result in singular information matrices.

Table 2 Optimal comparison depths d^* and optimal weights $w^*_{d^*}$ for the D-optimal designs $\xi^* = w^*_{d^*}\bar{\xi}_{d^*} + (1 - w^*_{d^*})\bar{\xi}_{d_1^*}$ in the case of full profiles ($S = K$)

	S							
	5	6	7	8	9	10	11	12
d^*	2	2	2	3	3	3	4	4
$w^*_{d^*}$	0.667	0.714	0.750	0.667	0.700	0.727	0.667	0.692
d_1^*	4	5	6	6	7	8	8	9
$w^*_{d_1^*}$	0.333	0.286	0.250	0.333	0.300	0.273	0.333	0.308

Table 3 D-efficiencies of the designs $\bar{\xi}_1$ and $\bar{\xi}_{d^*}$ with single comparison depth d^* from the optimal designs ξ^* in Table 2 in the case of full profiles ($S = K$)

K	5	6	7	8
d^*	2	2	2	3
$\mathrm{eff}_D(\bar{\xi}_{d^*})$	0.982	0.991	0.993	0.996
$\mathrm{eff}_D(\bar{\xi}_1)$	0.858	0.807	0.764	0.723

The optimality of the so obtained designs has been checked numerically by virtue of the Kiefer-Wolfowitz equivalence theorem. For full profiles $S = K$, the corresponding values of the normalized variance function $V(d, \xi^*)/p$ are recorded in Table 4, where maximal values less than or equal to 1 establish optimality.

5 Discussion

For paired comparisons in a linear model without interactions optimal designs require that the alternatives in the choice sets show distinct levels in each attribute subject to the profile strength (Graßhoff et al. 2004). Moreover, in a first-order interactions model pairs have to be used for an optimal design in which approximately one half of the attributes are distinct and one half of the attributes coincide, subject to the profile strength (Graßhoff et al. 2003). In a second-order interactions model both types of pairs have to be used for an optimal design in which either all attributes have distinct levels or approximately one half of the attributes are distinct and one half of the attributes coincide, subject to the profile strength and the total number of attributes available (see Nyarko and Schwabe 2019). Here it is shown that, in a third-order interactions model, two types of pairs have to be used, in which the numbers of distinct attributes are symmetric with respect to about half of the profile strength, to obtain a D-optimal design for the whole parameter vector. Optimal designs may be concentrated on one, two, three or four different comparison depths depending on the number of the profile strengths. The invariance considerations used here can be extended to larger numbers of levels for each attribute.

Table 4 Values of the variance function $V(d, \xi^*)$ for ξ^* from Table 2 in the case of full profiles $S = K$ (boldface **1** corresponds to the values at the optimal comparison depths d^* and d_1^* included in ξ^*)

	d											
K	1	2	3	4	5	6	7	8	9	10	11	12
5	0.938	**1**	0.938	**1**	0.938							
6	0.850	**1**	0.950	0.950	**1**	0.850						
7	0.792	**1**	0.982	0.952	0.982	**1**	0.792					
8	0.759	0.998	**1**	0.954	0.954	**1**	0.998	0.759				
9	0.693	0.958	**1**	0.966	0.945	0.966	**1**	0.958	0.693			
10	0.644	0.925	**1**	0.985	0.958	0.958	0.985	**1**	0.925	0.644		
11	0.609	0.901	0.999	**1**	0.973	0.960	0.973	**1**	0.999	0.901	0.609	
12	0.566	0.860	0.979	**1**	0.982	0.963	0.963	0.982	**1**	0.979	0.860	0.566

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Compliance with ethical standards

Conflicts of interest The author declares that he has no conflict of interest.

Appendix

Proof of Lemma 1 The quantities $h_1(d), h_2(d)$ and $h_3(d)$ can be obtained as in Graßhoff et al. (2003) and Nyarko and Schwabe (2019). The quantity $h_4(d)$ can be obtained on similar lines. First note that for the levels $i, j = -1, 1$ we have $i^2 = 1$ and $ij = -1$, $(i-j)^2 = 4$ for $i \neq j$.

