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This paper is devoted to the analysis of small central composite designs obtained with a regular fraction of resolution III*. We show that it is then possible to find explicitely mean square estimators, predicted response, variance dispersion graphs and D-efficiency. Such designs, well chosen, can be an alternative to classical CCD when the priority is to reduce the number of runs.

Keywords Central composite designs; regular fractions of resolution III* or V; variance dispersion graphs; D-efficiency.

Mathematics Subject Classification 62K20

1 Introduction

This paper deals with the analysis of experimental designs for response surfaces when the main goal is to reduce the number of runs. Apart from its theoretical interest this problem is of prime importance in every situation in which experiments are expensive, difficult to achieve, time-consuming, *etc.*

One extremely useful type of designs are central composite designs (CCD) suggested by Box and Wilson (1951) and Box and Hunter (1957). Such CCD are well known and widely used in practice. But a main structural problem of these designs is the size of the factorial part which is constituted by 2^m runs in the case of a complete CCD for m factors or 2^{m-k} runs by using a regular fraction of resolution V built with k generators (see Box and Hunter, 1961). In some cases the size of this part is too important, for example with 4 factors the factorial part has 16 runs (and the CCD at least 24 runs adding the axial part) for a surface response model with only 15 unknown parameters. However it is sometimes possible to still reduce the factorial part, following Hartley (1959), using a regular fraction of resolution III*. These designs are often smaller than classical CCD (they are even satured in some cases), but their analyse is somewhat more complicated.

In order to implement a central composite design it is useful to explicitly obtain the form of the least square estimators and the predicted response. In a global point of view concerning the quality of the predicted responses it is also interesting to use variance dispersion graphs (see Giovannitti-Jensen and Myers, 1989). Such VDG are in general obtained with computer programs that optimize quadratics forms on every centered sphere (see, for example, Vining, 1993). Finally it is important to evaluate the efficiency of the design, for example in order to choose an appropriate value for the distance α between the center and the axial points. Our goal is then to extend these results and methods, well known for classical CCD, to the case of small CCD built with fractions of resolution III*.

The paper is organized as follows. The beginning (section 2) is devoted to recalls, notations and general results for classical CCD. The section 3 is dedicaced to the analyse of small CCD. A final section concludes with the problem of the practical implementation of these designs.

2 Classical CCD

2.1 Response surface designs

We make some recalls in this part concerning experimental designs for response surfaces. See also, for more details, books of Box and Draper (1987) or Khuri and Cornell (1996). Consider in the following a random phenomenon depending on m quantitative factors. An experiment is then associated to the vector $x =^t (x_1, ..., x_m)$ and we assume that the observed response in x, called $Y(x)$, can be approximated by the classical second order model:

$$Y(x) = \beta_0 + \sum_{i=1}^{m} \beta_i x_i + \sum_{i=1}^{m} \beta_{ii} x_i^2 + \sum \sum_{i<j} \beta_{ij} x_i x_j + \varepsilon(x) \tag{1}$$

The matricial formulation for such model is then:

$$Y = X\beta + \varepsilon$$

with Y the vector of the n observations , ε the vector of the n random errors, β the vector of the p unknown parameters ($p = (m+1)(m+2)/2$ here) and X the $n \times p$ model matrix. We call design matrix the $n \times m$ matrix D with the row u made up of the m coordinates of the u-th design point. Let L_j $(1 \leq j \leq m)$ be the j-th column of D and $\odot$ the Hadamard product operator (*i.e. if* $u, v \in \mathbb{R}^n$ then $u \odot v \in \mathbb{R}^n$ is such that $(u \odot v)_i = u_i v_i$ for $i = 1, ..., n$). The model matrix has then the following form:

$$X = [\ \mathbb{I}_n \mid D_Q \mid D \mid D_I\ ]$$

with $D = D_L = [\ L_1 \mid \ \ldots \ \mid L_m\ ]$ associated to the linear effects, $D_Q = [\ L_1 \odot L_1 \mid \ldots \mid L_m \odot L_m\ ]$ associated to the quadratic effects and $D_I = \left[\ L_1 \odot L_2 \mid \ldots \mid L_{(m-1)} \odot L_m\ \right]$ associated to the interaction effects. The arbitrary order for the columns of X is chosen in order to simplify the expression of some following results. Similarly, the vector β of the unknown parameters of the model is partitionned in ${}^t\beta = ({\beta_0}, {}^t\beta_Q, {}^t\beta_L, {}^t\beta_I)$.

2.2 Construction and properties of classical CCD

In the following a CCD for m factors is called classical when it is made from:

a) a factorial part constituted by a full factorial design or by a regular fraction of resolution V (or more),

b) an axial part constituted by the points on the axes at a same distance α from the origin of the experimental domain,

c) a central part constituted by $n_0 \in \mathbb{N}$ repeated runs at the origin of the experimental domain.

Note that such design has a total of $n = 2^{m-k} + 2m + n_0$ runs when the regular fraction is built with k generators ($k = 0$ in the case of a full factorial design). Some properties of classical CCD are listed below, see Borkowski (1995) or Tinsson (2010) for the proofs.

1) The moment matrix of each classical CCD is a block-diagonal matrix under the following canonical form (with $\mathbb{I}_m$ the vector of m ones, I_m the identity matrix and $J_m = \mathbb{I}_m {}^t\mathbb{I}_m$):

$$M = \frac{1}{n}{}^tXX = \frac{1}{n} diag\,(A, B) \ \text{ with}$$

$$A = \begin{bmatrix} n & s_2{}^t\mathbb{I}_m \\ s_2\mathbb{I}_m & (s_4 - s_{22})\, I_m + s_{22} J_m \end{bmatrix} \text{ and } B = \begin{bmatrix} s_2 I_m & 0 \\ 0 & s_{22} I_{(m-1)m/2} \end{bmatrix}. \tag{2}$$

So all the odd moments up to order 4 are zero and the even moments satisfy the following relations ($\forall\ i, j = 1, ..., m$ with $i \neq j$):

$$n\left[i^2\right] = s_2 = 2^{m-k} + 2\alpha^2\ ,\ n\left[i^2 j^2\right] = s_{22} = 2^{m-k}\ ,\ n\left[i^4\right] = s_4 = 2^{m-k} + 2\alpha^4.$$

