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D-optimal weighted paired comparison designs

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D-optimal weighted paired comparison designs

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Abstract: As a generalization of the paired comparison designs, the experimental design which considers the weighted difference between responses is studied. D-optimal designs are constructed for a model with main effects and first order interactions. The experimental region is a hypercube or a hypersphere.

Key words and phrases: D-optimal designs; weighted paired comparison; approximate theory; linear models.
1. Introduction

Consider the model

\[ Y = \beta_1 x_1 + \cdots + \beta_n x_n + \beta_{12} x_1 x_2 + \cdots + \beta_{n-1n} x_{n-1} x_n, \]  

(1.1)

where \( x \in \chi, \chi \subseteq \mathbb{R}^n \) the experimental region.

If we define

\[ f(x) = (x_1, \ldots, x_n, x_1 x_2, \ldots, x_{n-1} x_n)', \]

we can consider the weighted difference between responses

\[ (1 - \alpha)f(x) - \alpha f(y) \]

with \( x, y \in \chi \) and \( 0 \leq \alpha \leq 1 \). This relation has been suggested by J. Van Casteren (UIA, University of Antwerp).

In the case \( \alpha = 0 \), we consider \( f(x) \) and \( y \) will disappear from all computations. This corresponds to the standard experimental design. The case \( \alpha = \frac{1}{2} \) accords to the paired comparison design, where observations are made by representing objects in pairs to one or more judges. Other values of \( \alpha \) can lead to new interpretations.

The information matrix can be generalized as follows:

\[ M_\alpha(\epsilon) = \sum_{i=1}^{N} \lambda(u_i, v_i) p_i ((1 - \alpha)f(u_i) - \alpha f(v_i))((1 - \alpha)f(u_i) - \alpha f(v_i))' \]  

(1.2)

where \( N \) is the number of runs, \( \sum p_i = 1 \) and \( \lambda(u_i, v_i) \) is the loss function. We assume that \( \lambda(x, y) = 1 \) for all \( x, y \in \chi \).

The variance of the estimated weighted response difference between the points \( x \) and \( y \) can be defined as

\[ d_\alpha(x, y, \epsilon) = ((1 - \alpha)f(x) - \alpha f(y))' M_\alpha^{-1}(\epsilon) ((1 - \alpha)f(x) - \alpha f(y)). \]  

(1.3)

From these definitions it is clear that \( \alpha = \beta \) and \( \alpha = 1 - \beta \) describe the same design.

Now we can generalize theorems, analogous to theorems in the standard experimental situation. Some of them are given in section 2.

In section 3, we will construct \( D \)-optimal designs for model (1.1) with a hypercube as experimental region \( \chi \). In section 4, \( \chi \) is a hypersphere.
2. Generalization of definitions and theorems

The most important theorem in constructing $D$-optimal designs is the equivalence theorem.

**Theorem 2.1:**

a. The following assertions are equivalent:
   
   1. $\det (M_\alpha(\epsilon^*)) = \max_{\epsilon} \det (M_\alpha(\epsilon))$,
   
   2. $\max_{x,y \in X} \lambda(x,y)d_\alpha(x,y,\epsilon^*) = \min_{x,y \in X} \max_{\epsilon} \lambda(x,y)d_\alpha(x,y,\epsilon)$,
   
   3. $\max_{x,y \in X} \lambda(x,y)d_\alpha(x,y,\epsilon^*) = m$, the number of parameters.

b. The information matrix of all designs satisfying (1)–(3) coincide.

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

**Theorem 2.2:** If $(x,y)$ is a pairs of a $D$-optimal design $\epsilon^*$, then

$$d_\alpha(x,y,\epsilon^*) = m,$$

where $m$ is the number of parameters.

For reasons of symmetry, the information matrix defined in (1.2) has the following structure:

$$M_\alpha(\epsilon) = \begin{pmatrix}
\gamma_\alpha I_n \\
z_\alpha I_{\frac{1}{2}n(n-1)}
\end{pmatrix},$$

where $p_\alpha I_n$ is related to the main effects and $z_\alpha I_{\frac{1}{2}n(n-1)}$ to the first-order interactions. So the covariance matrix equals

$$M_\alpha^{-1}(\epsilon) = \begin{pmatrix}
\gamma_\alpha I_n \\
\delta_\alpha I_{\frac{1}{2}n(n-1)}
\end{pmatrix}$$

(2.1)

with $\gamma_\alpha = \frac{1}{p_\alpha} > 0$ and $\delta_\alpha = \frac{1}{z_\alpha} > 0$.

