D-Optimality For Designs With Different Numbers of Runs

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ABSTRACT

A per-run measure of D-optimality is given for designs with unequal numbers of runs. The measure is illustrated with examples. Although the number of runs may vary with the design, the parameter set should be similar and perhaps the same for all designs being considered. Some comments are made relative to this and illustrated with examples.

INTRODUCTION

Situations arise wherein an investigator desires to determine the relative merits of a group of treatment designs which have different numbers of runs. For example, several fractional replicates may be under consideration for a particular investigation. If one uses D-optimality, i.e., the determinant of X'X where X is the design matrix for a single-degree-of-freedom set of parameters, the design with the larger number, r, of runs, may turn out to have the larger value simply because there are more runs. In order to offset this and to take account of the number of runs it is suggested that the following *per-run D-optimality* measure could be used:

$$|X'X|/r = D_r \quad ,$$

where $|.|$ is the value of the determinant.

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The above measure may be criticized on the ground that it does not take into account the increase in every diagonal element of X'X when more runs are included. To take account of this, it is suggested that D-optimality for fractions with different numbers of runs be measured by

$$\left|\frac{1}{r} X'X\right| = D_{rm} .$$

This corresponds to using variances and covariances rather than sums of squares and cross products. Such a measure as this appears to overcompensate and hence is not used here.

Some examples illustrating these measures are presented below. Also, the selection of a relevant set of parameters as the estimable parameter set is a problem. It is noted that this set may vary from fraction to fraction.

EXAMPLE 1

Let design 1 be the fractional replicate for r = 9 runs obtained from a latin square of order 3. The design is:

Row	Column 0	Column 1	Column 2
0	0	1	2
1	2	0	1
2	1	2	0

→

Combinations ($\mathbf{Y}$)

0	0	0	0		1	2	2	0
0	1	2	1		2	0	2	2
0	2	1	2		2	1	1	0
1	0	1	1		2	2	0	1
1	1	0	2					

The corresponding contrast design matrix X, parameter vector $\boldsymbol{\beta}$ and observation vector $\mathbf{Y}$ is

$$X\boldsymbol{\beta} = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 0 & -2 & -1 & 1 & 0 & -2 \\ 1 & 1 & 1 & -1 & 1 & 0 & -2 & -1 & 1 \\ 1 & 0 & -2 & 1 & 1 & 0 & -2 & 0 & -2 \\ 1 & 0 & -2 & 0 & -2 & 1 & 1 & -1 & 1 \\ 1 & 0 & -2 & -1 & 1 & -1 & 1 & 1 & 1 \\ 1 & -1 & 1 & 1 & 1 & -1 & 1 & -1 & 1 \\ 1 & -1 & 1 & 0 & -2 & 0 & -2 & 1 & 1 \\ 1 & -1 & 1 & -1 & 1 & 1 & 1 & 0 & -2 \end{bmatrix} \begin{bmatrix} M \\ A_1 \\ A_2 \\ B_1 \\ B_2 \\ C_1 \\ C_2 \\ D_1 \\ D_1 \end{bmatrix} = E \begin{bmatrix} Y_{0000} \\ Y_{0121} \\ Y_{0212} \\ Y_{1011} \\ Y_{1102} \\ Y_{1220} \\ Y_{2022} \\ Y_{2110} \\ Y_{2201} \end{bmatrix} = E(Y) \quad ,$$

where E $[\cdot]$ denotes expectation.

The determinant of X'X is

$$|X'X| = \begin{bmatrix} 9 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 6 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 18 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 6 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 18 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 6 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 18 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 6 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 18 \end{bmatrix} = 9 \cdot 6^4 \cdot 18^4 = 1,224,440,064.$$

Since there were r = 9 runs,

$$D_9 = |X'X|/_9 = 9 \cdot 6^4 \cdot 18^4 \ /9 = 6^4 \cdot 18^4 .$$

The aliasing structure and degrees of freedom for the above fractional replicate is:

Effect	Degrees of Freedom
$M \approx AB^2C$	1
$A \approx BC^2 + ABC^2$	2
$B \approx AC + ABC$	2
$C \approx AB^2 + AB^2C^2$	2
$AB \approx AC^2 + BC$	2

where $\approx$ means confounded with and the effects are geometrical components (see e.g., Federer, 1955). The estimable parameter set is M, A_1, B_1, C_1, A_2, B_2, C_2 and contrasts among the levels of the geometrical component of interaction AB.