2) For each design having a regular moment matrix under canonical form the inverse of this matrix can be explicitely found. This implies that the least square estimators $\widehat{\beta} = ({}^tXX)^{-1}\,{}^tXY$ of the model parameters are given by explicit formulas (see proposition 5.3 of Tinsson, 2010). Moreover the diagonal elements of $Var\left(\widehat{\beta}\right) = \sigma^2\,({}^tXX)^{-1}$ are given by ($\forall\ i, j = 1, ..., m$ with $i \neq j$ and denoting $\phi = ns_4 + n\,(m-1)\,s_{22} - ms_2^2$):

$$Var\left(\widehat{\beta}_0\right)=\frac{\sigma^2}{n}\left(1+\frac{ms_2^2}{\phi}\right),Var\left(\widehat{\beta}_i\right)=\frac{\sigma^2}{s_2},Var\left(\widehat{\beta}_{ij}\right)=\frac{\sigma^2}{s_{22}},$$
$$Var\left(\widehat{\beta}_{ii}\right)=\frac{\sigma^2}{s_4-s_{22}}\left(1+\frac{s_2^2-ns_{22}}{\phi}\right) \tag{3}$$

3) For each design having a regular moment matrix under canonical form the dispersion of the predicted response $\widehat{Y}(x)$ is explicitely given by (denoting $r^2={}^txx$):

$$Var\widehat{Y}(x)=\sigma^2\left[f(r)+\left(\frac{1}{s_4-s_{22}}-\frac{1}{2s_{22}}\right)\sum_{i=1}^{m}x_i^4\right]$$

with $f(r)=\left(\frac{1}{n}+\frac{ms_2^2}{n\phi}\right)+\left(\frac{1}{s_2}-2\frac{s_2}{\phi}\right)r^2+\left(\frac{1}{2s_{22}}+\frac{s_2^2-ns_{22}}{\phi(s_4-s_{22})}\right)r^4$.

It follows from this relation that a classical CCD is rotatable if and only if:

$$s_4=3s_{22}\Longleftrightarrow 2^{m-k}+2\alpha^4=3\left(2^{m-k}\right)\Longleftrightarrow\alpha=\left(2^{m-k}\right)^{1/4}.$$

4) Following Giovannitti-Jensen and Myers (1989), a graphical tool for the predictions capabilities of a design can be its variance dispersion graph (VDG). For each design having a regular moment matrix under canonical form its spherical variance V and its extremal predictions variances $Vmin$ and $Vmax$ are explicitely given by the following expressions (with $U_r=\left\{x\in\mathbb{R}^m\ /\ {}^txx=r^2\right\}$ and $\Psi=\int_{U_r}dx$):

$$\begin{aligned}
Vmin(r)&=\min_{x\in U_r}\left[Var\widehat{Y}(x)\right]=\sigma^2\left[f(r)+\frac{1}{m}\left(\frac{1}{s_4-s_{22}}-\frac{1}{2s_{22}}\right)r^4\right],\\
V(r)&=\Psi^{-1}\int_{U_r}Var\widehat{Y}(x)\,dx=\sigma^2\left[f(r)+\frac{3}{m+2}\left(\frac{1}{s_4-s_{22}}-\frac{1}{2s_{22}}\right)r^4\right],\\
Vmax(r)&=\max_{x\in U_r}\left[Var\widehat{Y}(x)\right]=\sigma^2\left[f(r)+\frac{3}{m+2}\left(\frac{1}{s_4-s_{22}}-\frac{1}{2s_{22}}\right)r^4\right].
\end{aligned} \tag{4}$$

Note that these formulas are true when $s_4>3s_{22}$. If $s_4<3s_{22}$ then $Vmin$ and $Vmax$ have to be permuted. The three curves are identical when $s_4=3s_{22}$, that is when the design is rotatable.

5) For each design having a moment matrix under canonical form its D-efficiency $\Phi_0=|{}^tXX|^{1/p}$ is explicitely given by:

$$\Phi_0(s_2,s_4,s_{22})=\left[(s_4-s_{22})^{m-1}s_2^m s_{22}^{m(m-1)/2}\phi\right]^{1/p}. \tag{5}$$

3 Small CCD

3.1 Recalls, definitions and notations

According to Box and Hunter (1957) notations we denote by the letter `j` the column L_j $(1\leq j\leq m)$ of the factorial part of the design matrix. Conventionally the Hadamard product of the columns `i` and `j` is now simply denoted by "`ij`" instead of "`i` $\odot$ `j`" and it is called a

word of lenght 2 (the lenght of a word is its number of letters). A regular fraction (of the full factorial design) is then defined by a set of k words called generators. These words generate a group, denoted G in the following, and called defining relation. For k independant generators the defining relation is constituted by 2^k elements and defines a design in 2^{m-k} runs. The resolution of such regular fraction is the length of the shortest word in the defining relation. Following Hartley (1959) we call regular fraction of resolution III* every regular fraction of resolution III such that its defining relation has no element of length 4.

Example. For $m = 6$ factors and $k = 2$ generators the regular fraction defined by $\mathbb{I}_{16} = \mathtt{123} = \mathtt{346}$ has a resolution III but not III* because $G = \{\mathbb{I}_{16}, \mathtt{123}, \mathtt{346}, \mathtt{1246}\}$. On the other side the regular fraction defined by $\mathbb{I}_{16} = \mathtt{123} = \mathtt{456}$ has a resolution III* because $G = \{\mathbb{I}_{16}, \mathtt{123}, \mathtt{456}, \mathtt{123456}\}$.

A central composite design is then called **small CCD** (see Draper, 1985) if and only if it is made from the sets given by a', b and c with (see section 2.2 for b and c):

a') a factorial part constituted by a regular fraction of resolution III*.

Note that it may be surprising, *a priori*, to use such a design in order to fit a response surface model with a resolution not equal to V. But the important point is that with a small CCD two-factors interactions are not aliased with each other. Two factor interactions could be aliased with linear effects (in our example $\mathtt{1} = \mathtt{23}$, $\mathtt{2} = \mathtt{13}$, *etc.*) but this is not a problem because the axial part provides additional information on the linear effects and then these aliases vanish (and the model matrix can be of full rank).

We compare now, in table 1, the sizes of classical CCD (with full factorial part or regular fraction of resolution V) and small CCD (up to $m = 8$, response surface models are rarely used with more factors). This table is constructed using the smallest possible regular fractions of resolution III* or V (so with the largest possible number of generators) and with no center point. General methods in order to obtain these smallest regular fractions are presented in Draper and Lin (1990). The columns represent respectively: the number of factors, the number of model's parameters, the size of full CCD, the size of CCD obtain with a regular fraction of resolution V and the size of small CCD. We also note in brackets the relative size of each design, that is its size scaled by the number of unknown parameters of the model:

$$\Phi = \frac{n}{p} = \frac{2n}{(m+1)(m+2)}.$$

Factors	Parameters	Full CCD	CCD res. V	CCD res. III*
2	6	8 (1.33)	no	no
3	10	14 (1.40)	no	10 (1.00)
4	15	24 (1.60)	no	16 (1.07)
5	21	42 (2.00)	26 (124)	26 (1.24)
6	28	76 (2.71)	44 (1.57)	28 (1.00)
7	36	142 (3.94)	78 (2.17)	46 (1.28)
8	45	272 (6.04)	80 (1.78)	80 (1.78)

Table 1

Sizes of complete and fractionnal CCD.

