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On Construction of Odd-fractional Factorial Designs

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Abstract: Fractional designs involve selection from a given set of experimental treatments as subset of treatments to make-up a specified design measure that has such statistical properties as balance, high relative efficiency, D-optimality etc. For decades statisticians have relied on the use Defining Contracts (DC), and Latin Squares (LS) to construct fractional factorial designs. But these methods are shown to have very limited range of applications and sometimes produce designs that are singular. This paper introduces the method of Concentric Balls (CB) for constructing non-singular fractional designs. Each ball consists of treatments that are of equal distance from the center and using a set of rules for selecting treatments from a ball the CB method yields a small set of admissible designs. The best member of this admissible set is the desired design:{Best in the sense of maximizing the determinant of the normalized information matrix or maximizing the relative efficiency of the factorial effects.}Numerical examples show that the CB method covers every range of experimental design conditions and can produce fractional designs that are D-optimal.

Keywords: Odd-fraction, concentric balls, relative efficiency

1 Introduction

Construction of fractional factorial designs is a topic that is extensively treated in most standard texts on design of experiments; see, e.g. Cochran and Cox (1957), Anderson and Mclean (1974). From n-independent, non-stochastic variables, where the *i*th variate, x_i appears at s_i-levels, we get $\tilde{N} = s_1 \times s_2 \times \ldots \times s_n$ treatments and consider three kinds of treatment spaces $\tilde{X}$:

i)The uniform or symmetric form; $\tilde{X}_s = \{x_1, x_2, \ldots, x_n;\ x_i = 1,2,\ldots,s_i, s_1 = s_2 = \ldots = s_n\}$,

ii)The non-uniform or asymmetric type; $\tilde{X}_A = \{x_1, \ldots, x_n; s_i \neq s_{i'}.\ for\ at\ least\ one\ pair\ of\ i, i'\}$

iii)The Irregular type; $\tilde{X}_R = [\tilde{X}_1 \oplus \tilde{X}_2;\ e.g. \tilde{X}_1 = \{x_1, x_2, \ldots, x_n; x_i = 1,2,\ldots,s_i\},$ $\tilde{X}_2 = \{x_1, x_2, \ldots, x_n;\ x_i = 1,2,\ldots,m_i\}, i = 1,2,\ldots,$ $n, s_i \neq m_i,$ is the number of levels of the *ith* variate in $\tilde{X}_2$].

Other geometric forms can also occur.eg. $\tilde{X} = \{x_1, x_2, \ldots, x_n; -1 < x_i < 1, i = 1,2,\ldots,n\}$ is a product of continuous intervals; however, the coverage of this report does not include continuous intervals.

As stated earlier, the problem of interest here is to construct an N-point design ($p \leq N < \tilde{N}$), i.e. an $\left(\frac{N}{\tilde{N}}\right) \times s_1 \times s_2 \times \ldots \times s_n$ fractional factorial design, p being the number of parameters in the response function $f(\underline{x})$. The fraction $\frac{N}{\tilde{N}}$ is considered an odd-fraction if N is not divisible by any s_i, otherwise it is a regular fraction.

For decades, the practice has been to construct fractional factorial designs using either Latin Squares (LS) or Defining Contrasts (DC); see, e.g. Anderson and Mclean. Two problems can arise from this approach:

a) The DC and LS methods are inapplicable, as in $\left(\frac{13}{27}\right) \times 3 \times 3 \times 3$.

b) The methods can produce singular or near singular designs as shown in table 3.3..., even when the relative efficiency of the design is considered good.

This paper introduces the Concentric Balls (CB) method of construction that has a wide range of applications and can produce an admissible set of equivalent designs, leaving the scientist to make a choice. The CB method proceeds as follows:

1) Arrange the $\tilde{N}$ support points into H groups or balls, so that support points that are of the same distance from the center are in one ball. Thus the *h*th ball, $\underline{g}_h = (\underline{x}_{h1}, \underline{x}_{h2}, \ldots, \underline{x}_{hn_h})'$ contains n_h support points, *h* = 1,2, . . ., H, $\underline{x}_{hk}$ is an *n*-component vector, k = 1,2, . . ., n_h,

where,

$$d_h = (\underline{x}'_{hk}\underline{x}_{hk})^{1/2} \text{ is the distance from the center, and } d_1 > d_2 > \ldots > d_H.$$

2) Partition $\underline{g}_h$ into sub-groups according to the number of negative signs and zeros appearing. at the support point $\underline{x}_{hk}$; see section three (3) of this paper.