For third-order interactions we consider attributes k, ℓ, m and r, say, and distinguish between pairs in which all four attributes are distinct, pairs in which three of these attributes k, ℓ and m, say, have distinct levels in the alternatives while the same level is presented in both alternatives for the remaining attribute, pairs in which two of these attributes k, ℓ, say, have distinct levels in the alternatives while the same level is presented in both alternatives for the remaining two attributes 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 three remaining attributes. Then $i_k i_\ell i_m i_r = j_k j_\ell j_m j_r$ in the first and third case, while $i_k i_\ell i_m i_r = -j_k j_\ell j_m j_r$ in the second and last case. Hence,

$$
\begin{aligned}
(i_k i_\ell i_m i_r - j_k j_\ell j_m j_r)^2 &= 0 \quad \text{for} \quad i_k \neq j_k,\ i_\ell \neq j_\ell,\ i_m \neq j_m \quad \text{and} \quad i_r \neq j_r,\\
(i_k i_\ell i_m i_r - j_k j_\ell j_m j_r)^2 &= 4 \quad \text{for} \quad i_k \neq j_k,\ i_\ell \neq j_\ell,\ i_m \neq j_m \quad \text{and} \quad i_r = j_r,\\
(i_k i_\ell i_m i_r - j_k j_\ell j_m j_r)^2 &= 0 \quad \text{for} \quad i_k \neq j_k,\ i_\ell \neq j_\ell,\ i_m = j_m \quad \text{and} \quad i_r = j_r,
\end{aligned}
$$

and

$$
(i_k i_\ell i_m i_r - j_k j_\ell j_m j_r)^2 = 4 \quad \text{for} \quad i_k \neq j_k,\ i_\ell = j_\ell,\ i_m = j_m \quad \text{and} \quad i_r = j_r,
$$

respectively, where the roles of the attributes k, ℓ, m and r may be interchanged.

For given attributes k, ℓ, m and r, the pairs with distinct levels in the four attributes occur $\binom{K-4}{S-4}\binom{S-4}{d-4}2^S$ times in $\mathcal{X}_d^{(S)}$, while those which differ in the three attributes occur $\binom{4}{3}\binom{K-4}{S-4}\binom{S-4}{d-3}2^S$ times in $\mathcal{X}_d^{(S)}$, while those which differ in the two attributes occur $\binom{4}{2}\binom{K-4}{S-4}\binom{S-4}{d-2}2^S$ times in $\mathcal{X}_d^{(S)}$ and, finally, those which differ only in one attribute occur $\binom{4}{1}\binom{K-4}{S-4}\binom{S-4}{d-1}2^S$ times. As a consequence, since the number N_d of paired comparisons in $\mathcal{X}_d^{(S)}$ equals $N_d = \binom{K}{S}\binom{S}{d}2^S$, for the third-order interactions the diagonal elements $h_4(d)$ in the information matrix are given by

$$\begin{aligned}
h_4(d) &= \frac{1}{N_d}\tbinom{K-4}{S-4}\left(\tbinom{S-4}{d-3}2^{S+4} + \tbinom{S-4}{d-1}2^{S+4}\right) \\
&= \frac{16(S-d)d(d-1)(d-2)}{K(K-1)(K-2)(K-3)} + \frac{16(S-d)(S-d-1)(S-d-2)d}{K(K-1)(K-2)(K-3)} \\
&= \frac{16d(S-d)(2d^2-2Sd+S^2-3S+4)}{K(K-1)(K-2)(K-3)}. \qquad (11)
\end{aligned}$$

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 "orthogonality" condition for single attributes. □

Proof of Theorem 2. First we note that the inverse of the information matrix of the design $\bar{\xi}$ is given by

$$\mathbf{M}(\bar{\xi})^{-1} = \begin{pmatrix} \frac{1}{h_1(\bar{\xi})}\mathbf{Id}_K & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \frac{1}{h_2(\bar{\xi})}\mathbf{Id}_{\binom{K}{2}} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \frac{1}{h_3(\bar{\xi})}\mathbf{Id}_{\binom{K}{3}} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \frac{1}{h_4(\bar{\xi})}\mathbf{Id}_{\binom{K}{4}} \end{pmatrix}.$$