This table shows that, in order to reduce the number of runs, small CCD can be very interesting for 3, 4, 6 and 7 factors. Moreover the cases 3 and 6 factors lead to saturated designs. See appendix A for more informations concerning these designs.

3.2 Structure of the moment matrix

We define in a first time some sets associated to every regular fraction of resolution III* obtained with k independant generators of lenght 3. The set E_3 contains all the triplets (i, j, k), with $i < j < k$, such that the word `ijk` is an element of G. The set E_2 contains all the pairs (i, j), with $i < j$, such that the interaction `ij` is aliased in G with one linear effect. The set E_1 contains all the simple values i such that the linear effect `i` is aliased in G with one interaction. Note that the k generators of the regular fraction are always disjoint (because if two elements of E_3 are not disjoint then the regular fraction cannot be of resolution III*). So:

$$card\,(E_3) = k \ , \ card\,(E_2) = k\binom{3}{2} = 3k \ , \ card\,(E_1) = k\binom{3}{1} = 3k.$$

Example. Using the previous example with $m = 6$ factors and the regular fraction generated by the relation $\mathbb{I}_{16} = \texttt{123} = \texttt{456}$ we have $k = 2$, $G = \{\mathbb{I}_{16}, \texttt{123}, \texttt{456}, \texttt{123456}\}$ and then:

$$E_3 = \{(1,2,3)\,,(4,5,6)\}\,,\ E_2 = \{(1,2)\,,(1,3)\,,(2,3)\,,(4,5)\,,(4,6)\,,(5,6)\}\,,\ E_1 = \{1,2,3,4,5,6\}\,.$$

Now for every small CCD the elements of the moment matrix are the same than these of the classical case, excepted for some non-zero moments $[ijk]$. In fact these moments are the k ones given by (denoting z_u the u-th row of D):

$$\forall\ (i,j,k) \in E_3\ ,\ [ijk] = \frac{1}{n}\sum_{u=1}^{n} z_{ui}z_{uj}z_{uk} = \frac{2^{m-k}}{n} = \frac{s_{22}}{n}.$$

Then the moment matrix of each small CCD has the following form (the block A was already given in (2)):

$$M = \frac{1}{n}{}^tXX = \frac{1}{n}diag\,(A, B^*) \text{ with } B^* = \begin{bmatrix} s_2 I_m & P^* \\ {}^tP^* & s_{22} I_{(m-1)m/2} \end{bmatrix}$$

with P^* an $m \times m\,(m-1)\,/2$ matrix containing only the two values 0 or s_{22}. More precisely if the i-th row of P^* is such that $i \notin E_1$ then it is a row of 0. If the i-th row of P^* is such that $i \in E_1$ then this row has only one non-zero value located in the column associated to the interaction aliased with `i`. So the matrix P^* is constituted by $3k$ non-zero elements (and also k non-zero rows). Since two generators of the regular fraction are disjoint note that if we remove every row and column of 0 in the matrix P^* we obtain the submatrix $s_{22}P$ with P a $3k \times 3k$ permutation matrix. More precisely P is then the alias matrix between linear and interaction effects. So it is always possible to rearrange the elements of β (and in parallel the columns of the matrix X) in the following order:

$${}^t\beta = \left(\beta_0, {}^t\beta_Q, {}^t\beta_L^{\text{na}}, {}^t\beta_I^{\text{na}}, {}^t\beta_L^{\text{a}}, {}^t\beta_I^{\text{a}}\right)$$

with $\beta_L^{\text{na}} \in \mathbb{R}^{m-3k}$ vector of the linear effects not aliased with an interaction effect, $\beta_I^{\text{na}} \in \mathbb{R}^{m(m-1)/2-3k}$ vector of the interaction effects not aliased with a linear effect, $\beta_L^{\text{a}} \in \mathbb{R}^{3k}$ vector of the linear effects aliased with an interaction effect and $\beta_I^{\text{a}} \in \mathbb{R}^{3k}$ vector of the interaction effects aliased with a linear effect. Using such order the moment matrix of each small CCD is then given by:

$$M = \frac{1}{n}{}^tXX = \frac{1}{n}diag\,(A, B_1, B_2) \text{ with} \tag{6}$$

$$B_1 = \begin{bmatrix} s_2 I_{m-3k} & 0 \\ 0 & s_{22} I_{(m-1)m/2-3k} \end{bmatrix} \text{ and } B_2 = \begin{bmatrix} s_2 I_{3k} & s_{22}P \\ s_{22}{}^tP & s_{22} I_{3k} \end{bmatrix}.$$

Example. For the small CCD for $m = 4$ factors generated by the relation $\mathbb{I}_8 =$ `124` we have $E_3 = \{(1,2,4)\}$, $E_2 = \{(1,2),(1,4),(2,4)\}$, $E_1 = \{1,2,4\}$ and then:

$${}^t\beta_L^{\text{na}} = \beta_3,\ {}^t\beta_I^{\text{na}} = (\beta_{13}, \beta_{23}, \beta_{34}),\ {}^t\beta_L^{\text{a}} = (\beta_1, \beta_2, \beta_4),\ {}^t\beta_I^{\text{a}} = (\beta_{12}, \beta_{14}, \beta_{24}).$$

Note also that the alias matrix P is given by (with its rows associated to, respectively, the linear effets `1`, `2` and `4` and its columns to the interaction effects `12`, `14` and `24`):

$$P = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix}.$$

3.3 Estimation of the model parameters

We consider in this section the resolution of the normal equations in order to find the least square estimators of the model (1). So we have to find $\hat{\beta}$ such that $({}^tXX)\,\hat{\beta} = {}^tXY$ and from relation (6), denoting $X = [\ \mathbb{I}_n \mid D_Q \mid D_L^{\rm na} \mid D_I^{\rm na} \mid D_L^{\rm a} \mid D_I^{\rm a}\ ]$, we obtain the three following results associated to the three blocks of M:

1) The estimators of general mean effect and quadratic effects satisfy:

$$\left[\begin{array}{cc} n & s_2\,{}^t\mathbb{I}_m \\ s_2\mathbb{I}_m & (s_4 - s_{22})\,I_m + s_{22}J_m \end{array}\right]\left(\begin{array}{c} \widehat{\beta}_0 \\ \widehat{\beta}_Q \end{array}\right) = \left(\begin{array}{c} {}^t\mathbb{I}_n Y \\ {}^tD_Q Y \end{array}\right).$$

So these estimators are exactly the same as in the case of a classical CCD (see 2.2 point 2) and their dispersions are also given in (3).

