A note on small size augmented pair designs

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Abstract

This paper is devoted to small size experimental designs for response surfaces. Our purpose is to investigate the class of augmented pair designs obtained from an initial saturated simplex design with only two or three levels. Then we are looking in this new class for D-optimal properties and blocking structures.
Keywords: *simplex designs, augmented pair designs, saturated designs, moment matrix, efficiency.*

1 Introduction

Experimental designs for fitting response surfaces with quantitative factors are well known, many books and articles treat this question (see, for example, Box and Draper [3] or Khuri and Cornell [7]). A problem of prime importance in response surface methodology is to obtain **small size** designs, that is designs with a number of experiments close to the number of unknown parameters in the model. Apart from its theoretical interest this problem is of crucial importance in every situation in which experiments are expensive, difficult or time-consuming.

Our purpose in this paper is to investigate a general iterative method for constructing saturated second order designs in the class of **augmented pair** designs introduced by Morris [9]. These saturated designs can be later augmented by adding center replications in order to make an analysis of variance or used, because of the small number of runs, as blocks. The construction of an augmented pair design begins, in a first step, by the choice of an initial design. In this paper the initial design is always a first order **saturated design**. Then we have to add one new design run, called $x(\alpha, s, t)$, for each pair of runs (x_s, x_t), $s < t$, of the initial design by setting :

$$x(\alpha, s, t) = \alpha (x_s + x_t).$$

In other words we consider the sum of all the pairs of runs with a multiplicative coefficient α. This method including only the pair of runs is a particular case of the general method proposed first by Box and Behnken [2] for simplex-sum designs. Our problem with such a construction is to choose an "optimal" value for the coefficient α. The idea of Spendley et *al.* [12] is to add to the initial simplex all the midpoints of its edges (so $\alpha = 1/2$). More recently, Morris [9] or Fang and Mukerjee [5] have proved that taking $\alpha = -1/2$ lead us to more efficient designs. Our objective in this paper is on one hand to provide a general understanding of this class when the initial design is a simplex and, on the other hand, to find some new interesting values for this multiplicative coefficient.

Our paper is organized as follow. The beginning is devoted to recalls, notations and general results about simplex designs and ASD. Section 3 deals with general properties of small size simplex-sum designs. The problem of optimality for such designs is studied in section 4. Blocking structures for ASD are introduced in section 5 and we conclude with the presentation of an example in section 6.

2 Augmented pair designs

2.1 Initial simplex design

An augmented pair design is derived from an initial design which is often a first-order classical design. In this paper we always consider that our initial design is a **saturated** first-order design (*i.e.* constituted by $n = m + 1$ experimental units when m quantitative factors are used). Such designs have received much attention in the past principally concerning the class of simplex designs which is very useful for fitting first order models when the factors are continuous and the region of interest is spherical (see Box [1]). Note that a design is classically called **simplex** design if, denoting X the model matrix:

$$n = m + 1 \text{ and } \frac{1}{\sqrt{m+1}} X \text{ is an orthogonal matrix.} \tag{1}$$

In order to have a maximum of three different levels (a, b and c) for each factor we consider in this paper the class of saturated designs such that their matrix have the following form introduced by Mee [8] (with $J_m = \mathbb{I}_m {}^t\mathbb{I}_m$ the $m \times m$ matrix of ones) :

$$D_1 = D_1(a, b, c) = \left[\frac{a\, {}^t\mathbb{I}_m}{(b-c) I_m + cJ_m} \right]$$

Such a design can be used to fit a first order model and the model matrix is then $X = [\mathbb{I}_n \mid D_1]$. The purpose of Mee [8] was to use these configurations as simplex designs. We easily verifies that D_1 is the matrix of a simplex design if and only if $a = \pm 1$ and the two possible choices for $a = -1$ are given by:

$$\begin{cases} a = -1 \\ b = \left(1 - (m-1)\sqrt{m+1}\right)/m \\ c = \left(1 + \sqrt{m+1}\right)/m \end{cases} \text{ or } \begin{cases} a = -1 \\ b = \left(1 + (m-1)\sqrt{m+1}\right)/m \\ c = \left(1 - \sqrt{m+1}\right)/m \end{cases}.$$

The two other choices for $a = 1$ are obtained by reversing all the signs in the previous relations.

We are not interested in this paper by the classical method for constructing simplex designs (see, for example, Khuri and Cornell [7]) because it follow from the choice of an upper triangular matrix in place of the block $(b-c)\, I_m + cJ_m$ of D_1 and generally needs a great number of different levels (for example 6 levels are needed for $m = 4$). In the same way, cyclic simplex designs introduced by Crosier [4] are not considered in this paper because they need in general more than 3 levels for each factor (for example 5 levels are needed for $m = 4$). Note that the particular cases of cyclic simplex designs for 3, 7 or 11 factors can nevertheless be used because we find then Plackett and Burman designs [10] (*i.e.* simplex designs with only two levels for each factor). Note also that it is classical and easier to consider for the initial design, like Fang and Mukerjee [5] do, a regular fraction of the vertices of $[-1,1]^m$. But with this choice the initial design cannot be a first order saturated design (except when $m \equiv 3$ [4] but we have then another time a Plackett and Burman design [10]).

2.2 Augmented design

Now we consider the following second-order model denoting $Y_{u,x}$ the observed value of the response when the treatment $x = {}^t(x_1, \ldots, x_m)$ of the experimental domain $\mathcal{E} \subset I\!R^m$ is applied to the experimental unit u :

$$Y_{u,x} = \beta_0 + \sum_{i=1}^{m} \beta_i x_i + \sum_{i=1}^{m} \beta_{ii} x_i^2 + \sum\sum_{i<j} \beta_{ij} x_i x_j + \varepsilon_{u,x}.$$

Such a model has then $p = (m+1)(m+2)/2$ unknown parameters. In order to fit this model we consider the augmented matrix D_2 whose rows consist of all possible sums of the pair of rows of D_1. Then we call **augmented simplex design** (ASD) every design constituted by the design matrix such that :

$${}^tD = \left[\alpha_1 {}^tD_1 \mid \alpha_2 {}^tD_2\right].$$

Note that D_1 has $n_1 = (m+1)$ rows and D_2 has $n_2 = \binom{m+1}{2}$ rows. So, the total of experimental units for such an ASD is $n = n_1 + n_2 = p$, it is then a **saturated** second order design. More generally we call ASD in the following every design of this form with the addition of $n_0 \in \mathbb{N}$ central replications. We suppose now that $\alpha_1 = 1$ and we denote by α (in place of $\alpha_2 > 0$) the radius multiplier. This hypothesis is not restrictive because we are only interested in the following by the ratio between α_1 and α_2. The value of α_1 is just a scale parameter and it is classical to give it the value 1 in order to put the design points of the simplex on the sphere of radius $\sqrt{m}$ (see section 3.1). We also denote by x_s and x_t the coordinates of two different points of the initial simplex design (*i.e.* two different rows of D_1). The augmented part of the design (*i.e.* the rows of D_2) is then constituted by the following points x_{st} such that :

$$\forall\ x_s, x_t \text{ with } x_s \neq x_t\ ,\ x_{st} = x_s + x_t.$$

In addition of the simplicity of this relation we can remark the sequential property of such a design. The experiments can be run in a first time with the initial simplex design and continued only if the fist order model does not fit well.