3) Apply the selection rules; see section two (2) to build up the required design.

These rules yield a small set of admissible designs whose determinants and relative efficiencies can be easily compared.

Application of the idea of grouping of treatments towards construction of D-optimal exact designs have been employed by Onukogu and Iwundu (2007); and for D-optimals designs for 2-level factorial models and autoregressive error by Yeh and Huang(2005). Construction and analysis of fractional factorial designs on a wider platform has been considered by Gunst and Mason (2009).A range of techniques for construction of asymmetric fractional factorials as well as conditions for nonexistence of the designs have been given by Dey and Rahul (1999). A way has offered by Oludugba and Madukaife (2009) for segregating fractional factorial designs on the basis of their D-optimal and loss of information values.

As long as interest in a factorial experiment is restricted to a limited number of parameters (factorial effects) research in fractional designs will continue to flourish.

In what follows, the basic algebra for the CB technique is discussed in section two, while numerical illustrations are given in section three.

2. Algebraic Basis

The experimental space will be represented by the triple $\{\tilde{X}, F_x, \Sigma_x\}$; $\tilde{X} = \{x_1, x_2, \ldots, x_n; x_i = 1,2,\ldots s_i, i = 1,2,\ldots n\}$ is a continuous, compact, metric space of trials, $F_x = \{f(\underline{x}); \underline{x} \in \bar{X}\}$ is a set of continuous, differentiable functions. $\Sigma_x = \{\sigma(\underline{x}); \underline{x} \in \tilde{X}\}$ is a set of continuous, non-negative error functions. Each set of the triple is considered finite and together they form a basis for in-depth study of the subject of design of experiments; see, e.g. Pazman (1987), Atkinson and Donev (1992), Onukogu (1997).

Let $f(\underline{x})$ be a first-order interactive function defined by

2.1) $\underline{f}(\underline{x}) = X_t\underline{t} + X_b\underline{b} + e$

$X_t = (x_{ij})$ is an $N \times p$ extended design matrix; the *p* parameters comprising the linear and interactive terms, $p = \frac{1}{2}(n^2 + n + 2)$,

X_b is an $N \times b$ block incidence matrix; $X'_bX_b = diag\{k_1, k_2, \ldots, k_b\}$; k_j being the size of the *j*th block,

$\underline{t}$ is a *p*-parameter vector of treatment effects

$\underline{e}$ is an *N*-component vector of random error

The determinant of the information matrix in (2.1) equals,

2.2) $\left(\prod_{j=1}^{b} k_j\right)\det(X'_tX_t)\det(I - R);\ R = (X'_tX_t)^{-1}X'_tX_b(X'_bX_b)^{-1}X'_bX_t$

is the matrix of loss of information.

A geometric meaning of loss of information as $\cos^2(.)$ of the angle of inclination of a treatment effect on the blocks has been treated by Onukogu.

Now, for an N-point design in one block (b = 1),

$R = \underline{r}\underline{r}'$; $\underline{r}' = (r_1, r_2, \ldots, r_p)$; $0 \le r_i \le 1, i = 1, 2, \ldots, p.$; r_i is the loss of information on the ith treatment effect. Hence, the geometric mean,

2.3) $\bar{r}(\xi_N) = \left\{ \prod_{i=1}^{p} \left(1 - r_i^2\right) \right\}^{1/p}$

gives a measure of the overall efficiency of the design ξ_N relative to a complete block design. Notice that for $r_i \ne 0$, $\bar{r}(.)$ is maximized when the design is balanced; ie. when $r_1 = r_2 = \ldots = r_p$. But $\bar{r}(.)$ does not take into account the determinant, $\det(X_t' X_t)$, and therefore can take non-zero values for singular designs. But by including the determinant, we get the criterion for comparing designs:

2.4) $\bar{d}(\xi_N) = \bar{m}(\xi_N)\bar{r}(\xi_N)$;

$\bar{m}(\xi_N) = \det(X_t' X_t / N)$

To maximize (2.4) the following selection rules are to be applied when making-up the design measure ξ_N :

i) $\max\left(\sum_{i=1}^{N} x_{ij}^2\right)$ (ii) $\min\left(\sum_{i=1}^{N} x_{ij}\right)$ (iii) $\min\left(\sum_{i=1}^{N} x_{ij} x_{ij'}, \; j = 1, 2, \ldots, p, \; j < j'\right)$

We recall that $X_t = (x_{ij})$ is the extended treatment matrix.