EXAMPLE 2

A competing design for three factors at three levels would be a response surface design with 4 center points and 2^3 corner points. $X\boldsymbol{\beta} = E(\mathbf{Y})$ would be

$$
\begin{bmatrix}
1 & 1 & 1 & 1 & -1 & 1 & -1 & -1 & -1 \\
1 & 1 & 1 & -1 & -1 & -1 & -1 & 1 & 1 \\
1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
1 & 1 & 1 & -1 & 1 & -1 & 1 & -1 & -1 \\
1 & -1 & 1 & 1 & -1 & -1 & 1 & -1 & 1 \\
1 & -1 & 1 & -1 & -1 & 1 & 1 & 1 & -1 \\
1 & -1 & 1 & 1 & 1 & -1 & -1 & 1 & -1 \\
1 & -1 & 1 & -1 & 1 & 1 & -1 & -1 & 1 \\
1 & 0 & -2 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & -2 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & -2 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & -2 & 0 & 0 & 0 & 0 & 0 & 0
\end{bmatrix}
\begin{bmatrix}
M \\ A_1 \\ A_2 \\ B_1 \\ C_1 \\ A_1B_1 \\ A_1C_1 \\ B_1C_1 \\ A_1B_1C_1
\end{bmatrix}
= E
\begin{bmatrix}
Y_{002} \\ Y_{022} \\ Y_{000} \\ Y_{020} \\ Y_{202} \\ Y_{222} \\ Y_{200} \\ Y_{220} \\ Y_{111} \\ Y_{111} \\ Y_{111} \\ Y_{111}
\end{bmatrix} .
$$

Note that the contrasts are different than for design 1 and that A_2, B_2, and C_2 are completely confounded with each other, which is the reason for omitting B_2 and C_2 in the parameter vector $\boldsymbol{\beta}$.

An estimable parameter set is M, A_1, A_2, B_1, C_1, A_1B_1, A_1C_1, B_1C_1, and $A_1B_1C_1$. The absolute value of the determinant of $X'X$ is:

$$
\begin{bmatrix}
12 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 8 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 24 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 8 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 8 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 8 & 0 & 0 & 0 \\
0 & 0 & 0 & 8 & 0 & 0 & 8 & 0 & 0 \\
0 & 0 & 0 & 0 & 8 & 0 & 0 & 8 & 0 \\
0 & 0 & 0 & 0 & 0 & 8 & 0 & 0 & 8
\end{bmatrix}
= 12(24)(8^7) = 603{,}979{,}776 .
$$

The aliasing structure in terms of the geometrical effects is rather complex. For the aliasing structure in terms of contrasts as given in $\boldsymbol{\beta}$ above, the aliasing structure may be obtained as follows. Let X_{27} be the contrast matrix for a 3^3 factorial. Partition X_{27} as

$$X_{27} = \begin{bmatrix} X_{9\times 9} & X_{9\times 18} \\ X_{18\times 9} & X_{18\times 8} \end{bmatrix}$$

where $X_{9\times 9}$ is the first nine rows of the above X matrix which is the design matrix for the vector of means for the nine distinct treatments. Then, $X_{9\times 9}\,\boldsymbol{\beta} + X_{9\times 18}\,\boldsymbol{\beta}_0 = E(\mathbf{Y})$ where $\boldsymbol{\beta}_0$ is the parameter vector for the remaining contrasts from a 3^3 factorial not included in $\boldsymbol{\beta}$ above. Then

$$\boldsymbol{\beta} + \left(X'_{9\times 9}X_{9\times 9}\right)^{-1}X'_{9\times 9}X_{9\times 18}\,\boldsymbol{\beta}_0 = \boldsymbol{\beta} + A\boldsymbol{\beta}_0 = \left(X'_{9\times 9}X_{9\times 9}\right)^{-1}X'_{9\times 9}E(\mathbf{Y}) \ ,$$

where A denotes the aliasing structure of other effects with those in $\boldsymbol{\beta}$.

