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FURTHER RESULTS ON A-OPTIMAL SECOND-ORDER DESIGNS OVER CUBIC REGIONS

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ABSTRACT. Designs are presented which are A-optimal over a cubic experimental region for estimating all, and also for estimating two subsets of the parameters in a second-order polynomial regression model. The subsets of interest correspond to coefficients of the pure quadratic terms and all the second-order terms, respectively. The performance of each optimal design relative to the other two is examined. Optimal central composite designs are also obtained for the three design situations. The efficiency of these and some integer designs requiring a practicable number of trials is investigated.

1. INTRODUCTION

Consider the standard linear regression model $y = f'(x)\theta + \epsilon$ where x is the control variable, θ is a vector of unknown parameters, $f'(x)$ is a vector of linearly independent functions on the design space $\mathcal{X}$ and ϵ is the zero-mean error with variance σ^2 independent of x. An experimental design ξ is a probability measure on $\mathcal{X}$. If N uncorrelated observations are taken according to ξ and ξ has mass $\xi(x_i) = n_i N^{-1}$ at $x_i, i = 1, \ldots, r$, then n_i observations are taken at x_i. The variance-covariance matrix of the least squares estimator $\hat{\theta}$ of θ is given by $cov(\hat{\theta}) = (\sigma^2/N)M^{-1}(\xi)$ where $M(\xi) = \int_{\mathcal{X}} f(x)f'(x)\xi(dx)$ is the information matrix of ξ. The design is usually chosen so as to minimize (or maximize) some scalar function of $M(\xi)$. Amongst the most widely discussed criteria are the D- and A- criteria. Under the first, the objective is to maximize $|M(\xi)|$ while under the latter, we wish to minimize $\text{tr}M^{-1}(\xi)$, i.e. minimize the average variance.

Sometimes, the parameter vector θ may be partitioned into two components as $\theta' = (\theta_1', \theta_2')$ so that the experimenter is primarily interested in one treating the other as a vector of parameters of secondary interest. If $f'(x) = (f_1'(x), f_2'(x))$ is the corresponding partitioning of the regression functions, then the information matrix may be expressed as

$$M(\xi) = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix}$$

where $M_{ij}(\xi) = \int_{\mathcal{X}} f_i(x) f_j'(x) \xi(dx)$. If interest is in only θ_i then the appropriate information matrix is $M_{i.j}(\xi) = M_{ii} - M_{ij} M_{jj}^{-1} M_{ji}$. A design optimal in terms of $M(\xi)$ is not necessarily so in terms of $M_{i.j}(\xi)$ and vice versa.

In what follows, we shall consider second-order designs for regression over cubic regions. Note that a design is said to be of order d if it allows estimation of all the parameters in a polynomial model of degree d. A large volume of statistical literature on response surface designs is devoted to derivation of optimal designs for low order polynomial models. In particular, second-order D-optimal designs for cubic regions were first studied by Kôno (1962) but were more accessibly given by Nalimov, Golikova and Mikeshina (1970). Galil and Kiefer (1977b) carried out an extensive study of D-, A- and E-optimal second-order designs over cubic regions. Their derivation of A-optimal designs involved solving numerically a pair of sixth degree equations in two variables. An alternative derivation was provided in Huda (1990) which involved minimization of a convex univariate function. Atkinson (1973) using the D-criterion studied designs that were optimal for coefficients of all, pure quadratic, and second-order terms respectively. It is to be noted that the designs for second-order terms in the second-order model are useful for detecting departures from the simple first-order model. Similarly, the designs for pure quadratic terms are intended for detecting departures from the first-order model with interactions. In the present paper, we consider these designs under the A-optimality criterion. Only symmetric designs are considered since it is known (Kiefer, 1960) that for polynomial regression models over symmetric regions, under most criteria including A-optimality, there exist optimal designs which are symmetric. For a symmetric second-order design ξ, $M(\xi)$ has only three non-zero elements which are $\alpha_2 = \int_{\mathcal{X}} x_i^2 \xi(dx)$, $\alpha_4 = \int_{\mathcal{X}} x_i^4 \xi(dx)$ and $\alpha_{22} = \int_{\mathcal{X}} x_i^2 x_j^2 \xi(dx)$ $(i \neq j = 1, \ldots, k)$. Since $\mathcal{X} = \{x : |x_i| \leq 1\}$, these design moments satisfy the constraints $0 \leq \alpha_{22} \leq \alpha_4 \leq \alpha_2 \leq 1$ and further, non-singularity of $M(\xi)$ requires $\alpha_4 > \alpha_{22}$ and $\alpha_4 + (k-1)\alpha_{22} > k\alpha_2^2$.

