Chapter 1

EFFICIENT DESIGNS FOR PAIRED COMPARISONS WITH A POLYNOMIAL FACTOR

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Abstract In psychological research paired comparisons which demand judges to evaluate the trade-off between two alternatives have been shown to yield valid estimates of the judges' preferences. For this situation we present optimal and efficient designs in a response surface setting where the alternatives are modeled by a polynomial.

Keywords: paired comparisons, optimal design, equivalence theorem, symmetrization, polynomial regression, additive model, marginal design

Dedicated to Professor Valerii V. Fedorov
on occasion of his 60th birthday

Introduction

In psychological research paired comparisons which demand judges to evaluate the trade-off between two alternatives have been shown to yield valid estimates of the judges' preferences (Bateson, Reibstein and Boulding (1987)). In addition, over the past decades a sound measurement theoretical framework for paired comparisons has been established by mathematical psychologists (David (1963)). As a result of these developments, paired comparisons have been widely adopted as a method for data collection in the social sciences and especially in marketing research. Recently, psychometric methods and, in particular ideas of experimental design have attracted growing interest in psychological research (McClelland (1997)).

In this note, we present optimal and efficient designs for paired comparisons in a response surface setting where the alternatives are modeled by a linear, quadratic or cubic polynomial. These components can be readily used as bricks for constructing efficient designs for more than one active effect.

1. GENERAL SETTING

As in the monograph by van Berkum (1987) we confine ourselves to the solution of the design problem for the approximating linear model. To be more specific we consider the general linear model

$$\mu(t) = \beta_0 + f(t)^\top \beta$$

with an explicit constant term β_0 for modeling the value of an alternative $t \in \mathcal{T}$. Here f is a vector of known regression functions and β is the vector of parameters of interest. In contrast to standard design problems the values for the alternatives are not directly observable. Only observations $Y(s,t)$ are available for comparing pairs of alternatives s and t. Nevertheless, the observations are still properly described by a linear model

$$Y(s,t) = (f(s) - f(t))^\top \beta + Z(s,t)$$

with settings $x = (s,t)$ for the paired comparisons chosen from the design region $\mathcal{X} = \mathcal{T} \times \mathcal{T}$. Note that for paired comparisons the regression function is given by $x = (s,t) \to F(s,t) := f(s) - f(t)$. Note also that it is fahionable in the literature to model the value $\mu(t)$ without a constant term β_0 (cf. van Berkum (1987)) which results in the same model for the paired comparisons but which might be misleading for finding optimal designs. Additionally, different experiments are assumed to result in uncorrelated and homoscedastic errors Z.

Due to the general complexity of the problem we mainly consider generalized designs ξ which are defined as finitely supported probability measures on the design region $\mathcal{X}$. For the definition and properties of generalized (approximate) designs we refer to the seminal paper by Kiefer (1959) and the monograph by Fedorov (1972). However, we will also point out, how certain exact designs can be constructed which are highly efficient.

The quality of a design ξ is reflected by its information matrix $M(\xi)$ which is essentially proportional to the inverse of the covariance matrix for the best linear unbiased estimator of the parameter vector β. As a performance measure we use the most popular criterion of D–optimality which aims at maximizing the determinant of the information matrix $M(\xi)$. In the present setting the information matrix equals $\sum_{(s,t)}(f(s)-f(t))(f(s)-f(t))^\top\xi(s,t)$ where $(f(s)-f(t))(f(s)-f(t))^\top$ is the information contained in the paired comparison of s and t and $\xi(s,t)$ is the weight associated with it.