Using (1.3) and (2.1) the variance function $d_\alpha(x,y,\epsilon)$ can be computed:

$$d_\alpha(x,y,\epsilon) = \gamma_\alpha \sum_{i=1}^{n} ((1 - \alpha)x_i - \alpha y_i)^2 + \delta_\alpha \sum_{1 \leq i < j \leq n} ((1 - \alpha)x_i x_j - \alpha y_i y_j)^2.$$  

(2.2)
Property 2.3: If the variance function $d_\alpha(x, y, \epsilon)$ can be expressed as in (2.2), then for all $1 \leq i, j \leq n$

1. $d_\alpha((x_1, \ldots, x_i, \ldots, x_n), (y_1, \ldots, y_i, \ldots, y_n), \epsilon)$
   \[ = d_\alpha((x_1, \ldots, -x_i, \ldots, x_n), (y_1, \ldots, -y_i, \ldots, y_n), \epsilon), \]

2. $d_\alpha((x_1, \ldots, x_i, \ldots, x_j, \ldots, x_n), (y_1, \ldots, y_i, \ldots, y_j, \ldots, y_n), \epsilon)$
   \[ = d_\alpha((x_1, \ldots, x_j, \ldots, x_i, \ldots, x_n), (y_1, \ldots, y_j, \ldots, y_i, \ldots, y_n), \epsilon). \]

3. A hypercube as experimental region

The experimental region is defined by

\[ \chi = \{ x \in \mathbb{R}^n | x = (x_1, \ldots, x_n)' ; \quad -1 \leq x \leq 1, \ 1 \leq i \leq n \} \quad (3.1) \]

Lemma 3.1: Assume that $\epsilon$ is a design with covariance matrix as in (2.1) and $\chi$ as in (3.1). If the variance function $d_\alpha(x, y, \epsilon)$ attains its maximum at $(u, v)$, then

\[ |u_i| = |v_i| = 1 \quad \text{for all } 1 \leq i \leq n. \]

Proof: Suppose that for some $i$ we have $|u_i| < 1$ or $|v_i| < 1$.

Without loss of generality we may assume $|u_1| < 1$ (so we can assume that $\alpha \neq 1$).

Define $d_1 = d_\alpha((1, u_2, \ldots, u_n), (v_1, \ldots, v_n), \epsilon)$,

\[ d_2 = d_\alpha((-1, u_2, \ldots, u_n), (v_1, \ldots, v_n), \epsilon). \]

Since $d_\alpha(x, y, \epsilon)$ attains its maximum at $(u, v)$,

\[ d_1 - d_\alpha(u, v, \epsilon) = (1 - \alpha)(1 - u_1) \left[ \gamma_\alpha((1 - \alpha)(1 + u_1) - 2\alpha v_1) \right. \]

\[ + \delta_\alpha \sum_{j=2}^{n} ((1 - \alpha)u_j^2(1 + u_1) - 2\alpha v_1 u_j v_j) \leq 0 \]

\[ d_2 - d_\alpha(u, v, \epsilon) = (1 - \alpha)(1 - u_1) \left[ \gamma_\alpha((1 - \alpha)(1 - u_1) + 2\alpha v_1) \right. \]

\[ + \delta_\alpha \sum_{j=2}^{n} ((1 - \alpha)u_j^2(1 - u_1) + 2\alpha v_1 u_j v_j) \leq 0 \]

Combining these inequalities, we get

\[ 2\gamma_\alpha(1 - \alpha) + 2\delta_\alpha \sum_{j=2}^{n} (1 - \alpha)u_j^2 \leq 0, \]

which is a contradiction. \[ \Box \]
So the points \((x, y)\) of a \(D\)-optimal design have the form

\[
x = (1, \ldots, 1, 1, \ldots, 1)'
\]

\[
y = (1, \ldots, 1, -1, \ldots, -1)'
\]

with \(k_1 + k_2 = n\), or a derived form by using property 2.3.

**Definition 3.1:** \(S(k_1, k_2)\) with \(k_1 + k_2 = n\), is the set containing all pairs with \(k_1\) factors at the same level.

The set \(S(k_1, k_2)\) can be seen as a design with \(N = \binom{n}{k_1} 2^n\) runs and \(p_i = \frac{1}{N}\) for all \(1 \leq i \leq N\). Note that the number of runs can be reduced to \(\binom{n}{k_1} 2^{n-1}\) if \(\alpha = \frac{1}{2}\).