The referee has correctly pointed out that the A-optimality criterion, contrary to the D-optimality criterion, is not invariant under linear transformations. Likewise, E-optimality criterion also suffers from this lack of invariance property which may be considered a serious drawback in certain situations. However, results of Section 6 in Galil and Kiefer (1977a) for quadratic regression on hyperspheres seem to suggest that the transformations of an A-optimal design for the standard/unit region $\mathcal{X}$ when inplemented in a transformed region $\mathcal{X}'$ may not perform too badly except when $\mathcal{X}'$ is very large compared to $\mathcal{X}$. Further, their study showed that A-optimality may be superior to E-optimality in this regard.

As the referee suggested, it would be interesting to consider the performance of optimal designs for one criterion under another criterion. In particular, we could compare the designs of Atkinson (1973) with those to be derived here. However, in their study of the performance of optimal designs under variation of criterion, Galil and Kiefer (1977b) observed that for quadratic regression on hypercubes the A-optimal designs are fairly robust in their efficiencies under variation of criterion. We feel that further investigation along this line is redundant and therefore not pursued here.

2. A-OPTIMAL DESIGNS

Under A-optimality criterion, the objective is to minimize the average variance of the least squares estimators of the parameters of interest. Since we are only dealing with non-singular designs, the objective function reduces simply to the sum of the appropriate diagonal elements of $M^{-1}(\xi)$. Thus if the experimenter is primarily interested in the coefficients of the pure quadratic terms in a second-order model, under A-optimality criterion the appropriate objective function is readily seen to be

$$(0.1)\quad \begin{aligned} V_1(\xi) &= V_1(\alpha_2, \alpha_{22}, \alpha_4) \\ &= (k-1)/(\alpha_4 - \alpha_{22}) + 1/\{\alpha_4 + (k-1)\alpha_{22} - k\alpha_2^2\} \end{aligned}$$

which should be minimized with respect to α_2, α_{22} and α_4 subject to the constraints described above.

If interest is only in the coefficients of second-order terms, the objective function is

$$(0.2)\quad V_2(\xi) = V_2(\alpha_2, \alpha_{22}, \alpha_4) = V_1(\alpha_2, \alpha_{22}, \alpha_4) + k(k-1)/(2\alpha_{22})$$

and when interest is in all the parameters of the model the objective function is $\text{tr}M^{-1}(\xi)$ which may be written as

$$(0.3)\quad \begin{aligned} V_3(\xi) &= V_3(\alpha_2, \alpha_{22}, \alpha_4) = V_2(\alpha_2, \alpha_{22}, \alpha_4) + k/\alpha_2 + \\ & \{\alpha_4 + (k-1)\alpha_{22}\}/\{\alpha_4 + (k-1)\alpha_{22} - k\alpha_2^2\}. \end{aligned}$$

Let ξ_i denote the design minimizing $V_i(\xi)$ $(i = 1, 2, 3)$. Clearly, $V_i(\alpha_2, \alpha_{22}, \alpha_4)$ $(i = 1, 2, 3)$ are all strictly decreasing in α_4 so that the optimal designs should have $\alpha_4 = \alpha_2$ whence the objective functions in (1), (2), (3) reduce to

$$(0.4)\quad \begin{aligned} V_1(\alpha_2, \alpha_{22}) &= (k-1)/(\alpha_2 - \alpha_{22}) + 1/\{\alpha_2 + (k-1)\alpha_{22} - k\alpha_2^2\}, \\ V_2(\alpha_2, \alpha_{22}) &= V_1(\alpha_2, \alpha_{22}) + k(k-1)/(2\alpha_{22}), \\ V_3(\alpha_2, \alpha_{22}) &= V_2(\alpha_2, \alpha_{22}) + 1/\{\alpha_2 + (k-1)\alpha_{22} - k\alpha_2^2\}. \end{aligned}$$

Since $\alpha_4 = \alpha_2$, the optimal designs are supported only at points with coordinates 0 or ± 1.