Let us note the obvious fact that there is zero information in the pairs (t,t), i. e. in the comparison of t with itself. Moreover, it is also clear that the information for the pair (s,t) is the same as for (t,s), the pair with the internal order reversed. However, it is worthwhile to distinguish between the comparison of s with t and the comparison of t with s in view of the last section on models with more than one factor of influence - although those comparisons seem to be indistinguishable. As a side–effect we can always replace a design ξ by its symmetrized version $\bar{\xi}$ with respect to exchanging s and t and get the same information matrix, $M(\bar{\xi})=M(\xi)$, with the additional benefit $\sum_{(s,t)}(f(s)-f(t))\bar{\xi}(s,t)=0$. We will take advantage of that in the final section when constructing optimal designs for models where the response depends on more than one factor.

Our next remark is that invariance and equivariance properties are inherited by passing from the model μ for the value to the linear model for observing the paired comparison as long as the constant term is preserved: If the augmented regression function $(1,f)$ is linearly equivariant with respect to a transformation g, i. e. there is a matrix Q_g such that $(1,f(g(t)))=Q_g\cdot(1,f(t))$ for all $t\in\mathcal{T}$, and if, additionally, the first row of Q_g is the unit vector $(1,0,\ldots,0)$, then the regression function $F:(s,t)\to f(s)-f(t)$ of the paired comparison is also linearly equivariant. The corresponding transformation matrix for F is obtained by deleting the first row and column of Q_g.

In the following we will deal with polynomial response of degree p, i. e. $\mu(t)=\beta_0+\sum_{i=1}^p t^i\beta_i$ to model paired comparisons

$$Y(s,t)=\sum_{i=1}^p(s^i-t^i)\beta_i+Z$$

for a possibly continuously varying factor. According to the preceding considerations the following result is straightforward from the equivariance of polynomial regression:

Lemma 1. *If the design ξ^* is D–optimal for paired comparisons with polynomial response of degree p on the design region of the standard unit interval, $\mathcal{T} = [-1, 1]$, then the properly transformed design $g_{a,b} \circ \xi^*$ is D–optimal for paired comparisons with polynomial response of degree p on the general interval, $[a, b]$, where $g_{a,b}$ is the linear transformation which maps $[-1, 1]^2$ onto $[a, b]^2$.*

Hence, it is sufficient for D–optimality to work with the unit interval $\mathcal{T} = [-1, 1]$. Due to the equivariance with respect to sign changes and due to the quasi–concavity of the D–criterion also the following property is directly inherited:

Lemma 2. *If the design ξ^* is D–optimal for paired comparisons with polynomial response on the unit interval, $\mathcal{T} = [-1, 1]$, then ξ^* is symmetric, i. e. $\xi^*(s, t) = \xi^*(-s, -t)$. Moreover, its information matrix $M(\xi^*)$ has a chess–board structure, i. e. all entries with odd index sum vanish.*

2. LINEAR REGRESSION

For linear response, $\mu(t) = \beta_0 + t\beta$, i. e. $Y(s, t) = (s - t)\beta$, the information matrix reduces to a nonnegative number. It is well–known that this number will be maximized when ξ^* assigns all mass to the largest modulus of the regression function $F(s, t) = s - t$.

Theorem 1. *The design ξ^* is optimal for paired comparisons with linear response on the unit interval, $\mathcal{T} = [-1, 1]$, if and only if ξ^* is concentrated on $(1, -1)$ and $(-1, 1)$.*

Hence, the policy for linear response is to compare the extreme settings for the factor. Note that, in particular, the one–point designs concentrated on either the comparison $(1, -1)$ or on $(-1, 1)$ are optimal. The corresponding value for the variance of β equals $\frac{1}{4}$ which coincides with the minimal attainable variance for the slope in the directly observable model with response μ.