The information matrix of the set \(S(k_1, k_2)\) is denoted by \(M_\alpha(k_1, k_2)\) and the value of the variance function in a pair of \(S(k_1, k_2)\) by \(d_\alpha(k_1, k_2, \epsilon)\).

Using expression (2.2), we find

\[
d_\alpha(k_1, k_2, \epsilon) = \gamma_\alpha((1 - 2\alpha)^2 k_1 + k_2) + \delta_\alpha\left(k_1^2\right)(1 - 2\alpha)^2 + \delta_\alpha k_1 k_2 + \delta_\alpha\left(k_2^2\right)(1 - 2\alpha)^2
\]

\[
= \left[\gamma_\alpha k_1 + \delta_\alpha\left(k_1^2\right) + \delta_\alpha\left(k_2^2\right)\right](1 - 2\alpha)^2 + \gamma_\alpha k_2 + \delta_\alpha k_1 k_2.
\]

(3.2)

**Lemma 3.2:**

\[
M_\alpha(k_1, k_2) = \begin{pmatrix} p_\alpha I_n & z_\alpha I_{\frac{1}{2}n(n-1)} \\ \end{pmatrix},
\]

where

\[
p_\alpha = \frac{(1 - 2\alpha)^2 k_1 + k_2}{n},
\]

\[
z_\alpha = \frac{(1 - 2\alpha)^2 \left[k_1(k_1 - 1) + k_2(k_2 - 1)\right] + 2k_1 k_2}{n(n - 1)}.
\]

(3.3)

**Proof:** Denote \(S(k_1, k_2) = \{(x_1, y_1), \ldots, (x_N, y_N)\} \subseteq \chi^2\), \(x_i = (x_{i1}, \ldots, x_{in})', y_i = (y_{i1}, \ldots, y_{in})'\).

From expression (1.2) and the assumptions above, it follows that

\[
p_\alpha = \frac{1}{N} \sum_{i=1}^{N} ((1 - \alpha)x_{i1} - \alpha y_{i1})^2,
\]

\[
z_\alpha = \frac{1}{N} \sum_{i=1}^{N} ((1 - \alpha)x_{i1} x_{i2} - \alpha y_{i1} y_{i2})^2.
\]
So we have

\[ p_\alpha = \frac{1}{N} \left[ (1 - 2\alpha)^2 \binom{n-1}{k_2} \binom{n}{k_1} 2^n + \binom{n-1}{k_1} 2^n \right], \]

\[ z_\alpha = \frac{1}{N} \left[ (1 - 2\alpha)^2 2^n \left( \binom{n-2}{k_1} + \binom{n-2}{k_2} \right) + \binom{n-2}{k_1-1} 2^{n+1} \right]. \]

By substituting \( N = \binom{n}{k_1} 2^n \) we obtain expressions (3.3).

Now a \( D \)-optimal design \( \epsilon \) can be constructed which is the union of some \( S(k_1, k_2) \).
Using the equivalence theorem 2.1, we have to find the maximal value of \( d_\alpha(x, y, \epsilon) \) to proof the \( D \)-optimality.

**Lemma 3.3:** If the variance function can be expressed as in (3.2), then \( d_\alpha(k_1, k_2, \epsilon) \) is maximal for \( k_1 = \frac{1}{2}(n-1) \).

**Proof:** According to (3.2) and \( k_2 = n - k_1 \), we have to maximize

\[ \left[ \gamma_\alpha k_1 + \delta_\alpha \binom{k_1}{2} + \delta_\alpha \binom{n-k_1}{2} \right] (1 - 2\alpha)^2 + \gamma_\alpha(n-k_1) + \delta_\alpha k_1(n-k_1) \]

over \( k_1 (0 \leq k_1 \leq n-1) \) to find the maximum value of \( d_\alpha(k_1, k_2, \epsilon) \).

\[ \frac{\partial d_\alpha(k_1, k_2, \epsilon)}{\partial k_1} = 4\alpha(\alpha - 1)\left[ \gamma_\alpha + \delta_\alpha k_1 - \delta_\alpha(n-k_1) \right] = 0 \]

for all \( 0 \leq \alpha \leq 1 \). This holds for

\[ k_1 = \frac{-2\delta_\alpha + n}{2}. \]