EXAMPLE 3

Consider the design given in Table 8A.8 in Cochran and Cox (1957) for $k = 3$ factors A, B, and C. The contrast matrix X, the parameter set vector $\boldsymbol{\beta}$, and the vector of observations $\mathbf{Y}$ are:

$$X\boldsymbol{\beta} = \begin{bmatrix}
1 & -1 & -1 & -1 & 1 & 1 & 1 & -1 & c & c & c & c^2 \\
1 & 1 & -1 & -1 & -1 & -1 & 1 & 1 & c & c & c & c^2 \\
1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 & c & c & c & c^2 \\
1 & 1 & 1 & -1 & 1 & -1 & -1 & -1 & c & c & c & c^2 \\
1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 & c & c & c & c^2 \\
1 & 1 & -1 & 1 & -1 & 1 & -1 & -1 & c & c & c & c^2 \\
1 & -1 & 1 & 1 & -1 & -1 & 1 & -1 & c & c & c & c^2 \\
1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & c & c & c & c^2 \\
1 & a & 0 & 0 & 0 & 0 & 0 & 0 & e & d & d & de \\
1 & -a & 0 & 0 & 0 & 0 & 0 & 0 & e & d & d & d \\
1 & 0 & a & 0 & 0 & 0 & 0 & 0 & d & e & d & de \\
1 & 0 & -a & 0 & 0 & 0 & 0 & 0 & d & e & d & de \\
1 & 0 & 0 & a & 0 & 0 & 0 & 0 & d & d & e & d^2 \\
1 & 0 & 0 & -a & 0 & 0 & 0 & 0 & d & d & e & d^2 \\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & d & d & d & d^2 \\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & d & d & d & d^2 \\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & d & d & d & d^2 \\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & d & d & d & d^2 \\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & d & d & d & d^2 \\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & d & d & d & d^2
\end{bmatrix}
\begin{bmatrix} M \\ A_1 \\ B_1 \\ C_1 \\ A_1B_1 \\ A_1C_1 \\ B_1C_1 \\ A_1B_1C_1 \\ A_2 \\ B_2 \\ C_2 \\ A_2B_2 \end{bmatrix}
= E \begin{bmatrix} Y_{000} \\ Y_{200} \\ Y_{020} \\ Y_{220} \\ Y_{002} \\ Y_{202} \\ Y_{022} \\ Y_{222} \\ Y_{(a+1)11} \\ Y_{(-a+1)11} \\ Y_{1(a+1)1} \\ Y_{1(-a+1)1} \\ Y_{11(a+1)} \\ Y_{11(-a+1)} \\ Y_{111} \\ Y_{111} \\ Y_{111} \\ Y_{111} \\ Y_{111} \\ Y_{111} \end{bmatrix} .$$

Note that the mean of the last column needs to be subtracted from each element of that column to form a contrast set. In the above $a = 2^{.75} \cong .6818$, $c = .3172$, $d = -.6828$, $e = 2.1456$, $de = -1.4651$, $d^2 = .4663$, and $c^2 = .1006$.

The parameters A_2C_2, B_2C_2, and $A_2B_2C_2$ are not estimable parameters together with the above set. Since there are 15 distinct combinations, three additional parameters are estimable. These were not determined but could be if desired.