3 Some properties of ASD

3.1 Geometric properties

The general definition (1) of simplex designs implies that :

$$\left(\frac{1}{m+1}\right) X^t X = I_{m+1} \text{ with } X = [\mathbb{I}_n \mid D_1] \,.$$

So every simplex design satisfies :

$$D_1{}^t D_1 = (m+1)\, I_{m+1} - J_{m+1}.$$

In other words, if x_s and x_t are the coordinates of two different points of the simplex design we have then:

$$\|x_s\|^2 = \|x_t\|^2 = m \text{ and } (x_s \mid x_t) = -1. \tag{2}$$

For the augmented part, relation (2) implies that:

$$\|x_{st}\|^2 = \|x_s + x_t\|^2 = \|x_s\|^2 + \|x_t\|^2 + 2\,(x_s \mid x_t) = 2\,(m-1)\,. \tag{3}$$

So the non-central design points of a simplex-sum design lie on the surface of two different centered spheres. More precisely, denoting $S\,(x) = \{v \in I\!\!R^m \ / \ {}^t vv = x^2\}$, every ASD associated to the matrix ${}^t D = [{}^t D_1 \mid \alpha {}^t D_2]$ is constituted by:

$$\begin{cases} \text{an initial part on the sphere} & S(\sqrt{m}), \\ \text{an augmented part on the sphere} & S(|\alpha|\, \sqrt{2\,(m-1)}). \end{cases} \tag{4}$$

This last result implies in the following that $\alpha \in [L_{\min}, L_{\max}]$ with $L_{\max} = -L_{\min} = \sqrt{m/2\,(m-1)}$ in order to consider the classical spherical domain of radius $\sqrt{m}$.

3.2 Radius multiplier properties

We have seen in previous sections that construction and geometrical interpretation of ASD are easy. The main problem is now the choice of the value for the radius multiplier α. The usual choices are given below:

1) The most usual value used in practice for the radius multiplier is $\alpha = 1/2$ (see Spendley et *al.* [12]). This method of construction of the augmented part is called in the following the **classical method**. The principal advantage of this method is due to the simplicity of α and to a simple geometric interpretation (the augmented points are then at the midpoints of the edges of the initial simplex).

2) Morris [9] has proposed a method for constructing augmented pair designs. His idea is to take an initial design of small size (not only a simplex design like here) and to add an augmented part such that "*for each factor, the value selected in the new run is the negative of the average of the two values from the s-th and t-th run*". In other words, the **method of Morris** implies the choice $\alpha = -1/2$. The principal advantages of this method is on one hand to give more efficient designs than for the classical method and, on the other hand, to obtain a three-level augmented design if the initial design has only two levels for each factor.

3) Another goal can be the structure of **equiradial** design. In that case it is clear from (4) that the radius multiplier must verify:

$$|\alpha| \sqrt{2(m-1)} = \sqrt{m} \quad \text{so} \quad \alpha = \pm \sqrt{\frac{m}{2(m-1)}}.$$

This choice may be interesting in order to achieve some properties like D-optimality (see section 4.2) because all the experimental units are then at the boundary of the experimental domain (but such a design can be singular if, for example, there is no central point).

3.3 Moments properties

Box and Behnken [2] have defined the more general class of simplex-sum design (SSD) such that every SSD is associated to the following matrix:

$${}^tD = \left[\alpha_1 {}^tD_1 \mid \alpha_2 {}^tD_2 \mid ... \mid \alpha_k {}^tD_k\right]$$

where $k \leq m$ and D_s $(1 \leq s \leq k)$ is a matrix whose rows consist of all possible sums of the rows of D_1 taken s at a time. They have proved that when $k = m$ the set of runs must be scaled to specific radius multipliers in order to obtain a **rotatable** design (see table 2 of their paper for the corresponding values of $\alpha_1, ..., \alpha_k$) *i.e.* a design such that all the odd moments up to order 4 are zero and the even moments satisfy:

$$\forall\ i, j = 1, ..., m \text{ with } i \neq j\ ,\ \left[i^2\right] = \lambda_2\ ,\ \left[i^2 j^2\right] = \lambda_4 \text{ and } \left[i^4\right] = 3\lambda_4.$$

Our goal in this section is to look for rotatable ASD (*i.e.* rotatable SSD in the particular case $k = 2$). We prove in a first time (see appendix A) that for every ASD the following properties are satisfied:

$$\begin{cases} \text{all the moments of order 1 are zero,} \\ \text{all the odd moments of order 2 are zero and } \left[i^2\right] = \lambda_2. \end{cases}$$

In order to extend these properties to high-order moments we also prove in appendix A that all the moments of order 3 of an ASD are zero if and only if (for $m \neq 3$):

$$\alpha = \frac{-1}{\sqrt[3]{m-3}}.$$

Unfortunately this value of α does not imply that all the odd moments of order 4 are zero. So we can conclude that ASD cannot be **rotatable** designs.

4 Optimality of ASD

4.1 Maximin criterion

An easy way to evaluate the efficiency of ASD is to use the **maximin** criterion introduced by Johnson et *al.* [6]. This criterion (independent of the chosen model) leads us to select designs that maximize the smallest interpair distance of the design's points. Then if $(x_u)_{u=1,..,.n}$ are the experimental units of a given design $\mathcal{D}$ we have to maximize the following quantity for a chosen norm:

$$Mm\left(\mathcal{D}\right) = \min \left\| x_u - x_v \right\| \text{ for all } x_u, x_v \in \mathcal{D} \text{ with } x_u \neq x_v.$$

From the geometric properties given in section 3.1 it is then possible to find explicitly the value of $Mm\left(\alpha\right)$ for every saturated ASD of radius multiplier α. In fact, relations (2) and (3) imply the existence of the following different interpair distances for the usual Euclidian norm (with s, t, u, v four different integers):

$$\begin{aligned}
d_1^2 &= \left\| x_s - x_t \right\|^2 = \left\| x_s \right\|^2 + \left\| x_t \right\|^2 - 2\left(x_s \mid x_t\right) = 2\left(m+1\right). \\
d_2^2 &= \left\| \alpha x_{st} - x_u \right\|^2 = \left\| \alpha x_s + \alpha x_t - x_u \right\|^2 = 2\alpha^2\left(m-1\right) + 4\alpha + m, \\
d_3^2 &= \left\| \alpha x_{st} - x_s \right\|^2 = \left\| \alpha x_s + \alpha x_t - x_s \right\|^2 = 2\alpha^2\left(m-1\right) + 2\alpha\left(1-m\right) + m. \\
d_4^2 &= \left\| \alpha x_{st} - \alpha x_{su} \right\|^2 = \alpha^2 \left\| x_t - x_u \right\|^2 = 2\alpha^2\left(m+1\right), \\
d_5^2 &= \left\| \alpha x_{st} - \alpha x_{uv} \right\|^2 = \alpha^2 \left\| x_s + x_t - x_u - x_v \right\|^2 = 4\alpha^2\left(m+1\right).
\end{aligned}$$