Realising that the number of support points in $\underline{g}_1$ is $n_1 = 2^n \ge p = \frac{1}{2}(n^2 + n + 2)$;

then, for the response function (2.1),the optimal N-point design is constructed from $\underline{g}_1$ only. But, this is not the case for a complete quadratic function,

2.5) $f(\underline{x}) = a_{00} + \sum_{i=1}^{n} a_{0i} x_i + \sum_{i<i'} a_{ii'} x_i x_{i'} + \sum_{i=1}^{n} a_{ii} x_i^2 + e$

The starting point of the CB procedure is dependent on the relative values of N and p. When $N = p$, the procedure obtains the design as follows:

a) At the initial step take ($p - n - 1$) support points from $\underline{g}_1$ and the rest of ($N - p + n$ +1) from $\underline{g}_2, \underline{g}_3 \cdots$ by application the rules in (2.4) above. This yields a set of r admissible designs $S_A^{(0)} = \{\xi_{N(1)}, \xi_{N(2)}, \cdots \xi_{(N)(r)}\}$.

b) Compute $\bar{m}\left(\xi_N^{(0)}\right) = \max_i \bar{m}\left(\xi_{N(i)}\right); \xi_{N(i)} \in S_A^{(0)}$

c) At the k^{th} step take ($p + k - n - 1$) support points from $\underline{g}_1$ and the rest from $\underline{g}_2, \underline{g}_3 \ldots$ and compute $\bar{m}\left(\xi_{N(k)}^{(k)}\right) = \max_i \bar{m}\left(\xi_{N(i)}\right); \xi_{N(i)} \in S_A^{(k)}$

d) Stop, if $\bar{m}\left(\xi_N^{(k-1)}\right) \le \bar{m}\left(\xi_N^{(k)}\right) \ge \bar{m}\left(\xi_N^{(k+1)}\right)$

For $N >> p$, the above sequence can begin by taking p or p+1 points from $\underline{g}$. It seems that by properly relating the number of points to be taken from $\underline{g}_1$ to the ratio p/N, it should be possible to develop a non-iterative procedure for constructing optimal fractional factorial designs for quadratic response functions.

3. Numerical Examples

Given are trivariate first-order interactive response surface,

3.1) $f(x_1, x_2, x_3) = a_{00} + a_{10}x_1 + a_{20}x_1 + a_{30}x_3 + a_{12}x_1x_2 + a_{13}x_1x_3 + a_{23}x_2x_3 + e$

and a cubic surface, $\tilde{X}_1 = \{x_1, x_2, x_3; x_i = -1, 0, 1, i = 1, 2, 3\}$.

Using each of the three methods, we consider the construction of two fractional factorial designs:

a) $\left(\frac{9}{27}\right) \times 3 \times 3 \times 3$, for a regular fraction, and

b) $\left(\frac{11}{27}\right) \times 3 \times 3 \times 3$, for an odd-fraction.

The treatment table is given by

3.2 Table of Treatments For $x_1(-,0,+) \times x_2(-,0,+) \times x_3(-,0,+)$ cubic surface

−	−	−	−	0	−	−	+	−	0	−	−	o	o	−			
−	−	0	−	0	0	−	+	0	0	−	0	o	o	o			
−	−	+	−	0	+	−	+	+	0	−	+	o	o	+			

0	+	−	+	−	−	+	0	−	+	+	−
0	+	0	+	−	0	+	0	0	+	+	0
0	+	+	+	−	+	+	0	+	+	+	+

Using for instance $x_1x_2^2x_3$ as defining contrast; see, e.g. Anderson and Mclean, for details, the DC method produces the design

$$\xi_{9(DC)} = \begin{pmatrix} - & - & - \\ - & 0 & 0 \\ - & + & + \\ 0 & 0 & - \\ 0 & - & + \\ 0 & + & 0 \\ + & + & - \\ + & - & 0 \\ + & 0 & + \end{pmatrix}$$