3. QUADRATIC REGRESSION

Next we consider the situation where each alternative in the paired comparisons is modeled by a quadratic polynomial, i. e. the response is given by

$$Y(s, t) = (s - t)\beta_1 + (s^2 - t^2)\beta_2 + Z(s, t) \qquad s, t \in [-1, 1].$$

As has been pointed out by Silvey (1972) the possible support points of an optimal design are those points where the boundary of a circumscribing ellipsoid touches the image $\{(s - t, s^2 - t^2); s, t \in [-1, 1]\}$ of the regression function $F(s, t)$. This geometric approach suggests that an optimal design will be of the

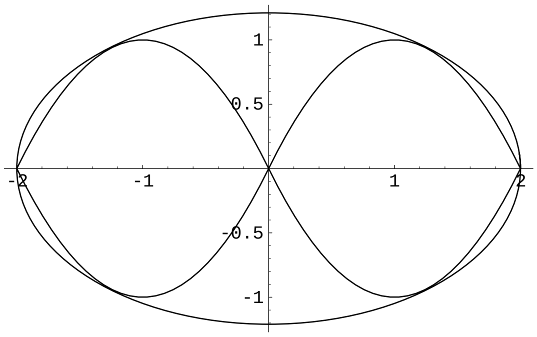

Figure 1.1 The image $\{F(s,t)\}$ with its circumscribing ellipsoid for quadratic response

form

$$\xi_{\tau,w} = \tfrac{1}{4}w(\epsilon_{(1,\tau)} + \epsilon_{(\tau,1)} + \epsilon_{(-1,-\tau)} + \epsilon_{(-\tau,-1)}) + \tfrac{1}{2}(1-w)(\epsilon_{(1,-1)} + \epsilon_{(-1,1)}),$$

where $\epsilon_{(s,t)}$ denotes the Dirac measure concentrated on (s,t) and the optimal setting τ and weight w have to be determined (see Figure 1.1). The equal weights $\frac{1}{4}w$ associated with the support points $(1,\tau)$, $(\tau,1)$, $(-1,-\tau)$, $(-\tau,-1)$ and $\frac{1}{2}(1-w)$ associated with the points $(1,-1)$, $(-1,1)$ are motivated by the natural requirement that the design should be invariant under the reflections at both diagonals of $\mathcal{X} = [-1,1]^2$. The information matrix $M(\xi_{\tau,w})$ for the design $\xi_{\tau,w}$ is diagonal and equals

$$M(\xi_{\tau,w}) = \begin{pmatrix} w(1-\tau^2) + 4(1-w) & 0 \\ 0 & w(1-\tau^2)^2 \end{pmatrix}.$$

The determinant of $M(\xi_{\tau,w})$ is given by

$$|M(\xi_{\tau,w})| = w(1-\tau^2)^2(w(1-\tau)^2 + 4(1-w))$$

which is maximized by the weight

$$w(\tau) = \frac{2}{(3-\tau)(\tau+1)}$$

where the setting τ is fixed. Hence,

$$|M(\xi_{\tau,w(\tau)})| = \frac{(1-\tau)^2(1+\tau)}{3-\tau}$$

is maximized for the optimal setting $\tau^* = 2 - \sqrt{5} \approx -0.236068$. The corresponding optimal weight $w^* = w(\tau^*) = 1/(\sqrt{5}-1) \approx 0.8090$ is closely related to the golden section number.

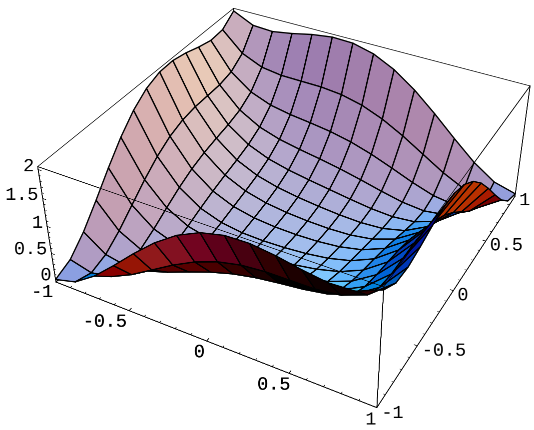

Figure 1.2 Variance function for the D–optimal quadratic design

The information matrix of the design ξ_{τ^*,w^*} is given by

$$M(\xi_{\tau^*,w^*}) = \begin{pmatrix} 2 & 0 \\ 0 & 4(5\sqrt{5}-11) \end{pmatrix}$$

resulting in the variance function

$$d(s,t) = (s-t)^2 \left(\frac{1}{2} + \frac{(s+t)^2}{20\sqrt{5}-44)} \right)$$

(see Figure 1.2).