Since \( k_1 \) can take all values in \( \{0, 1, \ldots, n-1\} \) for all \( n \), it is necessary that \( \gamma_\alpha = q\delta_\alpha \) with \( q \in \mathbb{Z} \). So using (3.3) we should have

\[ \frac{n}{(1 - 2\alpha)^2 k_1 + (n-k_1)} = q \frac{n(n-1)}{(1 - 2\alpha)^2 [k_1(k_1 - 1) + (n-k_1)(n-k_1 - 1)] + 2k_1(n-k_1)} \]

\[ \iff [(1 - 2\alpha)^2 k_1 + (n-k_1)](n-1)q - (1 - 2\alpha)^2 [k_1(k_1 - 1) + (n-k_1)(n-k_1 - 1)] - 2k_1(n-k_1) = 0 \]

\[ \iff (1 - 2\alpha)^2 \left[ k(k-1) + (n-k)(n-k-1) - q(n-1)k \right] - \left[ q(n-1)(n-k) - 2k(n-k) \right] = 0, \]

(1)

(2)
for all $0 \leq \alpha \leq 1$. This holds for $(1) = (2) = 0$, so
\[
k(k-1) + (n-k)(n-k-1) + q(n-1)k = q(n-1)(n-k) - 2k(n-k)
\]
\[\iff q = \frac{k(k-1) + (n-k)(n-k-1) + 2k(n-k)}{(n-1)(n-k) + (n-1)k}
\]
\[\iff q = 1
\]
\[\iff \frac{\gamma_{\alpha}}{\delta_{\alpha}} = 1.
\]

Furthermore $d_{\alpha}(k_1, k_2, \epsilon)$ is maximal for $k_1 = \frac{1}{2}(n-1)$ since
\[
\frac{\partial^2 d_{\alpha}(k_1, k_2, \epsilon)}{\partial k_1^2} = 8\alpha(\alpha - 1)\delta_{\alpha} < 0.
\]

\[\square
\]

**Lemma 3.4:** If $k_1 = \frac{1}{2}(n-1)$ and $k_2 = \frac{1}{2}(n+1)$, then $d_{\alpha}(k_1, k_2, \epsilon) = \frac{1}{2}n(n+1)$, the number of parameters.

**Proof:** If $k_1 = \frac{1}{2}(n-1)$ and $k_2 = \frac{1}{2}(n+1)$, then
\[
\gamma_{\alpha} = \delta_{\alpha} = \frac{2n}{(1-2\alpha)^2(n-1) + (n+1)}.
\]

Using (3.2)
\[
d_{\alpha} = \frac{2n}{(1-2\alpha)^2(n-1) + (n+1)} \left[ \frac{n^2 - 1}{4}(1-2\alpha)^2 + \frac{(n+1)^2}{4} \right]
\]
\[= \frac{n(n^2 - 1)(1-2\alpha)^2 + n(n+1)^2}{2(1-2\alpha)^2(n-1) + 2(n+1)}
\]
\[= \frac{n(n+1)[(n-1)(1-2\alpha)^2 + (n+1)]}{2[(n-1)(1-2\alpha)^2 + (n+1)]}
\]
\[= \frac{n(n+1)}{2}.
\]

\[\square
\]
Theorem 3.5: Following design $\epsilon$ is D-optimal
1. $n$ is odd.
   $\epsilon$ exists of the pairs of $S\left(\frac{1}{2}(n - 1), \frac{1}{2}(n + 1)\right)$ given the same weight $\frac{1}{N}$, where $N = \left(\frac{n}{4(n-1)}\right)^2n$, the number of runs.

   \[
   M_\alpha(\epsilon) = \begin{pmatrix}
   p_\alpha I_n \\
   z_\alpha I_{\frac{n}{2}}n(n-1)
   \end{pmatrix},
   \]

   where

   \[
   p_\alpha = z_\alpha = \frac{(1 - 2\alpha)^2(n - 1) + (n + 1)}{2n}.
   \]

2. $n$ is even.
   $\epsilon$ exists of the pairs of $S\left(\frac{1}{2}n, \frac{1}{2}n\right)$ given the same weight $\frac{1}{N}$ and of $S\left(\frac{1}{2}n - 1, \frac{1}{2}n + 1\right)$ given the same weight $\frac{1}{N}$, where $N = \left(\frac{n+2}{2(n+1)}\right)^2n$, the number of runs and $\nu = \frac{n+2}{2(n+1)}$.

   \[
   M_\alpha(\epsilon) = \begin{pmatrix}
   p_\alpha I_n \\
   z_\alpha I_{\frac{n}{2}}n(n-1)
   \end{pmatrix},
   \]

   where

   \[
   p_\alpha = z_\alpha = \frac{(1 - 2\alpha)^2n + (n + 2)}{2(n + 1)}.
   \]

Proof: According to theorem 2.1, we have to show that $d_\alpha(x, y, \epsilon) \leq \frac{1}{2}n(n + 1)$ for all $x, y \in \chi$. In lemma 2.3 it is proved that $d_\alpha(k_1, k_2, \epsilon)$ is maximal for $k_1 = \frac{1}{2}(n - 1)$.