, whereas the Latin square method gives

$$\xi_{9(LS)} = \begin{pmatrix} - & - & - \\ - & + & 0 \\ - & 0 & + \\ 0 & - & 0 \\ 0 & 0 & - \\ 0 & + & + \\ + & - & + \\ + & 0 & - \\ + & + & - \end{pmatrix}$$

The groups and subgroups required for the CB method are:

$$\underline{g}_1 = \left(\begin{array}{c|c} - - - & \underline{g}_{10} \\ \hline - - + & \\ - + - & \underline{g}_{11} \\ + - - & \\ \hline + + - & \\ + - + & \underline{g}_{12} \\ - + + & \\ \hline + + + & \underline{g}_{13} \end{array}\right) \quad \underline{g}_2 = \left(\begin{array}{c|c} - - 0 & \\ - 0 - & \underline{g}_{20} \\ 0 - - & \\ \hline - + 0 & \underline{g}_{21} \\ + - 0 & \\ \hline - 0 + & \underline{g}_{22} \\ + 0 - & \\ \hline 0 - + & \underline{g}_{23} \\ 0 + - & \\ \hline + + 0 & \\ + 0 + & \underline{g}_{24} \\ 0 + + & \end{array}\right) \quad \underline{g}_3 = \left(\begin{array}{c|c} 0\,0 - & \\ 0 - 0 & \underline{g}_{30} \\ - 0\,0 & \\ \hline 0\,0 + & \\ 0 + 0 & \underline{g}_{31} \\ + 0\,0 & \end{array}\right) \quad g_4 = (0 \quad 0 \quad 0)$$

Application of the rules under (2.4) gives two equivalent designs, $\xi^{(1)}_{9(CB)} = \begin{pmatrix} g_1 \\ g_{10} \end{pmatrix}$, $\xi^{(2)}_{9(CB)} = \begin{pmatrix} g_1 \\ g_{13} \end{pmatrix}$.

The determinants of these designs are reported in Table (3.3)

3.3 Determinants, Det(.) And Relative Efficiencies, RE(.) For Three Methods of Constructing Fractional Designs for First-Order Interactive Functions

Serial Number	Fractional Design	METHOD OF CONSTRUCTION					
		DC		LS		CB	
		Det(.)	RE(.)	Det(.)	RE(.)	Det(.)	RE(.)
1	$\left(\frac{9}{27}\right)\times 3\times 3\times 3$	3.51246 x E-05	0.98331	3.51246 x E-05	0.98331	41.4103 x E-02	0.99985
2	$\left(\frac{11}{27}\right)\times 3\times 3\times 3$	NA	NA	NA	NA	69.9511 x E-02	0.9988
3	$\left(\frac{14}{30}\right)\times 2\times 3\times 5$	NA	NA	31.3339 x E-02	1.0000	72.7571 x E-02	0.99875
4	$\left(\frac{17}{30}\right)\times 2\times 3\times 5$	NA	NA	NA	NA	92.35486 x E-02	0.9999

NA means Not Applicable.

Similarly, for the $\left(\frac{11}{27}\right)\times 3\times 3\times 3$ odd-fraction the CB method produces two equivalent designs:

$$\xi^{(1)}_{11(CB)} = \begin{pmatrix} \underline{g}_1 \\ \underline{g}_{11} \end{pmatrix}, \quad \xi^{(2)}_{11(CB)} = \begin{pmatrix} \underline{g}_1 \\ \underline{g}_{12} \end{pmatrix}$$

Both the DC and LS methods are inapplicable in this case of odd-fraction.

If the space of trials is non-uniform asymmetric tri-variate surface, $\widetilde{X}_2 = \{x_1, x_2, x_3; x_1(-,+)\times x_2(-,0,+)\times x_3(-2,-1,0,1,2)\}$,

We consider the construction of two designs:

c) $\left(\frac{14}{30}\right)\times 2\times 3\times 5$ for regular fraction, and

d) $\left(\frac{17}{30}\right)\times 2\times 3\times 5$ for odd-fraction.