The distance d_1 is between two points of $S(\sqrt{m})$, d_2 and d_3 are distances between a point of $S(\sqrt{m})$ and a point of the sphere $S(\left|\alpha\right| \sqrt{2\left(m-1\right)})$ and d_4 and d_5 are distances between two points of $S(\left|\alpha\right| \sqrt{2\left(m-1\right)})$ (note that distance d_5 does not exist when $m < 3$). So the maximin criterion can be derived (when $m \geq 3$) from the following function :

$$Mm\left(\alpha\right) = \min\left(d_1, d_2, d_3, d_4, d_5\right).$$

But it is clear that $d_4 \leq d_5$, $d_4 \leq d_1$ (because $-1 \leq \alpha \leq 1$), $d_3 \leq d_2$ if $\alpha \geq 0$ and $d_2 \leq d_3$ if $\alpha \leq 0$. These results imply that we have the very simple following expression for Mm (and for every number of factors m) :

$$Mm\left(\alpha\right) = \min\left(d_3, d_4\right) \text{ if } \alpha \geq 0 \text{ and } Mm\left(\alpha\right) = \min\left(d_2, d_4\right) \text{ if } \alpha \leq 0. \quad (5)$$

If we add now a central point to the ASD we have to consider the two following other distances :

$$d_6^2 = \left\| x_s \right\|^2 = m \text{ and } d_7^2 = \left\| \alpha x_{st} \right\|^2 = 2\alpha^2\left(m-1\right).$$

It is clear in this case that $d_7^2 \leq d_4^2$ and also $d_7^2 \leq d_6^2$ (because $\left|\alpha\right| \leq \sqrt{m/2\left(m-1\right)}$) so if a central point is added the function Mm is now defined by:

$$Mm\left(\alpha\right) = \min\left(d_3, d_7\right) \text{ if } \alpha \geq 0 \text{ and } Mm\left(\alpha\right) = \min\left(d_2, d_7\right) \text{ if } \alpha \leq 0. \quad (6)$$

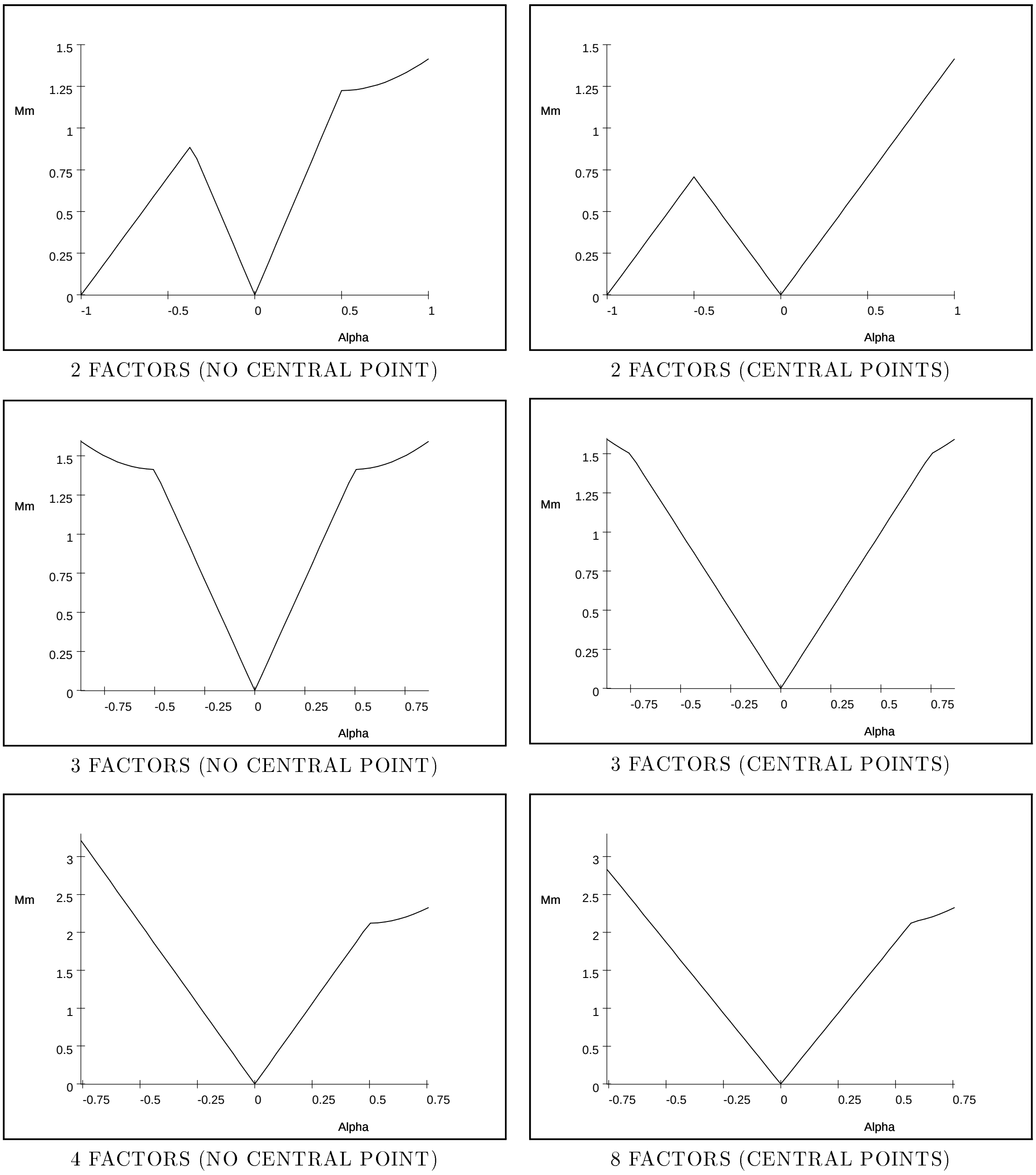
The figure 1 gives some graphical representations of the function Mm for $\alpha \in [L_{\min}, L_{\max}]$. Results (5) and (6) lead us easily to the following theorem:

Theorem 1. Consider an ASD for m factors and $n_0 \in \mathbb{N}$ central points. The most efficient designs for the **maximin** criterion are given by radius multipliers such that:

$$1)\ \alpha_{opt} = L_{\max} \quad \text{if } m = 2, \qquad 2)\ \alpha_{opt} = \pm L_{\max} \quad \text{if } m = 3,$$

$$3)\ \alpha_{opt} = L_{\min} \quad \text{if } m > 3.$$

Note that these results are true with or without central points added to the initial simplex design (that is with $n_0 > 0$ or $n_0 = 0$).



2 FACTORS (NO CENTRAL POINT) — 2 FACTORS (CENTRAL POINTS)

3 FACTORS (NO CENTRAL POINT) — 3 FACTORS (CENTRAL POINTS)

4 FACTORS (NO CENTRAL POINT) — 8 FACTORS (CENTRAL POINTS)

FIGURE 1

Maximin criterion Mm for $2, 3, 4$ and 8 factors.

Note also that this criterion is unable to make a choice between the classical radius multiplier $\alpha = 1/2$ and the radius multiplier of Morris $\alpha = -1/2$ because we always have $Mm\,(-1/2) = Mm\,(1/2)$.