For the above,

$$|X'X| = \begin{bmatrix} 20 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & b & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & b & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & b & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 8 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 8 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 8 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 8 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & f & g & g & h \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & g & f & g & h \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & g & g & f & h \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & h & h & h & i \end{bmatrix} = 20b^3 8^4 \,(2.0850)(12.9321)(15.9997)(23.4126),$$

where $b = 8+2^{2.5} \cong 13.6569$, $f = 14.6743$, $g = -1.3254$, $h = -6.5781$, and $i = 10.4065$. The determinant of $X'X$ omitting $A_1B_1C_1$ and A_2B_2 is $20(13.6569)^3 8^3 (3{,}077.9006) = 2{,}608{,}292{,}814(3077.9006)$.

Since there are 15 distinct combinations, there are 15 parameters in $\boldsymbol{\beta}$. There are $r = 20$ runs. The sum of squares among the six responses Y_{111} provides an error for testing effects. A usual way for partitioning degrees of freedom among the 20 observations is:

Source of Variation	Degrees of Freedom
Total	20
Correction for mean	1
First order efects (A_1,B_1,C_1)	3
Second order effects (A_2,B_2,C_2,A_1B_1,A_1C_1,B_1C_1)	6
Lack of fit (remaining parameters)	5
Error	5

COMPARISON OF DESIGNS

Note that designs can be compared on the basis of the set of parameters in $\boldsymbol{\beta}$, the determinants of X'X, and/or other criteria (see e.g., Raktoe *et al.*, 1981, Chapter 5). The usual situation in regard to D-optimality is that $\boldsymbol{\beta}$ is implicitly assumed to be fixed and the same for all the designs in the class being compared. For response surface situations, the restrictions are not so rigid regarding $\boldsymbol{\beta}$. Here $\boldsymbol{\beta}$ may be partitioned into first order parameters, second order parameters, and lack of fit parameters. The first two are clearly defined but the last is not. Lack of fit parameters for the $\boldsymbol{\beta}$ in Example 1 are AB $\cong$ AC^2 $\cong$ BC while for Example 3, they are $A_1B_1C_1$, A_2B_2, and three other parameters. In Example 2, the lack of fit parameter is $A_1B_1C_1$ and the second order parameters are A_2, A_1B_1, A_1C_1, and B_1C_1; A_2 is completely confounded with B_2 and C_2 which may not be a problem if A_2,B_2 and C_2 all respond in the same direction.

Despite the above, an investigator might be interested in the design in Example 1 plus the fold-over fraction (see Raktoe and Federer, 1986), with r = 18 runs versus the design of Example 3 with r = 20 runs. Then for whatever set of parameters under consideration the X'X matrices are determined for each design. Then, to compare the relative efficiencies of the two designs, one takes the determinants of X'X for each design and divides by the number of runs; then, the ratio of these two values, i.e., D_{18}/D_{20} is one measure of the relative efficiencies of the two designs. A fold-over design for the design in Example 1 is:

Design of Example 1	Fold-Over Design
000	222
012	210
021	201
101	121
110	112
122	100
202	020
211	011
220	002

For the above 2/3rds fraction of a 3^3, the main effects are not confounded with two-factor interaction effects. For the parameter vector $\boldsymbol{\beta}' = [M, A_1, B_1, C_1, A_2, B_2, C_2, A_1B_1, A_1C_1, B_1C_1]$, the design matrix X is