2) The estimators of linear and interaction effects $\beta_L^{\rm na}$ and $\beta_I^{\rm na}$ satisfy:

$$\left[\begin{array}{cc} s_2 I_{m-3k} & 0 \\ 0 & s_{22}I_{(m-1)m/2-3k} \end{array}\right]\left(\begin{array}{c} \widehat{\beta}_L^{\rm na} \\ \widehat{\beta}_I^{\rm na} \end{array}\right) = \left(\begin{array}{c} {}^tD_L^{\rm na}Y \\ {}^tD_I^{\rm na}Y \end{array}\right).$$

Again the situation for these estimators is similar to the case of a classical CCD and they are obtained by the very simple relations $\widehat{\beta}_L^{\rm na} = (1/s_2)\,{}^tD_L^{\rm na}Y$ and $\widehat{\beta}_I^{\rm na} = (1/s_{22})\,{}^tD_I^{\rm na}Y$. Their dispersions are also the same than the dispersions of parameters $\widehat{\beta}_i$ and $\widehat{\beta}_{ij}$ in (3).

3) The estimators of linear and interaction effects $\beta_L^{\rm a}$ and $\beta_I^{\rm a}$ satisfy:

$$\left[\begin{array}{cc} s_2 I_{3k} & s_{22}P \\ s_{22}\,{}^tP & s_{22}I_{3k} \end{array}\right]\left(\begin{array}{c} \widehat{\beta}_L^{\rm a} \\ \widehat{\beta}_I^{\rm a} \end{array}\right) = \left(\begin{array}{c} {}^tD_L^{\rm a}Y \\ {}^tD_I^{\rm a}Y \end{array}\right).$$

This situation is the only one that differs from the case of a classical CCD. But P is a permutation matrix, so $P^{-1} = {}^tP$ and we easily find that (if $s_2 \neq s_{22}$):

$$B_2^{-1} = \left[\begin{array}{cc} s_2 I_{3k} & s_{22}P \\ s_{22}\,{}^tP & s_{22}I_{3k} \end{array}\right]^{-1} = \frac{1}{s_2 - s_{22}}\left[\begin{array}{cc} I_{3k} & -P \\ -{}^tP & (s_2/s_{22})\,I_{3k} \end{array}\right]. \tag{7}$$

So these estimators are explicitely obtained by the following relations:

$$\widehat{\beta}_L^{\rm a} = \left(\frac{1}{s_2 - s_{22}}\right)\left({}^tD_L^{\rm a}Y - P^tD_I^{\rm a}Y\right) \text{ and } \widehat{\beta}_I^{\rm a} = \left(\frac{1}{s_2 - s_{22}}\right)\left(-P^tD_L^{\rm a}Y + \frac{s_2}{s_{22}}\,{}^tD_I^{\rm a}Y\right).$$

Finally note that the dispersion of each $\widehat{\beta}_i$ in $\widehat{\beta}_L^{\rm a}$ and each $\widehat{\beta}_{ii}$ in $\widehat{\beta}_I^{\rm a}$ is given by:

$$Var\left(\widehat{\beta}_i\right) = \frac{\sigma^2}{s_2 - s_{22}} \text{ and } Var\left(\widehat{\beta}_{ij}\right) = \frac{s_2}{s_{22}\,(s_2 - s_{22})}\sigma^2.$$

3.4 Predicted response

The predicted response in x is given by $\widehat{Y}(x) = {}^t g(x)\,\hat{\beta}$ with $g(x)$ regression vector such that ${}^t g(x) = {}^t\left(1, x_1^2, ..., x_m^2, x_1, ..., x_m, x_1x_2, ..., x_{m-1}x_m\right)$. The value of $\widehat{Y}(x)$ can be easily found in practice using the results of the previous section. Our purpose now is to find its dispersion, that is:

$$Var\widehat{Y}(x) = \sigma^2\ {}^t g(x)\left({}^t XX\right)^{-1} g(x).$$

Using the order proposed in section 3.2 for β (and the columns of X) we obtain from (6):

$$Var\widehat{Y}(x) = \sigma^2\left(Q_1(x) + Q_2(x) + Q_3(x)\right) \text{ with:}$$

1) Q_1 quadratic form associated to the block A of the moment matrix, so it is similar to the case of a classical CCD and (see, for example, Tinsson, 2010):

$$\begin{aligned} Q_1(x) = \quad & \left(\frac{1}{n} + \frac{ms_2^2}{n\phi}\right) + \frac{1}{s_4 - s_{22}}\left(1 + \frac{s_2^2 - ns_{22}}{\phi}\right)\sum_{i=1}^{m} x_i^4 \\ & + 2\frac{s_2^2 - ns_{22}}{(s_4 - s_{22})\,\phi}\sum\sum_{i<j} x_i^2 x_j^2 - 2\frac{s_2}{\phi}\sum_{i=1}^{m} x_i^2 \end{aligned}$$

denoting again $\phi = ns_4 + n(m-1)s_{22} - ms_2^2$.

2) Q_2 quadratic form associated to the block B_1 of the moment matrix, so (note that β_L^{na} contains all the β_i such that $i \notin E_1$ and β_I^{na} all the β_{ij} such that $(i,j) \notin E_2$):

$$Q_2(x) = \frac{1}{s_2}\sum_{i \in \overline{E}_1} x_i^2 + \frac{1}{s_{22}}\sum\sum_{(i,j) \in \overline{E}_2} x_i^2 x_j^2.$$

3) Q_3 quadratic form associated to the block B_2 of the moment matrix, so we obtain from (7):

$$Q_3(x) = \frac{1}{s_2 - s_{22}}\left(\sum_{i \in E_1} x_i^2 + \frac{s_2}{s_{22}}\sum\sum_{(i,j) \in E_2} x_i^2 x_j^2 - 6\sum\sum\sum_{(i,j,k) \in E_3} x_i x_j x_k\right).$$