4.2 D-efficiency criterion

In order to evaluate an efficiency adapted to the chosen polynomial model of order two our purpose is now to consider the classical criterion of D-efficiency (see for example the book of Pukelsheim [11]). For an ASD obtained with an initial simplex design of matrix D_1 and a radius multiplier equal to α this criterion is given by (denoting X the model matrix of the ASD and $|.|$ the determinant):

$$d_\alpha = d_\alpha\,(D_1) = |M|^{\frac{1}{p}} \text{ with } M = (1/n)^t\, XX.$$

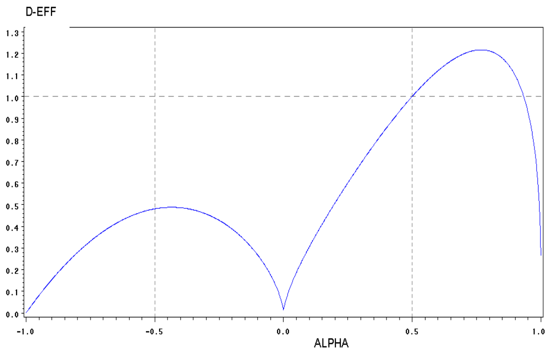
The goal is to maximize this criterion in order to obtain efficient designs. If we are interested by the efficiency of an ASD with respect to another ASD obtained with the same initial simplex design and a particular value α^* of the radius multiplier we have then to compute the ratio d_a/d_{α^*}. The following theorem concerns the choice of $\pm\alpha$ for the radius multiplier (see the proof in appendix B):

> **Theorem 2.** Consider the two ASD for m factors obtained with the same initial simplex design and the choice α or $-\alpha$ for the radius multiplier. We have then the following results for every positive radius multiplier α:
>
> 1) if $m = 2$ then $d_\alpha \geq d_{-\alpha}$, 2) if $m = 3$ then $d_\alpha = d_{-\alpha}$,
> 3) if $m > 3$ then $d_\alpha \leq d_{-\alpha}$.

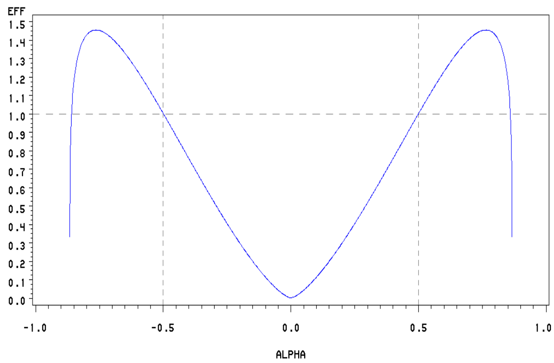
In other words the choice of a positive radius multiplier α would be better when two factors are analyzed. In all the other cases the choice of the negative radius multiplier $-\alpha$ is more judicious than the choice of α. This result is then a generalization of Morris one's only established for the value $1/2$.

Now we are interested by the determination of optimal values for the radius multiplier α. The problem of the maximization of d_α is very complex in our case due to the nontrivial form of the matrix ${}^tXX$ (see appendix B). So numerical computations have been made and some graphical representations are given below. Note that in this section tables and figures always compute D-efficiencies with respect to the classical value $\alpha = 1/2$ for the radius multiplier (*i.e.* $d_a/d_{0.5}$). The numerical results lead to the two following different situations.

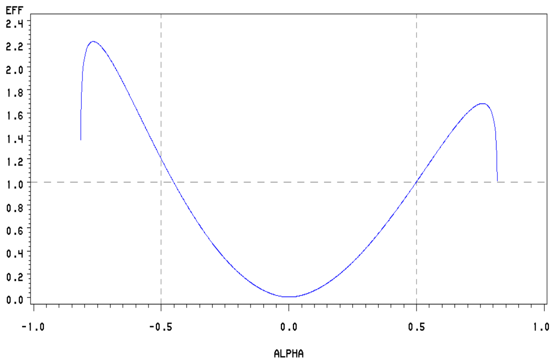
1) When no central experiment is used (see the three examples in figure 2) the optimal choice for the radius multiplier is not $L_{\min}$ or $L_{\max}$. This is because when $\alpha = \pm\sqrt{m/2\,(m-1)}$ all the experimental units of the ASD lie on the sphere $S(\sqrt{m})$ so the matrix X is not of full rank for a polynomial model of order two and then the efficiency is zero.



2 FACTORS (NO CENTRAL POINT)



3 FACTORS (NO CENTRAL POINT)



4 FACTORS (NO CENTRAL POINT)

FIGURE 2

D-efficiency for some saturated ASD.

We summarize in table 1 the optimal values of the radius multiplier and the corresponding efficiencies. We note that the proposed values lead us to most efficiency designs than the classical choice $\alpha = 0.5$ (or also $\alpha = -0.5$) especially for a great number of factors.

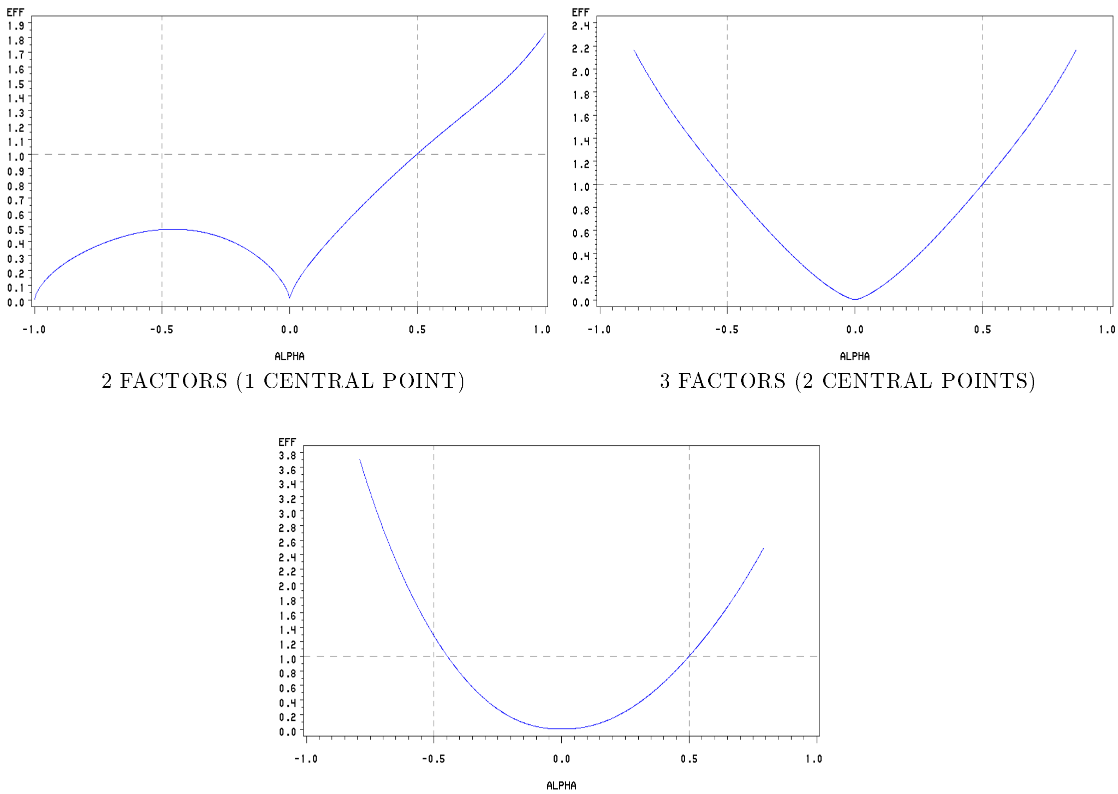
m	α opt.	D-efficiency	m	α opt.	D-efficiency
2	$+0.768$	1.215	6	-0.754	3.122
3	± 0.764	1.453	7	-0.749	3.388
4	-0.766	2.214	8	-0.745	3.580
5	-0.760	2.747			

TABLE 1

Optimal radius multiplier α and D-efficiencies for saturated ASD.