From (4), $V_1(\alpha_2, \alpha_{22})$ can be easily minimized algebraically. Partial differentiation shows that for any given α_2, V_1 is minimized with respect to α_{22} when $\alpha_{22} = \alpha_2^2$ and substitution of $\alpha_{22} = \alpha_2^2$ reduces $V_1(\alpha_2, \alpha_{22})$ to $V_1(\alpha_2) = k/(\alpha_2 - \alpha_2^2)$ which is a minimum when $\alpha_2 = 1/2$. Thus the design ξ_1 minimizing V_1 has $\alpha_4 = \alpha_2 = 1/2$, $\alpha_{22} = 1/4$ and $V_1 = 4k$, $V_2 = 2k(k+1)$ $V_3 = 2k^2 + 5k + 1$. Minimization of $V_2(\alpha_2, \alpha_{22})$ and $V_3(\alpha_2, \alpha_{22})$ are more difficult and need numerical methods. Changing variables from

(α_2, α_{22}) to (t, β) by substituting $\alpha_{22} = t\alpha_2$, $\beta = \alpha_2 k/\{1 + (k-1)t\}$ in (4) we may write

$$(0.5) \qquad \begin{aligned} V_2(\alpha_2, \alpha_{22}) &= V_2^*(t, \beta) = A(t)/\beta + B(t)/(1-\beta), \\ V_3(\alpha_2, \alpha_{22}) &= V_3^*(t, \beta) = C(t)/\beta + D(t)/(1-\beta), \end{aligned}$$

where

$$\begin{aligned} A(t) &= [1 + (k-1)\{1 + (k-1)t\}\{k/t + 1/(1-t)\}]k/\{1 + (k-1)t\}^2, \\ B(t) &= k/\{1 + (k-1)t\}^2, \qquad C(t) = A(t) + k^2/\{1 + (k-1)t\}, \\ D(t) &= B(t) + 1, \end{aligned}$$

and minimize V_2^*, V_3^* with respect to t and β subject to $0 \le t \le 1$ and $0 \le \beta \le k/\{1 + (k-1)t\}$. Now from (5) it is obvious that for any given $t \in (0,1)$, V_2^* and V_3^* are minimized with respect to β when $\beta = \sqrt{A(t)}/\{\sqrt{A(t)} + \sqrt{B(t)}\}$ and $\beta = \sqrt{C(t)}/\{\sqrt{C(t)} + \sqrt{D(t)}\}$, respectively. Substituting these values of β reduce the objective functions to $V_2^*(t) = \{\sqrt{A(t)} + \sqrt{B(t)}\}^2$ and $V_3^*(t) = \{\sqrt{C(t)} + \sqrt{D(t)}\}^2$ which can now be easily minimized with respect to the single variable t. The values of α_2 and α_{22} for the optimal designs ξ_2 and ξ_3 obtained by the method described above along with the values of V_1, V_2 and V_3 for these designs are displayed in Tables 1 and 2 which follow.