Note that $(s_2 - s_{22})^{-1} = s_2^{-1} + s_{22}/\left(s_2(s_2 - s_{22})\right)$ so using this relation in Q_3 it is possible to regroup the terms in $\sum_{i=1}^{m} x_i^2 = r^2$ and $\sum\sum_{i<j} x_i^2 x_j^2$ in the following way:

$$\begin{aligned} Var\widehat{Y}(x) = \quad & \left(\frac{1}{n} + \frac{ms_2^2}{n\phi}\right) + \left(\frac{1}{s_2} - 2\frac{s_2}{\phi}\right) r^2 \\ & + \left(\frac{1}{s_{22}} + 2\frac{s_2^2 - ns_{22}}{(s_4 - s_{22})\,\phi}\right)\sum\sum_{i<j} x_i^2 x_j^2 + \frac{1}{s_4 - s_{22}}\left(1 + \frac{s_2^2 - ns_{22}}{\phi}\right)\sum_{i=1}^{m} x_i^4 \\ & + \frac{s_{22}}{s_2(s_2 - s_{22})}\sum_{i \in E_1} x_i^2 + \frac{1}{s_2 - s_{22}}\sum\sum_{(i,j) \in E_2} x_i^2 x_j^2 - \frac{6}{s_2 - s_{22}}\sum\sum\sum_{(i,j,k) \in E_3} x_i x_j x_k \end{aligned}$$

Note also that:

$$r^4 = \left(\sum_{i=1}^{m} x_i^2\right)^2 = \sum_{i=1}^{m} x_i^4 + 2\sum\sum_{i<j} x_i^2 x_j^2 \text{ and then:}$$

Proposition 1. *For every small CCD the* **variance of the predicted response** *is given by:*

$$Var\widehat{Y}(x) = \sigma^2 \left[f(r) + \left(\frac{1}{s_4 - s_{22}} - \frac{1}{2s_{22}}\right) \sum_{i=1}^{m} x_i^4 + \frac{s_{22}}{s_2 (s_2 - s_{22})} \sum_{i \in E_1} x_i^2 + \frac{1}{s_2 - s_{22}} \sum\sum_{(i,j) \in E_2} x_i^2 x_j^2 - \frac{6}{s_2 - s_{22}} \sum\sum\sum_{(i,j,k) \in E_3} x_i x_j x_k \right]$$

with $f(r) = \left(\frac{1}{n} + \frac{m s_2^2}{n\phi}\right) + \left(\frac{1}{s_2} - 2\frac{s_2}{\phi}\right) r^2 + \left(\frac{1}{2s_{22}} + \frac{s_2^2 - n s_{22}}{(s_4 - s_{22})\phi}\right) r^4$
and $\phi = n s_4 + n(m-1) s_{22} - m s_2^2$.

This result implies immediately that a small CCD **cannot be a rotatable design** (the three last sums cannot vanish).

3.5 Variance dispersion graphs

We extend in this section the explicit results (4) to the case of small CCD. First, from proposition 1 the spherical variance is given by:

$$V(r) = f(r) + \left(\frac{1}{s_4 - s_{22}} - \frac{1}{2s_{22}}\right) \sum_{i=1}^{m} \Psi^{-1} \int_{U_r} x_i^4 dx + \frac{s_{22}}{s_2 (s_2 - s_{22})} \sum_{i \in E_1} \Psi^{-1} \int_{U_r} x_i^2 dx + \frac{1}{s_2 - s_{22}} \sum\sum_{(i,j) \in E_2} \Psi^{-1} \int_{U_r} x_i^2 x_j^2 dx - \frac{6}{s_2 - s_{22}} \sum\sum\sum_{(i,j,k) \in E_3} \Psi^{-1} \int_{U_r} x_i x_j x_k dx$$

But the geometry of the sphere U_r implies that:

$$\forall\ (i,j,k) \in E_3\ ,\ \int_{U_r} x_i x_j x_k dx = 0.$$

The other terms of $V(r)$ are classical non-zero spherical moments given by (see, for example, Giovannitti-Jensen and Myers, 1989):

$$\Psi^{-1} \int_{U_r} x_i^2 dx = \frac{r^2}{m}\ ,\ \Psi^{-1} \int_{U_r} x_i^2 x_j^2 d = \frac{r^4}{m(m+2)}\ ,\ \Psi^{-1} \int_{U_r} x_i^4 dx = \frac{3r^4}{m(m+2)}.$$

But $card(E_2) = card(E_1) = 3k$ and then:

Proposition 2. *For every small CCD the* **spherical variance** *is given by:*

$$V(r) = f(r) + \frac{3k s_{22}}{m s_2 (s_2 - s_{22})} r^2 + \frac{3}{m+2} \left(\frac{1}{s_4 - s_{22}} - \frac{1}{2s_{22}} + \frac{k}{m(s_2 - s_{22})}\right) r^4.$$

Now extremal variances are also needed in order to obtain VDG. So we have to minimize and maximize $Var\widehat{Y}(x)$ on the sphere of radius r^2. This problem has solutions because $Var\widehat{Y}$ is a continuous function (see proposition 1) to be optimized on a compact set. In order to find these solutions the Lagrange multipliers theorem can be used considering:

$$L(x,\Lambda) = L(x_1,...,x_m,\Lambda) = Var\widehat{Y}(x) + \Lambda\left(\sum_{i=1}^{m} x_i^2 - r^2\right).$$

So every critical point is such that $\partial L(x,\Lambda)/\partial x_i = 0$ ($\forall\ i \in \{1,...,m\}$) and $\partial L(x,\Lambda)/\partial\Lambda = 0$. Using this result with $Var\widehat{Y}(x)$ given at proposition 1 implies that a necessary (but no sufficient) condition to reach the minimum or the maximum prediction variance is to satisfy (note also that $\{1,...,m\} = E_1 \cup \overline{E_1}$):

$$\text{C1)}\quad \forall\ i \in E_1\ ,\quad \left[\left(\frac{2}{s_4 - s_{22}} - \frac{1}{s_{22}}\right)x_i^2 + \Lambda + \frac{s_{22}}{s_2(s_2 - s_{22})} + \left(\frac{1}{s_2 - s_{22}}\sum_{j/(i,j)\in E_2} x_j^2\right)\right]x_i - \frac{3}{s_2 - s_{22}}\sum\sum_{(j,k)/(i,j,k)\in E_3} x_j x_k = 0$$

$$\text{C2)}\quad \forall\ i \in \overline{E_1}\ ,\quad \left[\left(\frac{2}{s_4 - s_{22}} - \frac{1}{s_{22}}\right)x_i^2 + \Lambda\right]x_i = 0$$

$$\text{C3)}\quad \sum_{i=1}^{m} x_i^2 - r^2 = 0$$

Spherical variances of small CCD and explicit expressions of critical points for $m = 3,4,6,7$ are given in appendix A.

