Austral. J. Statist., **31**(1), 1989, 111–117

COMPUTER AIDED-CONSTRUCTION OF D-OPTIMAL 2^m FRACTIONAL FACTORIAL DESIGNS OF RESOLUTION V

NAM-KY NGUYEN

Phillip Institute of Technology
*Plenty Rd, Bundoora 3083, Australia**

AND ALOKE DEY
Indian Agricultural Statistics Research Institute
Library Av, New Delhi 110012, India

Summary

A new exchange algorithm for construction of 2^m D-optimal fractional factorial design (FFD) is devised. This exchange algorithm is a modification of the one due to Fedorov (1969, 1972) and is an improvement over similar algorithm due to Mitchell (1974) and Galil & Kiefer (1980). This exchange algorithm is then used to construct 54 D-optimal 2^m-FFD's of resolution V for $m = 4, 5, 6$.

Key words: Fractional factorial design; D-optimality; A-optimality; exchange algorithm.

1. Introduction

A fractional factorial design (FFD) is said to be of resolution V if it permits estimation of the mean, all main effects and all two factor interactions, under the assumption that all interactions between three or more factors are negligible in magnitude. Thus, a total number of parameters to be estimated in a resolution V design for 2^m-FFD is $p = 1 + m + {}_mC_2$.

An orthogonal resolution V plan for a 2^m-FFD is equivalent to an orthogonal array OA$(n, m, 2, 4)$, i.e. an OA with n assemblies, m constraints, 2 symbols and strength 4 (cf. Rao (1947)). When such an OA is available, it provides an optimal resolution V design with respect to

---

* New address: Gas and Fuel Corporation of Victoria, Box 1841 Q, Melbourne 3001, Australia

D-, A-, E-optimality criteria. In fact, this design is universally optimal (Kiefer, 1980). However, an OA providing an optimal resolution V design exists only if $n = 0$ (mod 4), a condition which may not always be possible to satisfy in practice. Thus, the need for optimal resolution V design for other values of n arises.

Srivastava & Chopra (1971) have considered A-optimal resolution V designs for 2^m-FFD for $m = 4$, 5 and 6 for practical values of n in the class of balanced designs. These designs are balanced in the sense that the variance-covariance matrix V of the parameter estimates is invariant under the permutation of the m factors. However, the balanced designs form only a subclass of designs and one may like to study the optimality of designs in the entire class. Such a study has been partially made by Kuwada (1982) who constructed optimal resolution V design 2^m-FFD for $m = 4, 5$ and 6 with respect to A-optimal criterion. Some of these designs are in fact superior to the corresponding designs of Srivastava & Chopra who restricted their attention to balanced designs.

The purpose of this study is to devise a computer algorithm for the construction of D-optimal resolution V 2^m-FFD. This algorithm is then used actually to construct 54 D-optimal 2^m-FFD of resolution V for $m = 4$, 5 and 6.

2. Some Matrix Results

In this section, we give some results in matrix algebra, which will be used in the sequel.

Consider the usual full rank linear model $y = X\beta + e$ where y is an n-component column vector of observations, X is an $n \times p$ matrix of known elements, β is a $p \times 1$ vector of unknown parameters and e is a $p \times 1$ vector of random residual components with $E(e) = 0$ and $D(e) = \sigma^2 I$ where E stands for the expectation operator and D denotes the dispersion matrix. The n rows of X are n p-dimensional vectors x_i', $i = 1, 2, \ldots, n$. These n vectors can be considered as n points in R^p. Let $M = X'X$ and assume M to be non-singular.

If x' is a row vector to be augmented to X, we have:

$$\det(M + xx') = \det(M)(1 + x'M^{-1}x) \qquad (2.1)$$

$$(M + xx')^{-1} = M^{-1} + wuu' \qquad (2.2)$$

where $w = -(1 + x'M^{-1}x)^{-1}$ and $u = M^{-1}x$.

Now let $M_x = M + xx'$. If x_i' is a row vector to be removed from the current X, we have:

$$\det(M_x - x_i x_i') = \det(M_x)(1 - x_i' M_x^{-1} x_i) \tag{2.3}$$

$$(M_x - x_i x_i')^{-1} = M_x^{-1} + w_i u_i u_i' \tag{2.4}$$

where $w_i = (1 - x_i' M_x^{-1} x_i)^{-1}$ and $u_i = M_x^{-1} x_i$.

Now, let x' be a row vector augmented to X and x_i' be a row vector removed from X simultaneously, i.e. x_i' and x' are exchanged. Then we have:

$$\det(M + xx' - x_i x_i') = \det(M)\{1 + D(x_i, x)\} \tag{2.5}$$

where:

$$D(x_i, x) = x' M^{-1} x - x_i' M^{-1} x_i (1 + x' M^{-1} x) + (x' M^{-1} x_i)^2 \, . \tag{2.6}$$

3. Method of Construction

The model for 2^m-FFD of resolution V is the usual full rank linear model $y = X\beta + e$ as in Section 2. The ith row of design matrix X is a p-dimensional row vector x_i':

$$x_i' = (1, x_{1i}, x_{2i}, \ldots, x_{mi}, x_{1i}x_{2i}, \ldots, x_{m-1i}x_{mi})$$

where $x_{hi} = \pm 1$, $h = 1, 2, \ldots, m$ and $i = 1, 2, \ldots, n$.