Table 1. A-optimal design for parameters of the second-order terms

k	t	α_2	α_{22}	$V_1(\alpha_2, \alpha_{22})$	$V_2(\alpha_2, \alpha_{22})$	$V_3(\alpha_2, \alpha_{22})$
2	0.6443	0.6091	0.3925	8.47	11.02	18.16
3	0.6827	0.6598	0.4505	13.48	20.14	30.81
4	0.7086	0.6918	0.4902	18.91	31.15	45.66
5	0.7279	0.7148	0.5203	24.71	43.93	62.52
6	0.7432	0.7326	0.5444	30.84	58.39	81.29
7	0.7558	0.7469	0.5645	37.26	74.46	101.89
8	0.7664	0.7588	0.5815	43.97	92.12	124.26
9	0.7756	0.7689	0.5964	50.93	111.30	148.34
10	0.7836	0.7777	0.6094	58.15	131.99	174.10

Table 2. A-optimal design for all the parameters

k	t	α_2	α_{22}	$V_1(\alpha_2, \alpha_{22})$	$V_2(\alpha_2, \alpha_{22})$	$V_3(\alpha_2, \alpha_{22})$
2	0.6579	0.5714	0.3759	8.51	11.17	17.89
3	0.6915	0.6148	0.4251	13.56	20.62	29.83
4	0.7153	0.6457	0.4619	19.07	32.06	43.84
5	0.7335	0.6695	0.4911	24.97	45.33	59.50
6	0.7481	0.6886	0.5152	31.22	60.33	76.83
7	0.7600	0.7044	0.5353	37.74	76.97	95.75
8	0.7702	0.7179	0.5529	44.57	95.22	116.22
9	0.7790	0.7296	0.5683	51.66	115.01	138.22
10	0.7868	0.7399	0.5821	59.02	136.32	161.70

The A-optimal designs obtained above put all their masses on points having coordinates 0 and ± 1 only since $\alpha_2 = \alpha_4$. Let S_j denote the set of points with j coordinates equal to ± 1 and the remaining $k - j$ coordinates equal to zero. We can always find optimal designs with mass $w_j / \binom{k}{j} 2^j$ at each point of S_j $(j = 0, 1, \ldots, k)$ by solving the equation $\sum_{j=0}^{k} w_j = 1$, $\sum_{j=0}^{k} w_j j/k = \alpha_2$ and $\sum_{j=0}^{k} w_j j(j-1)/k(k-1) = \alpha_{22}$, subject to the constraints $w_j \geq 0$ $(j = 0, 1, \ldots, k)$. In Tables 3,4 and 5 which follow we present some solutions, one for each k, which have only three non-zero w_j's.

Table 3. Selected A-optimal design ξ_1

k	w_0	w_1	w_2	w_3	w_4	w_5	w_6	w_7	w_8	w_9	w_{10}
2	.2500	.5000	.2500								
3		.7500		.2500							
4	.1250		.7500		.1250						
5		.3125		.6250		.0625					
6		.2501		.2497	.5002						
7		.1944			.7778			.0278			
8				.4001	.4999				.1000		
9					.8986	.0016				.0998	
10					.4170	.4996					.0834

Table 4. Selected A-optimal design ξ_2

k	w_0	w_1	w_2	w_3	w_4	w_5	w_6	w_7	w_8	w_9	w_{10}
2	.1763	.4328	.3909								
3	.1320		.6263	.2417							
4	.0931			.8910	.0159						
5			.1328	.5145		.3527					
6			.1941		.0218	.7841					
7		.0768				.4096	.5136				
8					.3707		.0433	.5860			
9	.0354							.8924		.0722	
10		.0440							.9709	.0851	

Table 5. Selected A-optimal design ξ_3

k	w_0	w_1	w_2	w_3	w_4	w_5	w_6	w_7	w_8	w_9	w_{10}
2	.2172	.3914	.3914								
3	.1968		.5698	.2334							
4	.1719		.2894	.5387							
5			.4944		.5035	.0021					
6			.2513		.0001	.7486					
7		.1557				.2846	.5597				
8		.1560	.0001				.8439				
9					.2645	.0001		.7354			
10		.0964	.0031					.9005			