A main practical problem is the choice of α (distance of the axial part from the origin). For a classical CCD α is often chosen in order to obtain the property of rotatability. For small CCD we have seen that it is impossible to have this property but we can try to minimise a measure of rotatability. A lot of such measures have been proposed in the literature (see, for example, the note of Ekman, 1994), we focus here on the area between the upper and lower curves of the VDG. In other words for a spherical domain of radius ρ and a small CCD obtain with the value α we consider the following measure of the rotatability:

$$Rot(\alpha) = \frac{1}{\rho}\int_0^{\rho} (Vmax(r) - Vmin(r))\,dr$$

Our goal is then to chose α in order to minimize the function Rot. Figure 1 shows the computed forms of these functions for $m = 3,4,6,7$ factors.

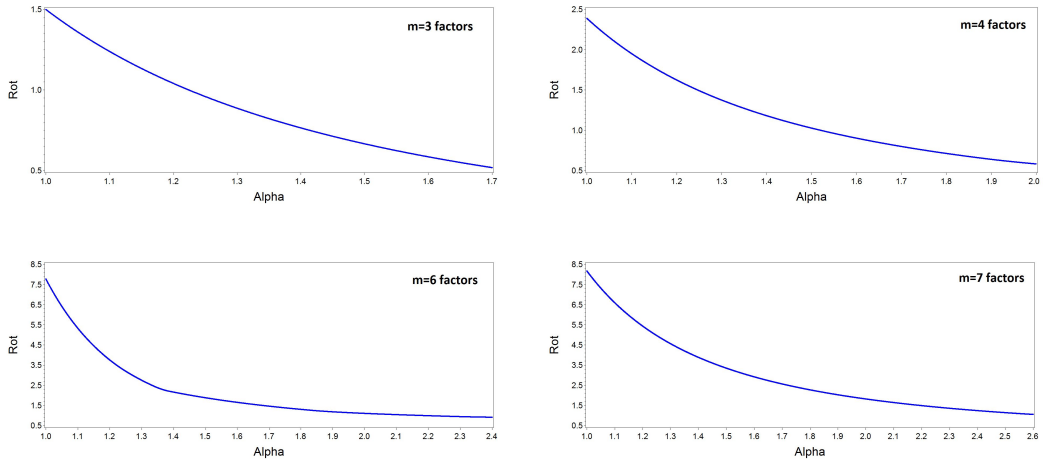

Figure 1

It is clear that the best choice, in order to reach a near-rotatability situation, is to take large values for α (like $\alpha = \sqrt{m}$ for putting the axial points at the boundaries of the spherical experimental domain).

3.6 Efficiency

We consider in this part the efficiency of small CCD using the classical criteria of D-efficiency. The main problem is to compare, for a fixed number of factors, the efficiency of a small CCD versus a classical CCD. First consider a classical CCD for m factors, in n_c runs, built with a regular fraction of resolution V with k_c independant generators, associated to the values $s_{2c} = 2^{m-k_c} + 2\alpha^2$, $s_{4c} = 2^{m-k_c} + 2\alpha^4$ and $s_{22c} = 2^{m-k_c}$. From (5) its D-efficiency is given by:

$$\Phi_{0c}(\alpha) = \left[\left(2\alpha^4\right)^{m-1} \left(2^{m-k_c} + 2\alpha^2\right)^m \left(2^{m-k_c}\right)^{m(m-1)/2} \phi_c(\alpha) \right]^{-1/p}.$$

with $\phi_c(\alpha) = n_c\left(2^{m-k_c} + 2\alpha^4\right) + n_c(m-1)\,2^{m-k_c} - m\left(2^{m-k_c} + 2\alpha^2\right)^2$.

Then consider a small CCD for m factors, resulting from a regular fraction of resolution III* with k independant generators, having n runs and associated to the values $s_2 = 2^{m-k} + 2\alpha^2$, $s_4 = 2^{m-k} + 2\alpha^4$ and $s_{22} = 2^{m-k}$. Its D-efficiency is $\Phi_0(\alpha) = |{}^tXX|^{-1/p}$ and its information matrix was given by relation (6), so:

$${}^tXX = \mathrm{diag}(A, B_1, B_2) \Rightarrow \Phi_0(\alpha) = \left(|A| \,.\, |B_1| \,.\, |B_2|\right)^{1/p}$$

The value of $|A|$ is the same than for a classical CCD (so $|A| = \left(2\alpha^4\right)^{m-1}\phi(\alpha)$), we have only

to évaluate the determinant of the two specific blocks of a small CCD, that is:

$$|B_1| = \begin{vmatrix} s_2 I_{m-3k} & 0 \\ 0 & s_{22} I_{(m-1)m/2-3k} \end{vmatrix} = s_2^{m-3k} s_{22}^{(m-1)m/2-3k}$$

and (using the notion of Schur complement):

$$|B_2| = \begin{vmatrix} s_2 I_{3k} & s_{22} P \\ {s_{22}}^t P & s_{22} I_{3k} \end{vmatrix} = |s_2 I_{3k}| \cdot \left| s_{22} I_{3k} - \frac{s_{22}^2}{s_2} {}^t P I_{3k} P \right| = |s_2 I_{3k}| \cdot \left| s_{22} I_{3k} - \frac{s_{22}^2}{s_2} I_{3k} \right|$$

because P is a permutation matrix (and then ${}^t PP = I_{3k}$). So:

$$|B_2| = |s_2 I_{3k}| \cdot \left| \left(s_{22} - \frac{s_{22}^2}{s_2} \right) I_{3k} \right| = s_2^{3k} s_{22}^{3k} \left(1 - \frac{s_{22}}{s_2} \right)^{3k}$$

In conclusion the D-efficiency of a small CCD is given by:

$$\Phi_0(\alpha) = \left[\left(2\alpha^4\right)^{m-1} \left(2^{m-k} + 2\alpha^2\right)^m \left(2^{m-k}\right)^{m(m-1)/2} \left(1 - \frac{2^{m-k}}{2^{m-k} + 2\alpha^2} \right)^{3k} \phi(\alpha) \right]^{1/p}$$

with $\phi(\alpha) = n\left(2^{m-k} + 2\alpha^4\right) + n(m-1)\, 2^{m-k} - m\left(2^{m-k} + 2\alpha^2\right)^2$. Note that the two efficiencies $\Phi_{0c}(\alpha)$ and $\Phi_0(\alpha)$ cannot be compared directly because the two designs do not have the same number of runs. It is then classical in this case to use the following efficiencies:

$$\psi_{0c}(\alpha) = \frac{\Phi_{0c}(\alpha)}{n_c} \text{ and } \psi_0(\alpha) = \frac{\Phi_0(\alpha)}{n}.$$