Just as in table 3.2, a corresponding treatment table is set-up and since 14 is divisible by 2, the Latin-Square method can be applied.

i)The first step is to set-up a Partial Latin Square (PLS), *L* using the letters *a* and *b*.

ii) Next, superimpose *L* on the first batch of 15 treatments where $x_1 = -1$, and then on the other batch of 15 treatment at $x_1 = 1$,

$$L = \begin{pmatrix} a & b & a \\ b & a & b \\ a & b & a \\ b & a & b \\ a & b & a \end{pmatrix}$$

iii) Finally, the treatments that coincide with the letter *b* are grouped together to form the design:

$$\xi_{14(PLS)} = \begin{pmatrix} - & 0 & -2 \\ - & - & - \\ - & + & - \\ - & 0 & 0 \\ - & - & + \\ - & + & + \\ - & 0 & 2 \\ + & 0 & -2 \\ + & - & - \\ + & + & - \\ + & 0 & 0 \\ + & - & + \\ + & + & + \\ + & 0 & 2 \end{pmatrix}, \qquad \det(.) = 31.3339 \text{ x } E^{-02}$$

On the contrary the CB method produces an optimal designs;

$$\xi_{14(CB)} = \begin{pmatrix} - & - & -2 \\ - & + & -2 \\ + & - & -2 \\ - & - & -2 \\ + & + & -2 \\ + & - & 2 \\ - & + & 2 \\ + & + & 2 \\ - & + & -2 \\ + & - & -2 \\ - & - & 2 \\ + & + & -2 \\ + & - & 2 \\ - & + & 2 \end{pmatrix} \quad \text{with } \det(.) = 72.759 \text{ x } E^{-02}$$

The CB construction of $\begin{pmatrix} 17 \\ 30 \end{pmatrix} \times 2 \times 3 \times 5$ also gives two equivalent designs:

$$\xi^{(1)}_{17(CB)} = \begin{pmatrix} & \underline{g}_1 & \\ & \underline{g}_1 & \\ - & - & -2 \end{pmatrix} \text{ and } \xi^{(2)}_{17(CB)} = \begin{pmatrix} & \underline{g}_1 & \\ & \underline{g}_1 & \\ + & + & 2 \end{pmatrix} \quad \text{with } \det(.) = 92.35486 \text{ x } E^{-02};$$

$$\underline{g}_1 = \begin{pmatrix} - & - & -2 \\ - & + & -2 \\ + & - & -2 \\ - & - & 2 \\ + & - & 2 \\ - & + & 2 \\ + & + & -2 \\ + & + & 2 \end{pmatrix}$$

Notice that all the CB designs for the first-order interactive functions are constructed from the first ball for all values of N. This however is not the case for quadratic response function defined in (2.5).
Apparently, two concentric balls are required to construct a design for quadratic functions. For example, two equivalent designs are obtained by the CB method for a $\begin{pmatrix} 10 \\ 27 \end{pmatrix} \times 3 \times 3 \times 3$; namely,

$$\xi^{(1)}_{10(CB)} = \begin{pmatrix} \underline{g}_{10} \\ \underline{g}_{11} \\ \underline{g}_{12} \\ \underline{g}_{31} \end{pmatrix} \text{ and } \xi^{(2)}_{10(CB)} = \begin{pmatrix} \underline{g}_{11} \\ \underline{g}_{12} \\ \underline{g}_{13} \\ \underline{g}_{30} \end{pmatrix} \text{ with } \overline{m}(.) = 1.04588 \text{ x } E^{-04}.$$

Similarly, for the asymmetric surface, the CB method gives two equivalent optimal designs for

$$\begin{pmatrix} 10 \\ 30 \end{pmatrix} \times 2 \times 3 \times 5; \text{namely, } \xi^{(1)}_{10(CB)} = \begin{pmatrix} \underline{g}_1 \\ \underline{g}_{40} \end{pmatrix} \textit{ and } \xi^{(2)}_{10(CB)} = \begin{pmatrix} \underline{g}_1 \\ \underline{g}_{42} \end{pmatrix};$$

$$\underline{g}_{40} = \begin{pmatrix} - & - & 0 \\ - & 0 & - \end{pmatrix}, \quad \underline{g}_{42} = \begin{pmatrix} + & + & 0 \\ + & 0 & + \end{pmatrix}, \quad \underline{g}_1 \text{ is given above.}$$

Summary and Conclusion

The paper has shown that DC method can be used to construct fractional factorial designs only when the factor levels are uniform and even at this, the relative efficiency of this method is comparatively inferior. On the other hand, the Latin square method can be applied both for uniform and non-uniform levels provided only that the fraction is regular. Of the three methods it is only the CB method that can construct odd-fractional factorial designs; designs with the highest level of efficiency; designs that are required to be balanced in one replication as well as designs that are D-optimal.

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