The total number of candidate vectors x is 2^m. Our problem is that for a given n, we have to choose n vectors x's out of 2^m candidate vectors such that $\det(X'X)$ is maximized. Here, n is not necessarily $\leq 2^m$ and the x's are not necessarily distinct.

Let $M = X'X$. The proposed exchange algorithm (EA) for finding D-optimal 2^m-FFD of resolution V consists of the following steps:

(i) Start with a randomly chosen non-singular n-point design. Compute M, M^{-1} and $\det(M)$.

(ii) Find a vector x among 2^m candidate vectors such that $x'M^{-1}x$ is maximum. This $x'M^{-1}x$ is V_{max}/σ^2, where V_{max} is the maximum variance of the predicted response of the current n-point design.

(iii) Find a vector x_i among n vectors of the current n-point design such that $D(x_i, x)$ is maximum. $D(x_i, x)$ is calculated by (2.6).

(iv) If $D(x_i, x)$ is less than a chosen positive small number say 10^{-5}, then terminate. Otherwise exchange vector x_i with x. Update $\det(M)$ by (2.5) and M^{-1} by (2.2) and (2.4). Then return to step (ii).

TABLE 1

D-optimal 2^4-FFD of resolution V

n	$\|X'X\|$	V_{max}	tr V	tr V_k	tr V_s
11	3.86547E+10	2.55556	1.48611	–	1.4861
12	1.37439E+11	2.50000	1.31250	1.31250	1.3125
13	4.81036E+11	2.42857	1.14286	1.14286	1.2639
14	1.64927E+12	2.33333	0.97917	0.97917	1.1875
15	5.49756E+12	2.20000	0.82500	0.82500	0.8250
16	1.75922E+13	0.68750	0.68750	0.68750	0.6875
17	2.96868E+13	0.68519	0.66204	0.66204	0.6620
18	5.00278E+13	0.68269	0.63668	0.63668	0.6375
19	8.41814E+13	0.68000	0.61143	0.61143	0.6270
20	1.41425E+14	0.67708	0.58631	0.58631	0.5863
21	2.37181E+14	0.63975	0.56134	0.63908	0.5613
22*	3.89639E+14	0.65714	0.53780	0.63720	0.5384
23	6.45688E+14	0.65517	0.51365	0.63575	0.5136
24	1.06873E+15	0.58333	0.48958	0.63462	0.4896
25	1.69215E+15	0.57895	0.46930	0.63370	0.4693
26*	2.68006E+15	0.60256	0.44888	0.63294	0.4518
27	4.29497E+15	0.53600	0.42750	0.63230	0.4275
28	6.59707E+15	0.53333	0.41042	–	0.4104

* trace V is strictly less than either of trace V_k or trace V_s.

This EA, like Mitchell's DETMAX (1974) and Galil & Kiefer's modified DETMAX or MD (1980) is another version of Fedorov's EA (1969, 1972) (cf. St. John & Draper (1975)). One advantage of this EA over DETMAX and MD is that double precision is not required in the computation of $\det(M + xx' - x_i x_i')$ since the straightforward formula (2.5) is used. In DETMAX, for example $(M + xx')^{-1}$ has to be evaluated before the evaluation of $\det(M + xx' - x_i x_i')$. Another advantage of this EA over DETMAX and MD is that an array of length 2^m need not be maintained in the computer to store 2^m values of $x'M^{-1}x$.

Like all previous EA's, this new EA does not always guarantee D-optimality as it may get "trapped" in the local optimum. In order to get a good design for given m and n, several tries should be made, each try

TABLE 2

D-optimal 2^5-FFD of resolution V

n	$\|X'X\|$	V_{max}	tr V	tr V_k	tr V_s
16	1.84467E+19	1.00000	1.00000	1.00000	1.0000
17	3.68935E+19	1.00000	1.96875	0.96875	0.9687
18	7.37870E+19	1.00000	1.93750	0.93750	0.9398
19	1.47574E+20	1.00000	0.90625	0.90625	0.9296
20	2.95148E+20	1.00000	0.87500	0.87500	0.9194
21	5.90296E+20	1.00000	0.84375	0.84375	0.8437
22	1.18059E+21	1.00000	0.81250	0.94643	0.8125
23*	2.36118E+21	1.00000	0.78125	0.94531	0.7979
24*	4.72237E+21	1.00000	0.75000	0.94444	0.7881
25*	9.44473E+21	1.00000	0.71875	0.94375	0.7815
26	1.88895E+22	1.00000	0.68750	0.94318	0.6875
27	3.77789E+22	1.00000	0.65625	0.65625	0.6563
28	7.55579E+22	1.00000	0.62500	0.62500	0.6300
29	1.51116E+23	1.00000	0.59375	0.59375	0.6199
30	3.02231E+23	1.00000	0.56250	0.56250	0.5830
31	6.04463E+23	1.00000	0.53125	0.53125	0.5313
32	1.20893E+24	0.50000	0.50000	0.50000	0.5000

* trace V is strictly less than either of trace V_k or trace V_s.

with a different starting design. In this study, 10 tries are made for each design with given m and n.