$$\begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 0 & -2 & -1 & 1 & 0 & -1 & 0 \\ 1 & 1 & 1 & -1 & 1 & 0 & -2 & -1 & 0 & 0 \\ 1 & 0 & -2 & 1 & 1 & 0 & -2 & 0 & 0 & 0 \\ 1 & 0 & -2 & 0 & -2 & 1 & 1 & 0 & 0 & 0 \\ 1 & 0 & -2 & -1 & 1 & -1 & 1 & 0 & 0 & 1 \\ 1 & -1 & 1 & 1 & 1 & -1 & 1 & -1 & 1 & -1 \\ 1 & -1 & 1 & 0 & -2 & 0 & -2 & 0 & 0 & 0 \\ 1 & -1 & 1 & -1 & 1 & 1 & 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & -1 & 1 & -1 & 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & 0 & -2 & 1 & 1 & 0 & -1 & 0 \\ 1 & -1 & 1 & 1 & 1 & 0 & -2 & -1 & 0 & 0 \\ 1 & 0 & -2 & -1 & 1 & 0 & -2 & 0 & 0 & 0 \\ 1 & 0 & -2 & 0 & -2 & -1 & 1 & 0 & 0 & 0 \\ 1 & 0 & -2 & 1 & 1 & 1 & 1 & 0 & 0 & 1 \\ 1 & 1 & 1 & -1 & 1 & 1 & 1 & -1 & 1 & -1 \\ 1 & 1 & 1 & 0 & -2 & 0 & -2 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 1 & -1 & 1 & 1 & -1 & 1 \end{bmatrix} \begin{bmatrix} M \\ A_1 \\ A_2 \\ B_1 \\ B_1 \\ B_2 \\ C_1 \\ C_2 \\ A_1B_1 \\ A_1C_1 \\ B_1C_1 \end{bmatrix} = E \begin{bmatrix} Y_{000} \\ Y_{012} \\ Y_{021} \\ Y_{101} \\ Y_{110} \\ Y_{122} \\ Y_{202} \\ Y_{211} \\ Y_{220} \\ Y_{222} \\ Y_{210} \\ Y_{201} \\ Y_{121} \\ Y_{112} \\ Y_{100} \\ Y_{020} \\ Y_{011} \\ Y_{002} \end{bmatrix}$$

$$|X'X| = \begin{bmatrix} 18 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 \\ 0 & 12 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 \\ 0 & 0 & 36 & 0 & 0 & 0 & 0 & 0 & 0 & -4 \\ 0 & 0 & 0 & 12 & 0 & 0 & 0 & 0 & 0 & 2 \\ 0 & 0 & 0 & 0 & 36 & 0 & 0 & 0 & 6 & 2 \\ 0 & 0 & 0 & 0 & 0 & 12 & 0 & 0 & 0 & -2 \\ 0 & 0 & 0 & 0 & 0 & 0 & 36 & 6 & 0 & 2 \\ 0 & 0 & 0 & 0 & 0 & 0 & 6 & 8 & -2 & 4 \\ 0 & 0 & 0 & 0 & 6 & 0 & 0 & -2 & 8 & 0 \\ 2 & 2 & -4 & 2 & 2 & -2 & 2 & 4 & 0 & 8 \end{bmatrix} = 268{,}469{,}821{,}440 \ .$$

Then $D_{18}/D_{20} = (268{,}469{,}821{,}440/18)/(80{,}300{,}177{,}774.6/20) = 3.34(20/18) = 3.7$, indicating the design with 18 runs (denoted as Example 4) is nearly four times better using D-optimality as a criterion. Note that the parameter set for the two designs is the same.

Another way to compare the designs is as follows:

Source of variation	Degrees of freedom for Example 1	2	3	4
Total	9	12	20	18
Correction for mean	1	1	1	1
First order effects	3	3	3	3
Second order effects	3	4	6	6
Lack of fit terms	2	1	5	8
Error among duplicates	0	3	5	0

Note that some "lack of fit" effects may sometimes to be nonexistent and hence could be considered to be a measure of error variation.

LITERATURE CITED

Cochran, W. G. and G. M. Cox (1957). *Experimental Designs*, 2nd edition, John Wiley and Sons, Inc., New York.

Federer, W. T. (1955). *Experimental Design - Theory and Application*, Macmillan, New York (republished by Oxford and IBH Publishing Co., New Delhi, 1968 and 1974).

Raktoe, B. L. and W. T. Federer (1968). A unified approach for constructing a useful class of non-orthogonal main effect plans in k^n factorials, *J. Royal Statistical Soc., Series B*, **30**, 371-380

Raktoe, B. L., A. Hedayat, and W. T. Federer (1981). *Factorial Designs*, John Wiley and Sons, Inc., New York.