2) When at last one central experiment is used (see the three examples in figure 3) then the model matrix X is always of full rank and we find that optimal configurations are obtained (like for the maximin criterion) when :

$$\alpha_{opt} = L_{\max} \text{ if } m = 2 \text{ , } \alpha_{opt} = \pm L_{\max} \text{ if } m = 3 \text{ and } \alpha_{opt} = L_{\min} \text{ if } m > 3.$$



2 FACTORS (1 CENTRAL POINT)

3 FACTORS (2 CENTRAL POINTS)

5 FACTORS (3 CENTRAL POINTS)

FIGURE 3

D-efficiency for some unsaturated ASD.

5 Blocking structures for ASD

5.1 Fixed block effects model

Let us suppose now that we have b blocks of sizes $k_1, ..., k_b$ associated to the block effects $\gamma_1, ..., \gamma_b$. Then we consider the following linear model denoting $Y_{u,l,x}$ the observed value of the response when the treatment $x = {}^t(x_1, \ldots, x_m)$ associated to the l-block $(1 \leq l \leq b)$ is applied to the experimental unit u :

$$Y_{u,l,x} = \gamma_l + \sum_{i=1}^{m} \beta_i x_i + \sum_{i=1}^{m} \beta_{ii} x_i^2 + \sum_{i<j}\sum \beta_{ij} x_i x_j + \varepsilon_{u,l,x}.$$

Note that in order to avoid the classical singularity of block models we have excluded the general mean effect β_0. Such a model has then $p^* = m(m+3)/2 + b$ unknown parameters. When we take only one block we find again the classical second-order model. In the following we denote by X^* the matrix of this model so $X^* = [B \mid W]$ with B the matrix of the characteristic functions of the blocs and W the matrix of the linear, quadratic and interaction effects. Recall that a blocked design is said to be orthogonally blocked if and only if :

$$ {}^{t}W\left(I_n - \frac{1}{n}J_n\right)B = 0. \tag{7} $$

We are then looking for orthogonally blocked configurations of ASD.

5.2 Blocked ASD

Two different methods are investigated in this section in order to obtain to types of ASD orthogonally blocked in two blocks.

1) First method. A very simple and classical choice consists in the duplication of an ASD. The two blocks are then obtained by the repetition of the same experiments. We recommend in this case to use a saturated ASD for the blocks in order to minimize the total number of experiments. More precisely the number of experiments n and the number of unknown parameters p^* in the model are then given by:

$$ n = (m+1)(m+2) \text{ and } p^* = \frac{m(m+3)+4}{2}. $$

We easily verifies that such a configuration is always orthogonally blocked. Moreover if the user does not want to duplicate the experiments we have the same result with any ASD with radius multiplier α for the first block and any other ASD with radius multiplier $\pm\alpha$ for the second block.

2) Second method. The drawback of the first method is the number of experiments which cannot be less than $(m+1)(m+2)$. This is maybe too large when experiments are expensive. In this case another logical way in order to obtain two blocks for the ASD is given below :

$$ \begin{cases} \text{Block 1 :} & \text{initial part of the ASD and } n_{01} \text{ central points,} \\ \text{Block 2 :} & \text{augmented part of the ASD and } n_{02} \text{ central points.} \end{cases} $$

Note that the two block's sizes are respectively $k_1 = m + 1 + n_{01}$ and $k_2 = m(m+1)/2 + n_{02}$. Such a design is then saturated for the block effects model if and only if $n_{01} + n_{02} = 1$. We always assume in the following that $n_{01} + n_{02} \geq 1$. In order to obtain an orthogonally blocked configuration we have then the following result (see appendix C for the proof) :

> **Theorem 3.** Consider a blocked ASD in two blocks given by the initial part of the design (with n_{01} central points) and the augmented part of the design (with n_{02} central points). An **orthogonally blocked** configuration for a radius multiplier α is obtained if and only if:
>
> $$ m(m+1) + 2n_{02} = 2(m+1+n_{01})(m-1)\alpha^2. $$

5.3 Optimality

The main interest of orthogonal blocked configurations is due to similar properties concerning the D-efficiency criterion than non-blocked designs. Indeed denoting $X = [\mathbb{I}_n \mid W]$ and using Schur complements we have:

$$\left|{}^tXX\right| = \left|\left[\begin{array}{cc} n & {}^t\mathbb{I}_nW \\ {}^tW\mathbb{I}_n & {}^tWW \end{array}\right]\right| = n\left|{}^tW\left(I_n - \frac{1}{n}J_n\right)W\right|.$$

If we consider a blocked design the model matrix is now $X^* = [B \mid W]$ so:

$${}^tX^*X^* = \left[\begin{array}{cc} {}^tBB & {}^tBW \\ {}^tWB & {}^tWW \end{array}\right] \text{ with } {}^tBB = diag\left(k_1, ..., k_b\right).$$

Then using another time Schur complements we obtain:

$$\left|{}^tX^*X^*\right| = \prod_{i=1}^{b} k_i \left|{}^tWW - {}^tWB\left({}^tBB\right)^{-1}{}^tBW\right|.$$

From the assumption of orthogonal blocking we have ${}^tW\left(I_n - 1/nJ_n\right)B = 0$ so:

$${}^tWB\left({}^tBB\right)^{-1}{}^tBW = \frac{1}{n^2}{}^tW\mathbb{I}_n\left({}^t\mathbb{I}_nB\left({}^tBB\right)^{-1}{}^tB\mathbb{I}_n\right){}^t\mathbb{I}_nW.$$

But ${}^t\mathbb{I}_nB\left({}^tBB\right)^{-1}{}^tB\mathbb{I}_n = \sum_{i=1}^{b} k_i = n$ and then:

$$\left|{}^tX^*X^*\right| = \prod_{i=1}^{b} k_i \left|{}^tW\left(I_n - \frac{1}{n}J_n\right)W\right|.$$

In conclusion when an orthogonally blocked design is used we have:

$$n\left|{}^tX^*X^*\right| = \left(\prod_{i=1}^{b} k_i\right)\left|{}^tXX\right|.$$

Numerical values of these two determinants are then proportional so:

> **Proposition 4.** Consider a blocked ASD orthogonally blocked for each value of the radius multiplier. Note α_{opt} a radius multiplier such that the non-blocked design is D-optimal. Then a **D-optimal configuration** is obtained for the blocked design using the same value α_{opt} for the radius multiplier.