Hence, we obtain for the variance function

$$\begin{aligned}
V((\mathbf{i},\mathbf{j}),\bar{\xi}) &= (\mathbf{f}(\mathbf{i})-\mathbf{f}(\mathbf{j}))^\top \mathbf{M}(\bar{\xi})^{-1}(\mathbf{f}(\mathbf{i})-\mathbf{f}(\mathbf{j})) \\
&= \frac{1}{h_1(\bar{\xi})}\sum_{k=1}^{K}(i_k-j_k)^2 \\
&\quad + \frac{1}{h_2(\bar{\xi})}\sum_{k<\ell}(i_k i_\ell - j_k j_\ell)^2 \\
&\quad + \frac{1}{h_3(\bar{\xi})}\sum_{k<\ell<m}(i_k i_\ell i_m - j_k j_\ell j_m)^2 \\
&\quad + \frac{1}{h_4(\bar{\xi})}\sum_{k<\ell<m<r}(i_k i_\ell i_m i_r - j_k j_\ell j_m j_r)^2. \qquad (12)
\end{aligned}$$

From the proof of Theorem 2 in Nyarko and Schwabe (2019), it can be seen that the first, second and third sum on the right hand side of (12) associated with the main effects, the first-order interactions and the second-order interactions equal $4d$, $4d(S-d)$ and $4d(3S^2-6dS+4d^2-3S+2)/6$, respectively.

For the terms associated with the third-order interactions, we have $(i_k i_\ell i_m i_r - j_k j_\ell j_m j_r)^2 = 4$, if $(i_k i_\ell i_m i_r)$ and $(j_k j_\ell j_m j_r)$ differ in three of the associated four attributes k, ℓ, m and r or in exactly one of these attributes, and $(i_k i_\ell i_m i_r - j_k j_\ell j_m j_r)^2 = 0$ otherwise. For a pair $(\mathbf{i},\mathbf{j}) \in \mathcal{X}_d^{(S)}$ of comparison depth d there are $(S-d)\binom{d}{3}$ third-order interaction terms for which the four attributes k, ℓ, m and r

differ in exactly three of the attributes, and there are $d\binom{S-d}{3}$ third-order interaction terms for which the four attributes k, ℓ, m and r differ in exactly one attribute. As a result, there are

$$\begin{aligned}
&(S-d)\binom{d}{3} + d\binom{S-d}{3} \\
&\quad = (S-d)d(d-1)(d-2)/6 + d(S-d)(S-d-1)(S-d-2)/6 \\
&\quad = d((S-d)(2d^2 - 2Sd + S^2 - 3S + 4))/6
\end{aligned}$$

non-zero entries (equal to 4) in the fourth sum on the right hand side of (12) and, hence, this sum equals $4d((S-d)(2d^2 - 2Sd + S^2 - 3S + 4))/6$.

By substituting this result into (12) for fixed K and S, it can be seen that the value of the variance function depends on the pair $(\mathbf{i}, \mathbf{j})$ only through its comparison depth d and so the proposed formula is obtained. □

Proof of Corollary 1. In view of Theorem 2 it is sufficient to note that the representation of the variance function follows immediately by inserting the values of $h_r(\bar{\xi}_d)$ from Lemma 1 and $p_r = \binom{K}{r}$, $r = 1, 2, 3, 4$. □

Proof of Theorem 3. Let ξ^* be an invariant D-optimal design with weights w_d^* on the comparison depths d for which the variance function $V(d, \xi^*)$ is equal to the number of parameters p for all d such that $w_d^* > 0$. By Theorem 2 the variance function $V(d, \xi^*)$ is a polynomial of degree 4 in the comparison depth d with negative leading coefficient. For integer d the variance function $V(d, \xi^*)$ may thus be equal to p for, at most, four different values of d. Now, by the Kiefer and Wolfowitz (1960) equivalence theorem itself $V(d, \xi^*) \le p$ for all $d = 0, 1, \ldots, S$. Hence, by the shape of the variance function we obtain that $V(d, \xi^*) = p$ may occur only at, at most two adjacent comparison depths d^* and $d^* + 1$ or d_1^* and $d_1^* + 1$, say, in the interior. □

Proof of Theorem 4. For the design ξ^* we obtain $h_1(\xi^*) = 8/15$, $h_2(\xi^*) = 2/15$, $h_3(\xi^*) = 1/30$ and $h_4(\xi^*) = 1/120$. Inserting this into the variance function of Theorem 2 yields $V(d, \xi^*) = 5d(-1/2d^3 + 5d^2 - 35/2d + 25)/4$, which results in $V(1, \xi^*) = V(2, \xi^*) = V(3, \xi^*) = V(4, \xi^*) = 15$. Hence, the variance function is bounded by the number of parameters $p = 15$ which establishes the D-optimality of ξ^* by virtue of the Kiefer-Wolfowitz equivalence theorem. □

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