Now, we want to show that the variance function $d(s,t)$ does not exceed 2 which proves the D–optimality of the design ξ_{τ^*,w^*} by virtue of the celebrated Kiefer–Wolfowitz equivalence theorem (Kiefer and Wolfowitz (1960)). Due to the symmetry of the variance function $d(s,t)$ we can restrict ourselves to the case $s \geq t$. Note that $d(t,t) = 0$.

First we consider the variance function on line segments parallel to the main diagonal, $s = t + c$, $c > 0$. Then $d(t+c,t)$ is a polynomial in t of degree two which attains its maximum on the boundary, $s = 1$ or $t = -1$. Due to the symmetry, again, we have $\sup_{s,t} d(s,t) = \sup_t d(1,t)$. Now, $d(1,t)$ is a polynomial in t of degree four with positive leading coefficient. Moreover, $d(1,1) = 0$, $d(1,-1) = d(1,\tau^*) = 2$ and, addititonally, the derivative $\frac{\partial}{\partial t} d(1,t)$ equals 0 for $t = \tau^*$. Thus, it follows that $d(1,t)$ and, hence, $d(s,t)$ is bounded by 2 which proves the D–optimality of the design ξ_{τ^*,w^*}.

Moreover, the shape of the variance function $d(s,t)$ establishes that the support of every D–optimal design has to be included in that of ξ_{τ^*,w^*}.

Theorem 2. *The design ξ^* is optimal for paired comparisons with quadratic response on the unit interval, $\mathcal{T} = [-1, 1]$, if and only if $\xi^*(1, \tau^*) + \xi^*(\tau^*, 1) = \xi^*(-\tau^*, -1) + \xi^*(-1, -\tau^*) = \frac{1}{2}w^*$ and $\xi^*(1, -1) + \xi^*(-1, 1) = 1 - w^*$ with $\tau^* = 2 - \sqrt{5}$ and $w^* = 1/(\sqrt{5} - 1)$.*

In particular, the three point design is D–optimal which assigns equal weights $\frac{1}{2}w^* \approx 0.4045$ to each of the pairs $(1, \tau^*)$ and $(-\tau^*, -1)$, respectively, and the remaining weight $1 - w^* \approx 0.1910$ to the extreme comparison $(1, -1)$.

Remarks. 1. van Berkum (1987) has obtained numerical solutions for optimal designs in the paired comparison setup with quadratic response when more than one influential factor is present. These solutions are in accordance with our theoretical findings that the extreme settings have to be compared with an intermediate setting exceeding the center point and, additionally, with each other. Note that the optimal settings for the objects under comparison differ from those suitable for the situation of directly observable values. In the latter case the D–optimal design is known to allocate equal weights to the three settings $t = -1$, 0 and 1, respectively.

2. Atkins and Cheng (1999) considered a related situation where responses are observed directly and coming in pairs with a specified within pair correlation. For that situation the optimal designs show the same structure as in the present setup of paired comparisons. In fact, it is worthwhile noting that the within pair correlation is eliminated by passing to paired comparisons.