This result can be directly applied for blocked ASD obtained by the first method of section 5.2. Such designs are orthogonally blocked for every value of the radius multiplier so optimal values for the radius multiplier are given when no central experiment is made by Table 1 (see section 4.2) and in the other cases by:

$$\alpha_{opt} = L_{\max} \text{ if } m = 2,\ \alpha_{opt} = \pm L_{\max} \text{ if } m = 3 \text{ and } \alpha_{opt} = L_{\min} \text{ if } m > 3.$$

The situation is more complex for the second method of construction because in that case we can construct an ASD orthogonally blocked for only one particular value of the radius multiplier (see theorem 3). However if an ASD is not orthogonally blocked then:

$$n\left|{}^tX^*X^*\right| \leq \left(\prod_{i=1}^{b} k_i\right)\left|{}^tXX\right|.$$

This result can be proved in the following way. First, when two blocks are used we can verify after some algebra that:

$$B\left({}^tBB\right)^{-1}{}^tB - 1/nJ_n = \delta B^{*t}B^*$$

with $B^* = (I_n - 1/nJ_n)\,B$ the centered form of B and $\delta = n/\left(2k_1\left(n-k_1\right)\right) > 0$. Then, denoting $\succcurlyeq$ the Loewner ordering:

$${}^tW\left(B\left({}^tBB\right)^{-1}{}^tB - 1/nJ_n\right)W = \delta\left({}^tWB^*\right)\left({}^tB^*W\right) \succcurlyeq 0.$$

So, in conclusion:

$$\begin{aligned}&{}^tW\left(I_n - B\left({}^tBB\right)^{-1}{}^tB\right)W \preccurlyeq {}^tW\left(I_n - 1/nJ_n\right)W\\ &\Rightarrow n\left|{}^tX^*X^*\right| \leq \left(\prod_{i=1}^{b} k_i\right)\left|{}^tXX\right|.\end{aligned}$$

This result allow us to consider another time the non-blocked case and to state the following proposition:

> **Proposition 5.** Consider a blocked ASD in two blocks that can be orthogonally blocked for only one value $\alpha^\perp$ of the radius multiplier. Note α_{opt} a radius multiplier such that the non-blocked design is D-optimal. Then a **D-optimal configuration** is obtained for the blocked design if we put $\alpha^\perp$ and the radius multiplier α such that:
>
> $$\alpha^\perp = \alpha_{opt} \text{ and } \alpha = \alpha_{opt}.$$

This result can then be directly applied for blocked ASD obtained by the second method of section 5.2. Such designs are always regular (because we assume that $n_{01} + n_{02} \geq 1$) so an optimal blocked configuration must be orthogonally blocked for the value $\pm L_{\max}$ of the radius multiplier. From theorem 3 applied with $\alpha = \pm L_{\max}$ (so $\alpha^2 = m/2\,(m-1)$) we obtain the following lemma:

> **Lemma 6.** Consider a blocked ASD in two blocks given by the initial part of the design (with n_{01} central points) and the augmented part of the design (with n_{02} central points). A **D-optimal configuration** is obtained taking $mn_{01} = 2n_{02}$ and a radius multiplier such that:
>
> $$\alpha_{opt} = L_{\max} \text{ if } m = 2,\ \alpha_{opt} = \pm L_{\max} \text{ if } m = 3,\ \alpha_{opt} = L_{\min} \text{ if } m > 3.$$

Small size regular blocked ASD are then listed in Table 2. The values of n_{01}, n_{02} and α_{opt} verifying lemma 6 are computed and the total number of experiments n is given concurrently to the number of unknown parameters p^*.

m	n_{01}	n_{02}	α_{opt}	**n**	p^*
2	1	1	+1.000	**8**	7
3	2	3	±0.866	**15**	11
4	1	2	−0.816	**18**	16
5	2	5	−0.791	**28**	22
6	1	3	−0.775	**32**	29
7	2	7	−0.764	**45**	36
8	1	4	−0.756	**50**	46

TABLE 2
Some D-optimal orthogonally blocked ASD.

From this table it is clear that this method of construction allow us to use economical optimal blocked designs.

6 Example of application

Consider a random phenomenon associated to 4 quantitative factors in a context of expensive trials. From the results of this paper we can propose to use one ASD. With the initial simplex design in three levels of section 2.1 such configuration has then the matrix design D given below for the value of the radius multiplier $\alpha = L_{\min} = -\sqrt{2/3} \simeq -0.816$.

$$D = \left[\frac{D_1}{\alpha D_2} \right] = \left[\begin{array}{rrrr} -1.000 & -1.000 & -1.000 & -1.000 \\ 1.927 & -0.309 & -0.309 & -0.309 \\ -0.309 & 1.927 & -0.309 & -0.309 \\ -0.309 & -0.309 & 1.927 & -0.309 \\ -0.309 & -0.309 & -0.309 & 1.927 \\ \hline -0.757 & 1.069 & 1.069 & 1.069 \\ 1.069 & -0.757 & 1.069 & 1.069 \\ 1.069 & 1.069 & -0.757 & 1.069 \\ 1.069 & 1.069 & 1.069 & -0.757 \\ -1.321 & -1.321 & 0.505 & 0.505 \\ -1.321 & 0.505 & -1.321 & 0.505 \\ -1.321 & 0.505 & 0.505 & -1.321 \\ 0.505 & -1.321 & -1.321 & 0.505 \\ 0.505 & -1.321 & 0.505 & -1.321 \\ 0.505 & 0.505 & -1.321 & -1.321 \end{array} \right].$$

We also consider in the following the addition of $n_0 = 3$ central experiments (so the total of trials is now $n = 18$). Table 3 computes then all the dispersions of the estimators (with best results bolfaced) and the (relative) D-efficiencies for such designs with respect to the classical value $\alpha = 1/2$ (*i.e.* the ratios $d_\alpha/d_{0.5}$). We find another time that the choice $\alpha = -0.5$ is globally better than $\alpha = +0.5$ but the best choice in terms of D-efficiency is given by $\alpha = L_{\min} = -0.816$ (*i.e.* by the design of matrix D).

Value of α	Var $\hat{\beta}_0$	Var $\hat{\beta}_i$	Var $\hat{\beta}_{ii}$	Var $\hat{\beta}_{ij}$	D-eff.
$+0.500$	**0.165**	0.392	0.206	0.596	1.000
-0.500	**0.165**	0.200	0.134	0.545	1.197
$+0.816$	0.333	0.217	0.153	0.156	1.971
-0.816	0.333	**0.071**	**0.070**	**0.098**	2.636

TABLE 3
Dispersion of the parameters ($\sigma^2 = 1$) and D-efficiency of the ASD.

We can make now a comparison between this ASD and a Fang and Mukerjee [5] design (FMD), that is an augmented pair designs obtained from a regular fraction. More precisely we consider the FMD associated with the 2^{4-1} regular fraction generated by the relations $\mathbb{I} = 124$ (example denoted by the matrix X_a in their paper). Such a design has then $n_1 = 8$ trials in the initial part and then $n_2 = \binom{8}{2} = 28$ trials for the augmented part. In order to compare this FMD with another design of same size we can then use the $n = 36$ trials obtained by a duplication of our ASD. Dispersion and efficiency results are then given in table 4 (with all the relative D-efficiencies computed with respect to the FMD with $\alpha = -0.5$). Note that for the FMD there are several different values of the dispersion for the linear effects and the interaction effects so the values given in table 4 are then the average dispersion. At last, the value $\alpha = \pm 0.577$ for the FMD is the maximal value of the radius multitplier in order to stay in the classical experimental spherical domain of radius $\sqrt{m}$ (it is derived from augmented points on the form $(\alpha, \alpha, \alpha, 0)$).