1. If $n$ is odd, $\frac{1}{2}(n - 1)$ is an integer.
   The maximal value of $d_\alpha(x, y, \epsilon)$ equals $d_\alpha\left(\frac{1}{2}(n - 1), \frac{1}{2}(n + 1), \epsilon\right) = \frac{1}{2}n(n + 1)$.

2. If $n$ is even, $\frac{1}{2}(n - 1)$ is not an integer. So the maximal value is one of the values $d_\alpha\left(\frac{1}{2}n, \frac{1}{2}n, \epsilon\right)$ and $d_\alpha\left(\frac{1}{2}n - 1, \frac{1}{2}n + 1, \epsilon\right)$. So

   \[
   M_\alpha(\epsilon) = \nu M_\alpha\left(\frac{1}{2}n, \frac{1}{2}n\right) + (1 - \nu)M_\alpha\left(\frac{1}{2}n - 1, \frac{1}{2}n + 1\right),
   \]

   with

   \[
   p_\alpha = \nu \left(\frac{1 - 2\alpha)^2 + 1}{2} + (1 - \nu)\right)\frac{(1 - 2\alpha)^2(n - 2) + (n + 2)}{2n}
   \]

   \[
   = \nu p_1 + (1 - \nu)p_2,
   \]

   \[
   z_\alpha = \nu \left(\frac{(1 - 2\alpha)^2(n - 2) + n}{2(n - 1)} + (1 - \nu)\right)\frac{(1 - 2\alpha)^2(n^2 - 2n + 4) + (n^2 - 4)}{2n(n - 1)}
   \]

   \[
   = \nu z_1 + (1 - \nu)z_2.
   \]
We can compute $\nu$ from

$$p_\alpha = z_\alpha \iff \nu(p_1 - p_2) + p_2 = \nu(z_1 - z_2) + z_2$$

$$\iff \nu = \frac{z_2 - p_2}{p_1 - p_2 - z_1 + z_2}$$

$$\iff \nu = \frac{n + 2}{2(n + 1)}.$$ 

We find $d_\alpha(\frac{1}{2}n, \frac{1}{2}n, \epsilon) = d_\alpha(\frac{1}{2}n - 1, \frac{1}{2}n + 1, \epsilon) = \frac{1}{2}n(n + 1).$

4. A hypersphere as experimental region

The experimental region is defined by

$$\chi = \left\{ x \in \mathbb{R}^n | x = (x_1, \ldots, x_n)', \sum_{i=1}^{n} x_i^2 \leq 1 \right\}$$

(4.1)

**Lemma 4.1:** Let $\epsilon$ be a design with covariance matrix as in (1.3) and $\chi$ as in (4.1). If the variance function $d_\alpha(x, y, \epsilon)$ attains its maximum at $(u, v)$, then

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

**Proof:** Suppose that $\sum u_i^2 < 1$ or $\sum v_i^2 < 1$.

Without loss of generality we may assume $\sum u_i^2 < 1$ (so we can assume that $\alpha \neq 1$).

Define $d_1 = d_\alpha((u_1^*, u_2, \ldots, u_n), (v_1, \ldots, v_n), \epsilon)$

$$d_2 = d_\alpha((-u_1^*, u_2, \ldots, u_n), (v_1, \ldots, v_n), \epsilon)$$

with

$$u_i^* = \sqrt{1 - \sum_{i=2}^{n} u_i^2}.$$ 

It is clear that $u_1^* > u_1$.

The rest of the proof is exactly similar to the proof of lemma 3.1 and completes it.

**Lemma 4.2:** If the variance function can be expressed as in (2.2), then in a pair $(x, y)$ with $\sum x_i^2 = \sum y_i^2 = 1$ it is the case that

$$d_\alpha(x, y, \epsilon) = 2\alpha(\alpha - 1)\gamma_\alpha \left[ 1 + \sum_{i=1}^{n} x_iy_i \right] + \alpha(\alpha - 1)\delta_\alpha \left[ 1 + \left( \sum_{i=1}^{n} x_iy_i \right)^2 \right]$$

$$+ \gamma_\alpha + \frac{1}{2}\delta_\alpha - \frac{1}{2}\delta_\alpha \sum_{i=1}^{n} \left( x_i^2 - \alpha(x_i^2 + y_i^2) \right)^2.$$ 