As explained by Lucas (1976) such value gives "*an indication of the information per point for the design*". Then it is possible to compute the relative D-efficiency of the small CCD (with respect to the classical CCD) with:

$$\text{Eff}(\alpha) = \frac{\psi_0(\alpha)}{\psi_{0c}(\alpha)} = \left(\frac{n_c}{n}\right) \frac{\Phi_0(\alpha)}{\Phi_{0c}(\alpha)}.$$

Finally we obtain the following explicit result:

Proposition 3. *The* **relative efficiency** *of each small CCD, with respect to the classical CCD, is given by:*

$$\text{Eff}(\alpha) = \left(\frac{n_c}{n}\right) \left[2^{m(m-1)(k_c-k)/2} \left(\frac{2^{m-k} + 2\alpha^2}{2^{m-k_c} + 2\alpha^2} \right)^m \left(1 - \frac{2^{m-k}}{2^{m-k} + 2\alpha^2} \right)^{3k} \left(\frac{\phi(\alpha)}{\phi_c(\alpha)} \right) \right]^{1/p}$$

with n number of runs for the small CCD, k number of generators for the small CCD and $\phi(\alpha) = n\left(2^{m-k} + 2\alpha^4\right) + n(m-1)\, 2^{m-k} - m\left(2^{m-k} + 2\alpha^2\right)^2$ (respectively n_c, k_c and $\phi_c(\alpha) = n_c\left(2^{m-k_c} + 2\alpha^4\right) + n_c(m-1)\, 2^{m-k_c} - m\left(2^{m-k_c} + 2\alpha^2\right)^2$ for the classical CCD).

Figure 2 shows these functions for $m = 3, 4, 6, 7$ factors.

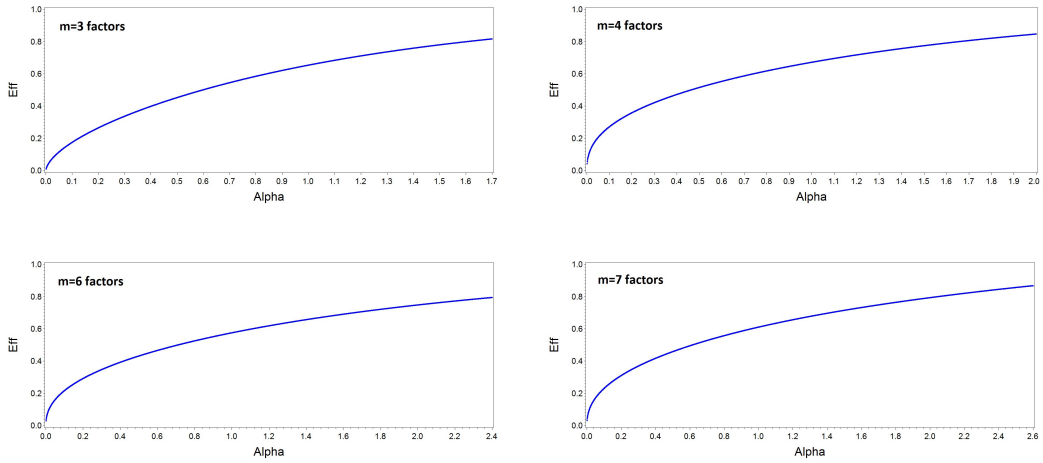

Figure 2

It is clear, another time, that the best choice, in order to improve the relative efficiency with respect to a classical CCD, is to take large values for α.

4 Conclusion

We have seen in this paper that a lot of explicit results can be extended to the class of small central composite designs. In particular no algorithmic methods are needed in order to obtain the D-efficiency of such design or a variance dispersion graph. Our main recommendation is to use **large values** for the parameter α (distance between the center and the axial points) in order to both maximize the D-efficiency of the design and minimize the value of the rotatability criterion derived from the variance dispersion graph (see section 3.5).

Note that in this paper small CCD have been only compared to classical CCD. No comparison have been made with other classical designs for surface response because small CCD are not in general the most efficient designs (classical CCD can be also more efficient like in section 3.6). But, in addition, small CCD may have some interesting properties. For example, if $m = 6$ factors are needed, the popular hybrid design $628A$ of Roquemore (1976) is at the same time saturated and rotatable. The small CCD is also saturated in this case, not rotatable, but it can be useful when a little number of levels are requested for the factors (the small CCD require a total of at most 5 distinct levels against 8 distinct levels for the hybrid design). For $m = 7$ factors the Box and Behnken (1960) design is rotatable. The small CCD does not satifsy this property but can be useful if expriments are very expensive because it needs only 46 runs against 57 for the Box and Behnken design.

Finally note also that small CCD are a very good option when a regular fraction of resolution III has been used in order to implement a first order model. If this model is not well fitted and a response surface model is needed then the choice of a small CCD is very pertinent if the budget in order to add new experiences is limited.

Appendix A. Constructions of small CCD and VDG.

1) For $m = 3$ factors, a small CCD can be obtained with the regular fraction given by $\mathbb{I}_4 = \mathtt{123}$. Such design has then $n = 10 + n_0$ runs (against $n = 14 + n_0$ for a classical CCD) and:

$$s_2 = 4 + 2\alpha^2,\ s_{22} = 4,\ s_4 = 4 + 2\alpha^4 \text{ so } \phi = (8 + 2n_0)\,\alpha^4 - 48\alpha^2 + (72 + 12n_0)$$

Furthermore, $k = 1$ and $E_1 = \{1, 2, 3\}$, $E_2 = \{(1, 2), (1, 3), (2, 3)\}$, $E_3 = \{(1, 2, 3)\}$. The spherical variance is then (see proposition 2):

$$V(r) = f(r) + \frac{s_{22}}{s_2(s_2 - s_{22})}r^2 + \frac{3}{5}\left(\frac{1}{s_4 - s_{22}} - \frac{1}{2s_{22}} + \frac{1}{3(s_2 - s_{22})}\right)r^4$$

The extremal variances can be computed using the following critical points (roots of the equations $C1$ and $C3$) such that:

$$\begin{array}{ll} (\pm a, 0, 0) & \text{with } a = r, \\ (\pm a, \pm a, \pm a) & \text{with } a = r/\sqrt{3}. \end{array}$$