	Value of α	Var $\hat{\beta}_0$	Var $\hat{\beta}_i$	Var $\hat{\beta}_{ii}$	Var $\hat{\beta}_{ij}$	D-eff.
FMD	-0.500	0.119	0.053	0.113	0.086	1.000
	-0.577	0.163	0.042	0.073	0.066	1.305
ASD	-0.500	**0.083**	0.100	0.067	0.273	0.728
	-0.816	0.167	**0.035**	**0.035**	**0.049**	1.925

TABLE 4
Comparison between ASD and Fang and Mukerjee design.

Then we can make the following conclusions concerning first the advantages of the FMD:

1) If we use a radius multiplier such that $\alpha \in [-0.5, 0.5]$ then the FMD with

$\alpha = -0.5$ is the best choice (like Fang and Mukerjee [5] have proved) and it is also better than the ASD with the same value of α.

2) For the radius multiplier $\alpha = -0.5$ the FMD has only three levels for each factors (instead of 7 for the ASD).

Now the main advantages of the ASD are given below:

1) If we use the radius multiplier $\alpha = -0.816$ then we obtain a more D-efficient design than every FMD.

2) The ASD is constituted by only $n = 15$ trials (if no central point is added) and not $n = 36$ trials like for the FMD.

3) If we use $n = 36$ trials then the ASD can be easily orthogonally blocked and central replications improve the analysis of variance.

7 Conclusion

We have seen in this paper that augmented simplex designs are very useful designs in order to obtain saturated or small-size configurations. But the main problem of such designs is the choice of the radius multiplier, especially when there is no central replications. One important conclusion for a practical use is that the classical value 1/2 for the radius multiplier is not a good choice because negative well-chosen values are better (for 3 factors or more. The other important conclusion concerns blocking structure for such design. We have proved that the hypothesis of orthogonally blocking is not difficult to obtain and the efficiency of these designs is then similar to the efficiency of the non-blocked case.

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Appendix A

We want to evaluate all the moments up to order 2 for an ASD. According to the notations of Box and Behnken [2], we have:

$$\left[1^{\delta_1} 2^{\delta_2} \dots k^{\delta m}\right] = \left[1^{\delta_1} 2^{\delta_2} \dots k^{\delta_m}\right]_1 + \alpha^{\delta} \left[1^{\delta_1} 2^{\delta_2} \dots k^{\delta_m}\right]_2$$

with $\left[1^{\delta_1} 2^{\delta_2} \dots k^{\delta_m}\right]$ the global moment of order $\delta = \delta_1 + ... + \delta_m$ and $\left[1^{\delta_1} 2^{\delta_2} \dots k^{\delta_m}\right]_s$ the moment of design D_s ($s = 1, 2$) multiplied by n_s/n with n_s the size of D_s. For the moments of order 1 we have then ($\forall\ i = 1, ..., m$) $[i] = [i]_1 + \alpha\, [i]_2$ with $[i]_1 = 0$ because columns of D_1 are orthogonal to $\mathbb{I}_{n_1}$. This result also implies that $[i]_2 = 0$ (see the paper of Box and Behnken [2] for the relation between $[i]_2$ and $[i]_1$). So all the moments of order 1 are zero for every ASD. With the same argument it is possible to show that all the odd moments of order 2 are zero. In fact, we have $[ij]_1 = 0$ (for every $i \neq j$) because columns or D_1 are orthogonal to each other and this result implies that $[ij]_2 = 0$ (see Box and Behnken [2]). Now the even moments of order 2 are given by ($\forall\ i = 1, ..., m$) $[i^2] = [i^2]_1 + \alpha^2 [i^2]_2$ with $[i^2]_1 = (m+1)/n$ from relation (1). For the augmented part, Box and Behnken [2] have proved that:

$$\forall\ i = 1, ..., m\ ,\ \left[i^2\right]_2 = \frac{m^2-1}{n} \text{ so } \left[i^2\right] = \lambda_2 = \frac{m+1}{n}\left(1+(m-1)\,\alpha^2\right).$$

For the moments of order 3 we consider in a first time (without loss of generality) the pure moments $[i^3]$. We have then ($\forall\ i = 1, ..., m$) , $[i^3] = [i^3]_1 + \alpha^3 [i^3]_2$. But Box and Behnken [2] have proved that:

$$\forall\ i = 1, ..., m\ ,\ \left[i^3\right]_2 = \frac{m-3}{m-1}\binom{m-1}{1}\left[i^3\right]_1 = (m-3)\left[i^3\right]_1.$$

So the moments $[i^3]$ of an ASD are given by:

$$\forall\ i = 1, ..., m\ ,\ \left[i^3\right] = \left(1+\alpha^3\,(m-3)\right)\left[i^3\right]_1.$$

Then:

$$\alpha = -\,(m-3)^{-1/3} \Rightarrow \forall\ i = 1, ..., m\ ,\ \left[i^3\right] = 0.$$

Note that this result is only a sufficient condition in order to obtain all the pure moments of ordre three equal to zero.This result is in fact a necessary and sufficient condition in the class of ASD because in general the initial simplex design doesn't statisfies the alternative propertie: $[i^3]_1 = 0$ for $i = 1, ..., m$. Box and Behnken [2] have also proved that $[i^2 j]_2 = (m-3)\,[i^2 j]_1$ and $[ijk]_2 = (m-3)\,[ijk]_1$ so all the moments of order 3 of the ASD are zero when this value of α is used ■

Appendix B

Our first purpose is to find here the general form of the moment matrix of every ASD. The model matrix of an ASD with $n_0 \geq 0$ central replications is:

$$X = \begin{bmatrix} \mathbb{I}_{n_1} & D_1 & D_1^Q & D_1^I \\ \mathbb{I}_{n_2} & \alpha D_2 & \alpha^2 D_2^Q & \alpha^2 D_2^I \\ \mathbb{I}_{n_0} & 0 & 0 & 0 \end{bmatrix}$$

with D_1^Q the matrix associated to the quadratic effects for the initial simplex and D_1^I for the interaction effects (D_2^Q and D_2^I are the same for the augmented part). Then the moment matrix is such that (with $\times$ denoting symmetric blocs):

$${}^tXX = \begin{bmatrix} n & {}^t\mathbb{I}_{n_1} D_1 + \alpha^t\mathbb{I}_{n2} D_2 & {}^t\mathbb{I}_{n_1} D_1^Q + \alpha^{2t}\mathbb{I}_{n2} D_2^Q & {}^t\mathbb{I}_{n_1} D_1^I + \alpha^{2t}\mathbb{I}_{n2} D_2^I \\ \times & {}^tD_1 D_1 + \alpha^{2t} D_2 D_2 & {}^tD_1 D_1^Q + \alpha^{3t} D_2 D_2^Q & {}^tD_1 D_1^I + \alpha^{3t} D_2 D_2^I \\ \times & \times & {}^tD_1^Q D_1^Q + \alpha^{4t} D_2^Q D_2^Q & {}^tD_1^Q D_1^I + \alpha^{4t} D_2^Q D_2^I \\ \times & \times & \times & {}^tD_1^I D_1^I + \alpha^{4t} D_2^I D_2^I \end{bmatrix}$$