(4.2)
Proof:

\[ d_\alpha(x, y, \epsilon) = \gamma_\alpha \sum_{i=1}^{n} \left( (1 - \alpha)^2 x_i^2 + \alpha^2 y_i^2 - 2\alpha(1 - \alpha) x_i y_i \right) \]
\[ + \delta_\alpha \sum_{1 \leq i < j \leq n} \left( (1 - \alpha)^2 x_i^2 x_j^2 + \alpha^2 y_i^2 y_j^2 - 2\alpha(1 - \alpha) x_i x_j y_i y_j \right) \]
\[ = \gamma_\alpha \left[ (1 - \alpha)^2 + \alpha^2 - 2\alpha(1 - \alpha) \sum_{i=1}^{n} x_i y_i \right] \]
\[ + \frac{1}{2} \delta_\alpha \left[ \left( \sum_{i=1}^{n} (1 - \alpha) x_i^2 \right)^2 + \left( \sum_{i=1}^{n} \alpha y_i^2 \right)^2 \right] \]
\[ - \frac{1}{2} \delta_\alpha \left[ \sum_{i=1}^{n} (1 - \alpha)^2 x_i^4 + \sum_{i=1}^{n} \alpha^2 y_i^4 \right] \]
\[ - \delta_\alpha \left( \sum_{i=1}^{n} \alpha(1 - \alpha) x_i y_i \right)^2 + \delta_\alpha \sum_{i=1}^{n} \alpha(1 - \alpha) x_i^2 y_i^2 \]
\[ = 2\alpha(\alpha - 1) \gamma_\alpha \left[ 1 + \sum_{i=1}^{n} x_i y_i \right] + \gamma_\alpha + \alpha(\alpha - 1) \delta_\alpha + \frac{1}{2} \delta_\alpha \]
\[ - \delta_\alpha \alpha(1 - \alpha) \left( \sum_{i=1}^{n} x_i y_i \right)^2 - \frac{1}{2} \delta_\alpha \sum_{i=1}^{n} \left( x_i^2 - \alpha(x_i^2 + y_i^2) \right)^2 \]

which completes the proof. \(\square\)

It is clear that property 2.3 also holds if the variance function \(d_\alpha(x, y, \epsilon)\) can be expressed as in (4.2).

Lemma 4.3: The upper bounds for \(d_\alpha(x, y, \epsilon)\) are obtained for a pair \((u, v)\), where

\[ \sum_{i=1}^{n} u_i^2 = \sum_{i=1}^{n} v_i^2 = 1, \]
\[ v_i^2 = \frac{1}{n} + \frac{1 - \alpha}{\alpha} \left( u_i^2 - \frac{1}{n} \right), \]
\[ \sum_{i=1}^{n} u_i v_i = -\frac{\gamma_\alpha}{\delta_\alpha}. \]

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Proof: We have to maximize $d_\alpha(x, y, \epsilon)$ under the conditions $\sum x_i^2 = \sum y_i^2 = 1$, i.e. to maximize

$$L = d_\alpha(x, y, \epsilon) - \lambda_1 \left(1 - \sum_{i=1}^{n} x_i^2 \right) (1 - \alpha) - \lambda_2 \left(1 - \sum_{i=1}^{n} y_i^2 \right) \alpha.$$ 

For all $1 \leq k \leq n$:

$$\frac{\partial L}{\partial x_k} = 2\alpha(\alpha - 1)\gamma_\alpha y_k + 2\alpha(\alpha - 1)\delta_\alpha \left(\sum_{i=1}^{n} x_i y_i \right) y_k - 2\delta_\alpha ((1 - \alpha)x_k^2 - \alpha y_k^2)(1 - \alpha)x_k + 2\lambda_1 x_k (1 - \alpha) = 0,$$

$$\frac{\partial L}{\partial y_k} = 2\alpha(\alpha - 1)\gamma_\alpha x_k + 2\alpha(\alpha - 1)\delta_\alpha \left(\sum_{i=1}^{n} x_i y_i \right) x_k + 2\delta_\alpha ((1 - \alpha)x_k^2 - \alpha y_k^2) \alpha y_k + 2\lambda_2 y_k \alpha = 0.$$ 

If we denote $\sum x_i y_i = q$, we have to solve the system

$$\alpha y_k \left(\gamma_\alpha + \delta_\alpha q\right) + x_k \left[\delta_\alpha ((1 - \alpha)x_k^2 - \alpha y_k^2) - \lambda_1 \right] = 0, \quad (1)$$

$$(1 - \alpha)x_k (\gamma_\alpha + \delta_\alpha q) - y_k \left[\delta_\alpha ((1 - \alpha)x_k^2 - \alpha y_k^2) + \lambda_2 \right] = 0, \quad (2')$$

for all $1 \leq k \leq n$ under the conditions $\sum x_i^2 = \sum y_i^2 = 1$.