Example 1. As an alternative to the D–optimal design ξ^* we propose a design ξ' with minimal support of the form $\{(1, \tau), (-\tau, -1)\}$. This is obtained by omitting the extreme comparison from ξ^* which bears the smallest weight. Since the number of support points coincides with the number of unknown parameters the D–optimal weights are uniform, i. e. $\frac{1}{2}$ on each pair. It remains to maximize the determinant $|M(\xi')| = (1 - \tau)^4(1 + \tau)^2$ of the information matrix. This is achieved for the setting $\tau' = -1/3$ with a resulting determinant $|M(\xi')| = 1024/729 \approx 1.4046$. As for the D–optimal design $|M(\xi^*)| \approx 1.4427$ we can calculate the D–efficiency of the design ξ' according to $\mathrm{eff}_D(\xi') = (|M(\xi')|/|M(\xi^*)|)^{1/2} \geq 98,6\%$ showing that ξ' is highly efficient. Due to the simple weight structure the design ξ' can be identified as an efficient exact design when the number n of paired comparisons is even. Then $\frac{1}{2}n$ observations are to be taken at each of the comparisons of $s = 1$ with $t = -\frac{1}{3}$ and $s = \frac{1}{3}$ with $t = -1$, respectively.

Example 2. The design ξ'' which assigns equal weight $\frac{1}{3}$ to the comparisons $(1, -1)$, $(1, 0)$ and $(0, -1)$ of the standard settings for directly observable alternatives results in a determinant $|M(\xi'')| = 4/3$ of the information matrix

$M(\xi'')$. Hence, ξ'' has a D–efficiency $\mathrm{eff}_D(\xi'') \geq 96\%$. The design ξ'' can be identified as an efficient exact design if the number of comparisons is a multiple of three.

4. CUBIC REGRESSION

For the cubic response

$$Y(s,t) = (s-t)\beta_1 + (s^2 - t^2)\beta_2 + (s^3 - t^3)\beta_3 + Z(s,t)$$

the optimization problem becomes even more complicated. Therefore we start with a characterization of the shape of the variance function $d(s,t) = (f(s) - f(t))^\top M(\xi)^{-1}(f(s) - f(t))$:

Lemma 3. *If the design ξ is symmetric with respect to sign change, $\xi(-s,-t) = \xi(s,t)$, then the variance function $d(s,t)$ attains its maximum at, at most, twelve points in $\mathcal{X} = [-1,1]^2$. These points can be characterized by three settings τ_1, τ_2 and $\tau_3 \in [-1,1]$, $\tau_2 < \tau_3$, according to $(s,t) = (1,-1)$, $(\tau_1, -\tau_1)$, $(1,\tau_2)$, and $(1,\tau_3)$ as well as their corresponding images under reflection with respect to the diagonals.*

Proof. According to Lemma 2 the information matrix $M(\xi)$ has a chess–board structure which is shared by its inverse $M(\xi)^{-1}$. Hence, the variance function can be written as

$$d(s,t) = (s-t)^2(c_1 + c_2(s+t)^2 + c_3(s^2 + st + t^2)^2 + c_4(s^2 + st + t^2))$$

for some constants $c_1, \ldots, c_4$, where, in particular, $c_3 > 0$. Note that the variance function itself is symmetric with respect to reflections at both diagonals. For notational convenience we only consider those pairs on one side of the main diagonal, $s \geq t$, keeping in mind that the variance function attains its minimum at the main diagonal, $d(t,t) = 0$.

On line segments parallel to the main diagonal, $s = t + c$, $c \neq 0$, the variance function $d(t+c,t)$ is a polynomial in t of degree four with positive leading term. Hence, due to the symmetry, $d(t+c,t)$ may attain its maximum only at the boundary, $s = 1$ or $t = -1$, or at the center of the line segment, $s = -t$. This consideration reduces the possible locations for the maxima of the variance function to the boundary of the design region and to the secondary diagonal, $s = -t$.

On the secondary diagonal the variance function $d(t,-t)$ is a polynomial in t of degree six with positive leading term. As $d(0,0) = 0$ and the variance function $d(t,-t)$ is symmetric to 0 it may attain its maximum only at the boundary, $t = 1$, or at, at most, one interior point $t = \tau_1 > 0$.