The efficiency of a design ξ relative to the optimal design ξ_i is simply the ratio of the variances $V_i(\xi_i)/V_i(\xi)$ and it indicates how good ξ is in estimating the parameter set for which ξ_i is A-optimal. In what follows we denote $V_j(\xi_j)/V_j(\xi_i)$ by E_{ij}. Thus E_{ij} is to stand for efficiency of design ξ_i relative to ξ_j in estimating the parameter set for which ξ_j is optimal $(i \neq j = 1, 2, 3)$. Since these designs are intended for detecting departures from simpler models we also compare them with the A-optimal first-order designs. For this, following Atkinson (1972) we use the ratio of the sum of the variances of the estimated coefficients of the linear terms when only a first-order model is fitted. In what follows, we let E_i denote this efficiency of ξ_i, $(i = 1, 2, 3)$. The efficiencies E_i, E_{ij} $(i \neq j = 1, 2, 3)$ are all displayed in Table 6 which follows. The efficiencies correspondig to $k = \infty$ are indicative of what would happen if the number of variables is very large.

Table 6. Efficiencies (in %) of the A-optimal designs

k	2	3	4	5	6	7	8	9	10	∞
E_1	50.00	50.00	50.00	50.00	50.00	50.00	50.00	50.00	50.00	50.00
E_{12}	91.81	83.91	77.87	73.22	69.51	66.48	63.97	61.83	59.99	25.00
E_{13}	95.57	90.62	86.15	82.26	78.92	76.04	73.53	71.32	69.36	25.00
E_2	60.91	65.98	69.18	71.48	73.26	74.69	75.88	76.89	77.78	100.00
E_{21}	94.46	89.02	84.61	80.94	77.82	75.15	72.78	70.68	68.79	00.00
E_{23}	98.53	96.83	96.02	95.18	94.51	93.97	93.53	93.17	92.87	100.00
E_3	57.14	61.48	64.57	66.95	68.86	70.44	71.79	72.96	73.99	100.00
E_{31}	93.97	88.47	83.89	80.10	76.88	74.19	71.79	69.69	67.78	00.00
E_{32}	98.60	97.67	97.16	96.91	96.78	96.74	96.75	96.78	96.82	100.00

3. CENTRAL COMPOSITE DESIGNS

A class of designs which is widely used and may require relatively fewer trials to implement is the class of central composite designs (CCDs). In the notation of previous section these are the designs with only w_1, w_k and possibly w_0 $(= 1 - w_1 - w_k)$ non-zero. These designs are also known as the star-point designs. In the present section we provide the A-optimal designs within this class. Although the optimal designs from this class will not usually be optimal among all designs, they require trials at fewer distinct points than those derived from any other combination of three S_is. The integer approximation to the CCDs are also likely to involve fewer trials.

For a CCD, $\alpha_2 = w_k + w_1/k = \alpha_4$ and $\alpha_{22} = w_k$. Thus the objective functions (1) - (3) reduce to

$$(0.6)\qquad \begin{aligned} V_1(w_1, w_k) &= k(k-1)/w_1 + 1/\{(kw_k + w_1/k) \\ &\quad -k(w_k + w_1/k)^2\}, \\ V_2(w_1, w_k) &= V_1(w_1, w_k) + k(k-1)/2w_k, \\ V_3(w_1, w_k) &= V_2(w_1, w_k) + k/(w_k + w_1/k) \\ &\quad +(kw_k + w_1/k)/\{(kw_k + w_1/k) \\ &\quad -k(w_k + w_1/k)^2\}. \end{aligned}$$

Direct minimization of these with respect to w_1 and w_k is difficult. However, using a change of variables from (w_1, w_k) to (s, z) by substituting

$w_1 = (1-w_0)s$, $w_k = (1-w_0)(1-s)$ and $(1-w_0) = z\{s+k^2(1-s)\}/\{s+k(1-s)\}^2$, (6) may be expressed as

$$(0.7)\quad \begin{aligned} V_1(w_1,w_k) &= U_1(s,z) = A_1(s)/z + B_1(s)/(1-z),\\ V_2(w_1,w_k) &= U_2(s,z) = A_2(s)/z + B_2(s)/(1-z),\\ V_3(w_1,w_k) &= U_3(s,z) = A_3(s)/z + B_3(s)/(1-z), \end{aligned}$$

for some functions A_1, A_2, A_3, B_1, B_2 and B_3 of s alone. These U_i's may first be minimized with respect to z and then with respect to s giving the optimal CCDs. The optimal CCDs η_j minimizing U_j $(j = 1,2,3)$ obtained by the above method are presented in Tables 7, 8 and 9 which follow. Further, the efficiency of these designs were computed and are presented in Table 10 in which C_{ij} denotes the efficiency of η_i with respect to ξ_j.