Solving the underbraced equations, we get

$$(1) = 0 \iff \sum_{i=1}^{n} x_i y_i = -\frac{\gamma_\alpha}{\delta_\alpha}.$$ 

and

$$(2) = 0 \iff y_k^2 = \frac{1 - \alpha}{\alpha} x_k^2 - \frac{\lambda_1}{\alpha \delta_\alpha}. \quad (4.4)$$

Substituting (4.4) in $\sum y_i^2 = 1$

$$\sum_{i=1}^{n} \left(\frac{1 - \alpha}{\alpha} x_k^2 - \frac{\lambda_1}{\alpha \delta_\alpha}\right) = 1$$

$$\iff \frac{1 - \alpha}{\alpha} - \frac{\lambda_1 n}{\alpha \delta_\alpha} = 1$$

$$\iff \lambda_1 = \frac{\delta_\alpha (1 - 2\alpha)}{n}.$$ 

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Then substituting $\lambda_1$ in (4.4), we find

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

For $(2') = 0$, we find $\lambda_2 = -\lambda_1$ and the same relation between $\hat{x}_k$ and $y_k$.

We can rewrite the variance function in (4.2) as:

$$d_{\alpha}(x, y, \epsilon) = 2\alpha(\alpha - 1)\gamma_{\alpha}(1 + q) + \alpha(\alpha - 1)\delta_{\alpha}(1 + q^2) + \gamma_{\alpha} + \frac{1}{2}\delta_{\alpha}$$

$$- \frac{1}{2}\delta_{\alpha} \frac{(1 - 2\alpha)^2}{n} - \frac{1}{2}\delta_{\alpha} \sum_{i=1}^{n} \left[ (1 - \alpha) \left( x_i^2 - \frac{1}{n} \right) - \alpha \left( y_i^2 - \frac{1}{n} \right) \right]^2.$$

So we can use the fact that

$$d_{\alpha}(x, y, \epsilon) \leq 2\alpha(\alpha - 1)\gamma_{\alpha}(1 + q) + \alpha(\alpha - 1)\delta_{\alpha}(1 + q^2) + \gamma_{\alpha} + \frac{1}{2}\delta_{\alpha} - \frac{1}{2}\delta_{\alpha} \frac{(1 - 2\alpha)^2}{n}.$$

If we maximize the right-hand side of the inequality to $q$, we find

$$q = -\frac{\gamma_{\alpha}}{\delta_{\alpha}}.$$

The upper bounds of $d_{\alpha}(x, y, \epsilon)$ are reached for the pairs $(u, v)$ satisfying (4.3), which completes the prove.

\[\square\]

**Definition 4.1:** $S^*_\alpha(k, l)$ with $0 \leq k \leq n - 2$ and $l$ a parameter, is the set containing the pairs $(x, y) = ((x_1, \ldots, x_n), (y_1, \ldots, y_n))$ where

$$(x_r, y_r) = \pm \left( \sqrt{1 + \frac{l}{1 - \alpha \sqrt{n}}}, \sqrt{1 - \frac{l}{\alpha \sqrt{n}}} \right),$$

$$(x_s, y_s) = \pm \left( \sqrt{1 - \frac{l}{1 - \alpha \sqrt{n}}}, \sqrt{1 - \frac{l}{\alpha \sqrt{n}}} \right),$$

$$(x_{r_i}, y_{r_i}) = \pm \left( \frac{1}{\sqrt{n}}, \frac{1}{\sqrt{n}} \right), \quad i = 1, \ldots, k,$$

$$(x_{s_j}, y_{s_j}) = \pm \left( \frac{1}{\sqrt{n}}, \frac{1}{\sqrt{n}} \right), \quad j = 1, \ldots, n - k - 2,$$

and $\{r, s, r_1, \ldots, r_k, s_1, \ldots, s_{n-k-2}\}$ is a permutation of $\{1, \ldots, n\}$.

$S^*_\alpha(k, l)$ can be seen as a design with $p_i = \frac{1}{N}$ for all $1 \leq i \leq N$, where $N$ is the number of runs.
The information matrix of set $S_\alpha^*$ is denoted by $M_\alpha^*(k,l)$ and the value of the variance function in a pair of $S_\alpha^*(k,l)$ by $d_\alpha(x,y,\varepsilon).