4. Results and Discussion

The values of $\det(X'X)$ of 54 constructed D-optimal 2^m-FFD of resolution V for $m = 4, 5$ and 6 together with trace V where $V = (X'X)^{-1}$, V_{max}, trace V_k and trace V_s are given in Tables 1, 2 and 3. V_k and V_s stand for the variance-covariance matrix of the designs obtained by Kuwada and by Srivastava & Chopra. For these designs, it was found that trace V is always less than or equal to the lesser of trace V_k and trace V_s. All in all, there are 14 new designs having trace V strictly smaller than either of trace V_k or trace V_s. As expected, none of the obtained designs is balanced in the sense of Srivastava & Chopra.

TABLE 3

D-optimal 2^6-FFD of resolution V

n	$\|X'X\|$	V_{max}	tr V	tr V_k	tr V_s
22*	6.27415E+28	1.34667	1.15167	-	1.6249
23*	1.47233E+29	1.34259	1.11569	-	1.1241
24*	3.44908E+29	1.33816	1.07974	-	1.1145
25*	8.06451E+29	1.33333	0.04382	-	1.1100
26*	2.17607E+30	1.35111	0.00278	-	1.1012
27	5.64036E+30	1.70222	0.97542	1.36458	0.9754
28*	1.52415E+31	1.70175	0.92544	1.00000	0.9487
29*	4.11788E+31	1.70130	0.87541	0.91518	0.9371
30	1.21694E+32	2.33333	0.83333	0.83333	0.9279
31	4.05648E+32	2.20000	0.75625	0.75625	0.7562
32	1.29807E+33	0.68750	0.68750	0.68750	0.6875
33	2.19050E+33	0.68519	0.67477	0.67477	0.6747
34	3.69140E+33	0.68304	0.66209	0.66209	0.6633
35	6.21276E+33	0.68103	0.64945	0.64945	0.6582
36	1.04439E+34	0.67917	0.63686	0.63686	0.6532
37	1.75370E+34	0.67742	0.62430	0.62430	0.6245
38	3.17438E+34	0.67511	0.60877	0.61178	0.6087
39*	5.31744E+34	0.67326	0.59627	0.66163	0.5992
40*	8.89748E+34	0.67129	0.58381	0.66106	0.5939

* trace V is strictly less than either of trace V_k or trace V_s.

For m = 5 it takes about $\frac{1}{2}$ minutes per try on an IBM AT-compatible personal computer with an 80287 math coprocessor. For $m = 6$ it takes about $2\frac{1}{2}$ minutes per try and 10 tries may not be enough for a particular value of n. Out of 10 tries, the best design with respect to D-optimality criterion is chosen. However, for m = 6 and for some values of n, it is not always true that the chosen designs have smaller trace and smaller V_{max} than the rejected designs because the choice is based on D-optimality criterion.

In concluding, we may remark that although we have presented results for $m = 4$, 5 and 6 only, the algorithm can be used for any values of m, for any resolution and for any factorial. Of course, for higher values of m and greater number of levels, the computer time requirement will be greater.

A PASCAL program listing of about 200 statements for constructing the designs in this paper can be obtained from the first author.

Acknowledgements

The authors would like to thank a referee for valuable suggestions and comments.

References

FEDOROV, V.V. (1969). Theory of optimal experiments. Preprint No.7 LSM, Izd-vo Moscow State University, Moscow, USSR.

FEDOROV, V.V. (1972). *Theory of optimal experiments.* Translated and edited by W.J. Studden and E.M. Klimko. New York: Academic Press.

GALIL, Z. & KIEFER, J. (1980). Time and space-saving computer methods, related to Mitchell's DETMAX, for finding D-optimal designs. *Technometrics* **22**, 301–313.

KIEFER, J. (1980). Optimal design theory in relation to combination designs. *Ann. Discrete Math.* **6**, 225–241.

KUWADA, M. (1982). On some optimal fractional 2^m factorial designs of resolution V. *J. Statist. Plann. Inference* **7**, 39–48.

MITCHELL, T.J. (1974). An algorithm for the construction of "D-optimal" experimental designs. *Technometrics* **16**, 203–211.

RAO, C.R. (1947). Factorial experiments derivable from combinatorial arrangements of arrays. *J. Roy. Statist. Soc. Suppl.* **9**, 118–139.

ST. JOHN, R.C. & DRAPER, N.R. (1975). D-optimality for regression designs: a review. *Technometrics* **17**, 15–22.

SRIVASTAVA, J.N. & CHOPRA, D.V. (1971). Balanced optimal 2^m fractional factorial designs of resolution V, $m \leq 6$. *Technometrics* **13**, 257–269.

Received August 1987; revised September 1988