Table 7. A-optimal CCD for coefficients of quadratic terms

k	s	z	w_1	w_k	α_2	α_{22}	V_1	V_2	V_3
2	2/3	2/3	0.5000	0.2500	0.5000	0.2500	8 .00	12.00	19.00
3	0.7500	0.7500	0.7500	0.2500	0.5000	0.2500	12.00	24.00	34.00
4	0.9109	0.6859	0.9090	0.0890	0.3162	0.0890	18.66	86.08	101.91
5	0.9439	0.6389	0.9439	0.0561	0.2449	0.0561	27.09	205.34	228.53
6	0.9619	0.6073	0.9619	0.0381	0.1984	0.0381	37.74	431.44	464.23
7	0.9725	0.5853	0.9725	0.0275	0.1664	0.0275	50.47	814.10	858.58
8	0.9793	0.5691	0.9793	0.0207	0.1431	0.0207	65.24	1417.90	1476.12
9	0.9839	0.5567	0.9839	0.0161	0.1254	0.0161	82.07	2318.09	2392.12
10	0.9879	0.5470	0.9879	0.0121	0.1116	0.0121	100.88	3589.25	3681.06

Table 8. A-optimal CCD for coefficients of second-order terms

k	s	z	w_1	w_k	α_2	α_{22}	V_1	V_2	V_3
2	0.6542	0.5246	0.4332	0.3925	0.6091	0.3925	8.47	11.02	18.16
3	0.6119	0.7686	0.6119	0.3881	0.5920	0.3881	12.97	20.70	30.30
4	0.5993	0.6917	0.5993	0.4007	0.5505	0.4007	21.88	36.85	47.36
5	0.5937	0.6410	0.5937	0.4063	0.5251	0.4063	34.97	59.58	71.89
6	0.5909	0.6055	0.5909	0.4091	0.5075	0.4091	51.81	88.47	102.83
7	0.5893	0.5794	0.5893	0.4107	0.4949	0.4107	72.06	123.19	139.72
8	0.5884	0.5593	0.5884	0.4116	0.4852	0.4116	97.78	163.81	182.57
9	0.5878	0.5436	0.5878	0.4122	0.4775	0.4122	123.09	210.43	231.47
10	0.5875	0.5308	0.5875	0.4125	0.4713	0.4125	153.57	262.66	286.01

Table 9. A-optimal CCD for all parameters

k	s	z	w_1	w_k	α_2	α_{22}	V_1	V_2	V_3
2	0.5099	0.6893	0.3910	0.3758	0.5714	0.3758	8.51	11.17	17.89
3	0.5910	0.7730	0.5691	0.4251	0.6148	0.4251	13.56	20.62	29.83
4	0.5677	0.7049	0.5677	0.4323	0.5742	0.4323	22.95	36.83	47.18
5	0.5659	0.6558	0.5659	0.4341	0.5473	0.4341	36.61	59.64	71.69
6	0.5660	0.6207	0.5660	0.4340	0.5283	0.4340	54.70	89.26	102.54
7	0.5668	0.5944	0.5668	0.4332	0.5142	0.4332	74.87	123.34	139.45
8	0.5679	0.5739	0.5679	0.4321	0.5031	0.4321	93.26	164.06	182.32
9	0.5686	0.5579	0.5686	0.4314	0.4946	0.4314	127.16	210.60	231.11
10	0.5696	0.5447	0.5696	0.4304	0.4874	0.4304	158.40	262.95	285.78