For the boundary we have to investigate only one segment of the boundary, say $s = 1$, due to the symmetry. On that segment $d(1,t)$ is a polynomial in t

of degree six with positive leading term. As $d(1,1) = 0$ the variance function $d(1,t)$ may attain the maximum only at $t = -1$ and at, at most, two different interior points, $t = \tau_2$ or $t = \tau_3$, $-1 < \tau_2 < \tau_3 < 1$.

Combining these arguments we see that the variance function $d(s,t)$ may attain its maximum, at most, at the points $(1,-1)$, $(\tau_1,-\tau_1)$, $(1,\tau_2)$ and $(1,\tau_3)$ as well as their corresponding images under reflections. □

As an immediate consequence we obtain the shape of the D–optimal design by virtue of the equivalence theorem of Kiefer and Wolfowitz (1960):

Theorem 3. *For paired comparisons with cubic response the D–optimal design ξ^* is supported by, at most, twelve pairs which can be characterized by three settings τ_1, τ_2 and $\tau_3 \in [-1,1]$, $\tau_2 < \tau_3$, according to $(s,t) = (1,-1)$, $(\tau_1,-\tau_1)$, $(1,\tau_2)$, and $(1,\tau_3)$ as well as their corresponding images under reflection with respect to the diagonals.*

For finding the D–optimal design it remains to specify six parameters, the optimal three location parameters $\tau_1,\ldots,\tau_3$ and the three corresponding optimal weights $w_1,\ldots,w_3$ which are to be uniformly distributed on the support sets $\{(\tau_1,-\tau_1),(-\tau_1,\tau_1)\}$, $\{(1,\tau_2),(-\tau_2,-1),(\tau_2,1),(-1,-\tau_2)\}$ and $\{(1,\tau_3),(-\tau_3,-1),(\tau_3,1),(-1,-\tau_3)\}$, respectively, where the remaining weight $1-w_1-w_2-w_3$ is meant to be assigned to $\{(1,-1),(-1,1)\}$. *The solution of this six–dimensional optimization problem is still under construction.* Again, the number of comparisons may be restricted to those pairs with $s > t$.

Example 3. Using a computer program by E. Rafajłowicz (personal communication) for optimizing the weights on an equidistant grid with step size 0.1 we could identify the pairs $(1,-1)$, $(0.6,-0.6)$, $(1,0.2)$ and $(-0.2,-1)$ as suitable candidate points for a highly efficient design with four different paired comparisons. In view of the symmetry this design has the shape required in Theorem 3 with $\tau_1 = 0.6$, $\tau_2 = 0.2$ and $w_3 = 0$. The optimal weights are found to be $w_1 = 0.3159$ for the pair $(0.6,-0.6)$, $\frac{1}{2}w_2 = 0.2423$ for each of the pairs $(1,0.2)$ and $(-0.2,-1)$ and the remaining weight $1-w_1-w_2 = 0.1996$ on the pair of extreme comparisons $(1,-1)$. The determinant of the information matrix can be calculated to $|M(\xi)| = 0.121566$. The corresponding variance function is plotted in Figure 1.3 and shows a good performance of the design.

A closer inspection of the variance function yields that it slightly exceeds the number $p = 3$ on the boundary at $(1,0.15)$ and on the secondary diagonal close to $(\tau_1,-\tau_1)$, with a value not larger than 3.004. In total the variance function $d(s,t)$ is apparently bounded by 3.004. According to Dette (1996) a lower bound for the D–efficiency is given by $\mathrm{eff}_D(\xi) \geq p/\sup_{s,t} d(s,t) \geq$

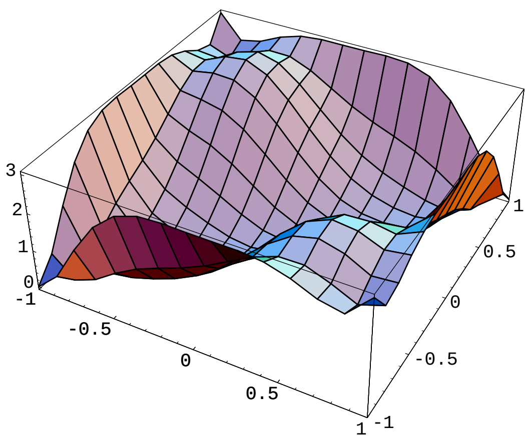

Figure 1.3 Variance function for the four point cubic design of Example 3

$3/3.004 = 99.8\%$. Hence, the present design is highly efficient and there may be hope that the D–optimal design is concentrated on four points.