This general form can be simplified in a first way because all the moments of the ASD up to order two are well known (see section 3.3). In a second way, using the results of Box and Behnken [2], we can express all the moments of the augmented part using only the moments of the initial part. These two treatments lead us to the following form only depending on the moments properties of the initial simplex design and the value of α :

$$ {}^{t}XX = \begin{bmatrix} A(\alpha) & B(\alpha) \\ {}^{t}B(\alpha) & C(\alpha) \end{bmatrix} \text{ with :} $$

$$ A(\alpha) = \begin{bmatrix} n & 0 \\ 0 & h_1(\alpha) I_m \end{bmatrix}, \; B(\alpha) = \begin{bmatrix} h_1(\alpha)\, {}^{t}\mathbb{I}_m & 0 \\ h_2(\alpha)\, {}^{t}D_1 D_1^Q & h_2(\alpha)\, {}^{t}D_1 D_1^I \end{bmatrix}, $$

$$ C(\alpha) = \begin{bmatrix} h_3(\alpha)\, {}^{t}D_1^Q D_1^Q + h_4(\alpha)(2I_m + J_m) & h_3(\alpha)\, {}^{t}D_1^Q D_1^I \\ h_3(\alpha)\, {}^{t}D_1^I D_1^Q & h_3(\alpha)^{t}\, D_1^I D_1^I + h_4(\alpha) I_m \end{bmatrix}, $$

$$ \text{and: } \begin{cases} h_1(\alpha) = (m+1)\left[1 + (m-1)\alpha^2\right], & h_2(\alpha) = \left[1 + (m-3)\alpha^3\right], \\ h_3(\alpha) = \left[1 + (m-7)\alpha^4\right], & h_4(\alpha) = (m+1)^2 \alpha^4. \end{cases} $$

So, using the Schur complements, we have:

$$ \left|{}^{t}XX\right|_{\alpha} = n h_1^m(\alpha) \left|C(\alpha) - {}^{t}B(\alpha) A^{-1}(\alpha) B(\alpha)\right|. $$

By definition h_1 is an even function of α and the matrix $C(\alpha)$ only depends on α by the even functions h_3 and h_4. We have then to consider only the following matrix (denoting $({}^{t}BA^{-1}B)_{\alpha}$ in place of ${}^{t}B(\alpha) A^{-1}(\alpha) B(\alpha)$):

$$ \left({}^{t}BA^{-1}B\right)_{\alpha} = \begin{bmatrix} \dfrac{h_1^2(\alpha)}{n} J_m + \dfrac{h_2^2(\alpha)}{h_1(\alpha)} {}^{t}D_1^Q D_1 {}^{t}D_1 D_1^Q & \dfrac{h_2^2(\alpha)}{h_1(\alpha)} {}^{t}D_1^Q D_1 {}^{t}D_1 D_1^I \\ \dfrac{h_2^2(\alpha)}{h_1(\alpha)} {}^{t}D_1^I D_1 {}^{t}D_1 D_1^Q & \dfrac{h_2^2(\alpha)}{h_1(\alpha)} {}^{t}D_1^I D_1 {}^{t}D_1 D_1^I \end{bmatrix}. $$

We have then:

$$ \begin{aligned} ({}^{t}BA^{-1}B)_{\alpha} - ({}^{t}BA^{-1}B)_{-\alpha} &= \Delta(\alpha) \begin{bmatrix} {}^{t}D_1^Q D_1 {}^{t}D_1 D_1^Q & {}^{t}D_1^Q D_1 {}^{t}D_1 D_1^I \\ {}^{t}D_1^I D_1 {}^{t}D_1 D_1^Q & {}^{t}D_1^I D_1 {}^{t}D_1 D_1^I \end{bmatrix} \\ &= \Delta(\alpha)\, {}^{t}\widetilde{X}\widetilde{X} \end{aligned} $$

denoting $\widetilde{X} = \begin{bmatrix} {}^{t}D_1 D_1^Q & {}^{t}D_1 D_1^I \end{bmatrix}$ and:

$$ \Delta(\alpha) = \frac{h_2^2(\alpha) - h_2^2(-\alpha)}{h_1(\alpha)} = \frac{4(m-3)\alpha^3}{h_1(\alpha)}. $$

So this last result implies the following relations for the Loewner ordering ($\forall\, \alpha \geq 0$ and $\forall\, m \geq 3$):

$$ \begin{aligned} ({}^{t}BA^{-1}B)_{\alpha} - ({}^{t}BA^{-1}B)_{-\alpha} \succcurlyeq 0 \; &\Rightarrow (C -{}^{t} BA^{-1}B)_{\alpha} \preccurlyeq (C -{}^{t} BA^{-1}B)_{-\alpha} \\ &\Rightarrow |{}^{t}XX|_{\alpha} \leq |{}^{t}XX|_{-\alpha}. \end{aligned} $$

The result is then well proved (the case for $m < 3$ is similar) ■

Appendix C

In order to obtain orthogonal blocking ASD we have to compute the matrix ${}^tW\left(I_n - 1/nJ_n\right)B$. Note that the structure of the two blocks implies that (using the notations of appendix B) :

$$B = \begin{bmatrix} \mathbb{I}_{k_1} & 0 \\ 0 & \mathbb{I}_{k_2} \end{bmatrix} \text{ and } W = \begin{bmatrix} W_1 \\ W_2 \end{bmatrix} = \begin{bmatrix} D_1 & D_1^Q & D_1^I \\ \alpha D_2 & \alpha^2 D_2^Q & \alpha^2 D_2^I \end{bmatrix}.$$

Then :

$$\left(I_n - \frac{1}{n}J_n\right)B = B - \frac{1}{n}\mathbb{I}_n\left({}^t\mathbb{I}_n B\right) = \frac{1}{n}\begin{bmatrix} k_2\mathbb{I}_{k_1} & -k_2\mathbb{I}_{k_1} \\ -k_1\mathbb{I}_{k_2} & k_1\mathbb{I}_{k_2} \end{bmatrix}.$$

We have seen in appendix A that for every ASD the block's moments verify (with the notations of Box and Behnken [2]) :

$$\forall\ i,j = 1,...,m \text{ with } i<j\ ,\ [i]_1 = [i]_2 = 0 \text{ and } [ij]_1 = [ij]_2 = 0.$$

So :

$${}^tW\left(I_n - \frac{1}{n}J_n\right)B = \begin{bmatrix} 0 & 0 \\ \left(k_2\left[i^2\right]_1 - k_1\alpha^2\left[i^2\right]_2\right)\mathbb{I}_m & \left(-k_2\left[i^2\right]_1 + k_1\alpha^2\left[i^2\right]_2\right)\mathbb{I}_m \\ 0 & 0 \end{bmatrix}.$$

Then such ASD is orthogonally blocked if and only if :

$$\forall\ i,j = 1,...,m\ ,\ k_2\left[i^2\right]_1 = k_1\alpha^2\left[i^2\right]_2.$$

From appendix A we have also :

$$\forall\ i,j = 1,...,m\ ,\ \left[i^2\right]_1 = \frac{m+1}{n} \text{ and } \left[i^2\right]_2 = \frac{m^2-1}{n}.$$

Then the ASD is orthogonally blocked if and only if :

$$k_2\left(\frac{m+1}{n}\right) = k_1\alpha^2\left(\frac{m^2-1}{n}\right) \Leftrightarrow k_2 = k_1(m-1)\alpha^2.$$

But the block's sizes are well known and then :

$$k_2 = k_1(m-1)\alpha^2 \Leftrightarrow m(m+1) + 2n_{02} = 2(m+1+n_{01})(m-1)\alpha^2 \quad \blacksquare$$

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