**Theorem 4.4:** Following design $\varepsilon$ is $D$-optimal:

$\varepsilon$ exists of the pairs of $S_\alpha^*(k,l)$ given the same weights $\frac{1}{N}$, where

1. for $n$ odd

\[ k = \frac{n - 3}{2}, \]
\[ l = 0, \]
\[ N = \left( \frac{n}{2(n - 1)} \right) 2^n, \]

2. for $n$ even

\[ k = \frac{n - 2}{2}, \]
\[ l = \frac{\sqrt{3}}{2} \frac{\alpha(1 - \alpha)}{\sqrt{1 - \alpha + \alpha^2}}, \]
\[ N = n(n - 1) \left( \frac{n - 2}{2} \right) 2^n. \]

The information matrix equals

\[
M_\alpha(\varepsilon) = \begin{pmatrix}
p_\alpha I_n & \\
\frac{1}{2} \frac{z_\alpha I_{\frac{1}{2} n(n-1)}}{n - 1}
\end{pmatrix},
\]

where

\[ p_\alpha = nz_\alpha = \frac{1}{2n^2} \left( n + 1 + (n - 1)(1 - 2\alpha)^2 \right). \]
Proof:
From the definition of $S^*_\alpha(k,l)$, we find

$$\sum_{i=1}^{n} x_iy_i = -\frac{1}{\sqrt{\alpha(1-\alpha)}} \left( \sqrt{(1-\alpha + l)(\alpha + l)} - \sqrt{(1-\alpha - l)(\alpha - l)} \right) + (2(k+1) - n) \frac{1}{n},$$

and

$$p_\alpha = \frac{1}{n^2} \left[ \left( \sqrt{(1-\alpha + l)(1-\alpha)} + \sqrt{(\alpha + l)\alpha} \right)^2 + \left( \sqrt{(1-\alpha - l)(1-\alpha)} - \sqrt{(\alpha - l)\alpha} \right)^2 + (1-2\alpha)^2k + (n-k-2) \right],$$

$$z_\alpha = \frac{1}{n^3(n-1)} \left[ 2 \left( \sqrt{(1-\alpha)^2 - l^2} + \sqrt{\alpha^2 - l^2} \right)^2 + (1-2\alpha)^2k(k-1) + (1-2\alpha)^2(n-k-2)(n-k-3) + 2k(n-k-2) + 2 \left( \sqrt{(1-\alpha + l)(1-\alpha)} + \sqrt{(\alpha + l)\alpha} \right)^2k + 2 \left( \sqrt{(1-\alpha + l)(1-\alpha)} - \sqrt{(\alpha + l)\alpha} \right)^2(n-k-2) + 2 \left( \sqrt{(1-\alpha - l)(1-\alpha)} - \sqrt{(\alpha - l)\alpha} \right)^2k + 2 \left( \sqrt{(1-\alpha - l)(1-\alpha)} + \sqrt{(\alpha - l)\alpha} \right)^2(n-k-2) \right].$$

In both cases $n$ even and $n$ odd, we find by substituting $k$ and $l$ that

$$\sum_{i=1}^{n} x_iy_i = -\frac{1}{n},$$

$$p_\alpha = n z_\alpha = \frac{1}{2n^2} (n+1 + (n-1)(1-2\alpha)^2).$$

Since $\gamma_\alpha = \frac{1}{p_\alpha}$ and $\delta_\alpha = \frac{1}{z_\alpha}$, $\delta_\alpha = n \gamma_\alpha$, we can compute the variance function in a pair $(x,y)$ of $S^*_\alpha(k,l)$

$$d^*_\alpha(x,y,\varepsilon) = \gamma_\alpha \left[ 2\alpha(\alpha - 1) \left( 1 - \frac{1}{n} \right) + \alpha(\alpha - 1)n \left( 1 + \frac{1}{n^2} \right) + 1 + \frac{n}{2} - \frac{n (1-2\alpha)^2}{n} \right]$$

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

the number of parameters. \(\square\)
5. Conclusion

In section 3 and 4 we derived a $D$-optimal approximate design for a model with main effects and first-order interactions. In general these designs can not be realised in practice. It is possible to construct exact designs (i.e. designs that can be realised in practice) with a high efficiency (see theorem 3.1.1 of Fedorov (1972)). In such a design, the product of the weights and the number of observations must be an integer. For practical applications, it is useful to construct designs with a small number of observations and a high efficiency.

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References