Example 4. As a simple alternative we propose a design ξ_0 with minimal support of the form $\{(\tau_1, -\tau_1), (1, \tau_2), (-\tau_2, -1)\}$. This is, similar to Example 1, obtained by omitting the extreme comparison which bears the smallest weight from the design of Example 3. Again, due to the support being minimal the D–optimal weights are uniform, i. e. $\frac{1}{2}$ on each pair. It remains to optimize the determinant $|M(\xi_0)| = \left(\frac{2}{3}\right)^3 (1-\tau_2^2)^2((2\tau_1^2 + (1-\tau_2)^2)(2\tau_1^6 + (1-\tau_2^3)^2) - (2\tau_1^4 + (1-\tau_2)(1-\tau_2^3))^2)$ of the information matrix with respect to the settings τ_1 and τ_2. A numerical solution is given by $\tau_1 = 0.645828$ and $\tau_2 = 0.208013$ with a resulting determinant $|M(\xi_0)| = 0.0987493$. Hence, the minimal support design ξ_0 has 93.3% D–efficiency compared to the four point design of the previous example and, hence, at least, 93.1% in total. Note that the settings τ_1 and τ_2 are very close to the corresponding solutions in Example 3. The design ξ_0 can be used as an efficient exact design when the number of observations is a multiple of n.

5. GENERATING OPTIMAL DESIGNS FOR ADDITIVE MODELS

Finally, we consider additive two–factor models $\mu(t_1, t_2) = \beta_0 + f_1(t_1)^\top\beta_1 + f_2(t_2)^\top\beta_2$ for the value of an alternative depending on two factors t_1 and t_2 which may be adjusted independently, $t = (t_1, t_2) \in \mathcal{T}_1 \times \mathcal{T}_2$. Thus the observations for the paired comparisons are described by

$$Y(s,t) = (f_1(s_1) - f_1(t_1))^\top \beta_1 + (f_2(s_2) - f_2(t_2))^\top \beta_2 + Z(s,t)$$

and no interactions occur among the components. Due to a result by Rafajłowicz and Myszka (1992) D–optimal designs can be constructed as the cross–product of the optimal designs in the corresponding marginal models (see also Schwabe (1996), section 5.2):

Theorem 4. *If the designs ξ_i^* are D–optimal for the marginal models given by the response functions $E(Y^{(i)}(s_i,t_i)) = (f_i(s_i) - f_i(t_i))^\top \beta_i$, $s_i, t_i \in \mathcal{T}_i$, $i = 1, 2$, and if, additionally, $\xi_2^* = \bar{\xi}_2^*$ is symmetric with respect to exchanging s_2 and t_2, then the product design $\xi_1^* \otimes \xi_2^*$ is D–optimal for paired comparisons in the additive model.*

Proof. Due to the orthogonality condition $\sum (f_2(s_2) - f_2(t_2)) \bar{\xi}_2^*(s_2, t_2) = 0$ the result follows immediately from Theorem 5.23 in Schwabe (1996). $\square$

Moreover, if ξ_1 and ξ_2 are competing designs in the marginal models which show high marginal D–efficiencies, $\mathrm{eff}_D(\xi_i) \leq 1 - \varepsilon$, then the corresponding product design $\xi_1 \otimes \xi_2$ has also D–efficiency of, at least, $1 - \varepsilon$. Hence, the optimal and efficient designs obtained in the previous sections can be used as bricks to build optimal or efficient designs for paired comparisons in additive models with more than one active effect.

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