2) For $m = 4$ factors, a small CCD can be obtained with the regular fraction given by $\mathbb{I}_8 = \mathtt{123}$. Such design has then $n = 16 + n_0$ runs (against $n = 24 + n_0$ for a classical CCD) and:

$$s_2 = 8 + 2\alpha^2,\ s_{22} = 8,\ s_4 = 8 + 2\alpha^4 \text{ so } \phi = (16 + 2n_0)\,\alpha^4 - 128\alpha^2 + (256 + 32n_0)$$

Furthermore, $k = 1$ and $E_1 = \{1, 2, 3\}$, $E_2 = \{(1, 2), (1, 3), (2, 3)\}$, $E_3 = \{(1, 2, 3)\}$. The spherical variance is then (see proposition 2):

$$V(r) = f(r) + \frac{3s_{22}}{4s_2(s_2 - s_{22})}r^2 + \frac{1}{2}\left(\frac{1}{s_4 - s_{22}} - \frac{1}{2s_{22}} + \frac{1}{4(s_2 - s_{22})}\right)r^4$$

The extremal variances can be computed using the following critical points (roots of the equations $C1$, $C2$ and $C3$) such that (denoting $\delta_1 = 2/(s_4 - s_{22}) - 1/s_{22}$, $\delta_2 = s_{22}/(s_2(s_2 - s_{22}))$, $\delta_3 = 1/(s_2 - s_{22})$ and $a^* = (3\delta_3 \pm \sqrt{9\delta_3^2 - 8(2\delta_1 + \delta_3)(\delta_2 - r^2\delta_1)})/4(2\delta_1 + \delta_3)$):

$$\begin{array}{ll} (\pm a, 0, 0, 0) & \text{with } a = r, \\ (\pm a, \pm a, \pm a, 0) & \text{with } a = r/\sqrt{3}, \\ (0, 0, 0, \pm b) & \text{with } b = r, \\ (\pm a, 0, 0, \pm b) & \text{with } a = \sqrt{r^2/2 - \delta_2/2\delta_1} \text{ and } b = \sqrt{r^2 - a^2}, \\ (\pm a, \pm a, \pm a, \pm b) & \text{with } a = a^* \text{ and } b = \sqrt{r^2 - 3a^2} \end{array}$$

Note that the two last solutions do not necessarily exist, expressions in the square roots must be positive.

3) For $m = 6$ factors, a small CCD can be obtained with the regular fraction given by $\mathbb{I}_{16} = \texttt{123} = \texttt{456}$. Such design has then $n = 28 + n_0$ runs (against $n = 44 + n_0$ for a classical CCD) and:

$$s_2 = 16 + 2\alpha^2,\ s_{22} = 16,\ s_4 = 16 + 2\alpha^4 \text{ so } \phi = (32 + 2n_0)\,\alpha^4 - 384\alpha^2 + (1152 + 96n_0)$$

Furthermore, $k = 2$ and $E_1 = \{1,2,3,4,5,6\}$, $E_2 = \{(1,2),(1,3),(2,3),(4,5),(4,6),(5,6)\}$, $E_3 = \{(1,2,3),(4,5,6)\}$. The spherical variance is then (see proposition 2):

$$V(r) = f(r) + \frac{s_{22}}{s_2(s_2 - s_{22})}r^2 + \frac{3}{8}\left(\frac{1}{s_4 - s_{22}} - \frac{1}{2s_{22}} + \frac{1}{3(s_2 - s_{22})}\right)r^4$$

The extremal variances can be computed using the following critical points (roots of the equations $C1$ and $C3$) such that:

$$\begin{array}{ll}
(\pm a, 0, 0, 0, 0, 0) & \text{with } a = r, \\
(\pm a, \pm a, \pm a, 0, 0, 0) & \text{with } a = r/\sqrt{3}, \\
(\pm a, 0, 0, \pm a, 0, 0) & \text{with } a = r/\sqrt{2}, \\
(\pm a, \pm a, \pm a, \pm a, \pm a, \pm a) & \text{with } a = r/\sqrt{6}.
\end{array}$$

4) For $m = 7$ factors, a small CCD can be obtained with the regular fraction given by $\mathbb{I}_{16} = \texttt{123} = \texttt{456}$. Such design has then $n = 46 + n_0$ runs (against $n = 78 + n_0$ for a classical CCD) and:

$$s_2 = 32 + 2\alpha^2,\ s_{22} = 32,\ s_4 = 32 + 2\alpha^4 \text{ so } \phi = (64 + 2n_0)\,\alpha^4 - 896\alpha^2 + (3136 + 224n_0)$$

Furthermore, $k = 2$ and $E_1 = \{1,2,3,4,5,6\}$, $E_2 = \{(1,2),(1,3),(2,3),(4,5),(4,6),(5,6)\}$, $E_3 = \{(1,2,3),(4,5,6)\}$. The spherical variance is then (see proposition 2):

$$V(r) = f(r) + \frac{6s_{22}}{7s_2(s_2 - s_{22})}r^2 + \frac{1}{3}\left(\frac{1}{s_4 - s_{22}} - \frac{1}{2s_{22}} + \frac{2}{7(s_2 - s_{22})}\right)r^4$$

The extremal variances can be computed using the following critical points (roots of the equations $C1$, $C2$ and $C3$) such that (denoting $\delta_1 = 2/(s_4 - s_{22}) - 1/s_{22}$, $\delta_2 = s_{22}/(s_2(s_2 - s_{22}))$, $\delta_3 = 1/(s_2 - s_{22})$ and $a^* = (3\delta_3 \pm \sqrt{9\delta_3^2 - 8(2\delta_1 + \delta_3)(\delta_2 - r^2\delta_1)})/4(2\delta_1 + \delta_3)$):

$$\begin{array}{ll}
(\pm a, 0, 0, 0, 0, 0, 0) & \text{with } a = r, \\
(\pm a, \pm a, \pm a, 0, 0, 0, 0) & \text{with } a = r/\sqrt{3}, \\
(\pm a, 0, 0, \pm a, 0, 0, 0) & \text{with } a = r/\sqrt{2}, \\
(\pm a, \pm a, \pm a, \pm a, \pm a, \pm a, 0) & \text{with } a = r/\sqrt{6}, \\
(0, 0, 0, 0, 0, 0, \pm b) & \text{with } b = r, \\
(\pm a, \pm a, \pm a, 0, 0, 0, \pm b) & \text{with } a = a^* \text{ and } b = \sqrt{r^2 - 3a^2}, \\
(\pm a, \pm a, \pm a, \pm a, \pm a, \pm a, \pm b) & \text{with } a = a^* \text{ and } b = \sqrt{r^2 - 6a^2}
\end{array}$$

Note that the two last solutions do not necessarily exist, expressions in the square roots must be positive.

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