Table 10. Efficiencies (in %) of A-optimal CCDs

k	2	3	4	5	6	7	8	9	10
C_{11}	100.00	100.00	85.74	73.83	63.59	55.48	49.05	43.86	39.65
C_{21}	94.45	92.52	73.13	57.19	46.32	38.86	32.73	29.25	26.05
C_{31}	93.98	88.47	69.71	54.63	43.88	37.47	34.31	28.31	25.25
C_{12}	91.83	83.92	36.19	21.39	13.53	9.15	6.50	4.80	3.68
C_{22}	100.00	97.29	84.53	73.73	66.00	60.44	56.24	52.89	50.25
C_{32}	98.56	97.67	84.57	73.65	65.42	60.37	56.15	52.85	50.19
C_{13}	94.16	87.74	43.02	26.04	16.55	11.15	7.87	5.78	4.39
C_{23}	98.51	98.45	92.57	82.77	74.72	68.53	63.66	59.71	56.54
C_{33}	100.00	100.00	99.92	83.00	74.99	68.66	63.74	59.80	56.58

4. INTEGER DESIGNS

All the optimal designs derived in earlier sections were continuous designs or design measures. In practice these have to be approximated by discrete or integer designs for which the masses are integer multiples of N^{-1}. Here we consider some integer designs, with n_j trials at each point of S_j $(j = 0, 1, 2, \ldots, k)$ for $k = 2, 3, 4$ and 5. Thus the integer designs of the CCD type and Kono type are both covered in this study. For each design the efficiency is derived for the first-order terms, for all the terms in the second-order model and for the two subsets of the parameters. All the efficiencies are presented in the table which follows. For the five factor designs the value of 1/2 for n_5 denotes 1/2 replicate of 2^5 factorial.

The results presented in the table show that for four or fewer factors, it is possible to find discrete CCD requiring a moderate number of trials whose performance is close to those of the optimal CCDs presented earlier. Most of the designs that are efficient for one experimental situation are efficient for the other two situations and also have high value of E. These designs are thus suitable both for testing for second-order departures from a first-order model and, depending on the outcome of the test, for fitting a model of either first- or second-order. However, for five factors, the designs require a large number of trials to achieve any reasonable efficiency. Thus the conclusions we derive using A-optimality are analogous to those derived by Atkinson (1973) who used D-optimality.

Table 11. Integer designs for a second-order model over cubic region

1-Central Composite Designs								
	Number of trials at each					Efficiency (in %) for		
	centre point	star point	Factorial point	Total number of trials	First order terms	Quadratic terms	second order terms	All terms
	n_0	n_1	n_k	N	E	E_1	E_2	E_3
(a)	k=2			maximum efficiencies		100	100	100
	1	1	1	9	66.67	88.89	**97.93**	92.95
	2	1	1	10	60.00	93.33	99.51	**99.53**
	1	1	2	13	76.92	**69.74**	56.20	61.52
	4	2	1	16	50.00	**100.00**	91.81	94.17
	6	3	4	34	64.71	86.63	96.98	**97.04**
	8	3	4	36	61.11	86.58	95.88	**98.40**
(b)	k=3			maximum efficiencies		100	97.29	100
	0	1	1	14	71.43	70.33	90.29	**92.65**
	0	4	1	32	50.00	**100.00**	83.91	87.75
	0	2	3	36	77.78	59.26	81.37	**89.44**
(c)	k=4			maximum efficiencies		85.74	85.53	92.92
	0	1	1	24	75.00	42.10	66.28	**75.80**
	0	2	1	32	62.50	62.06	85.10	**91.41**
(d)	k=5			maximum efficiencies		73.83	73.73	83.00
	0	1	1/2	26	69.23	37.51	63.14	**73.50**
	0	2	1/2	36	55.56	53.67	73.50	**82.98**
	0	1	1	42	80.95	23.52	44.75	54.90
	0	4	1/2	56	42.86	68.70	68.52	**76.75**
	0	3	2	94	74.47	31.20	55.75	**65.76**
	0	8	1/2	96	33.33	**76.19**	50.93	57.49

2-Other Designs											
k	n_0	n_1	n_2	n_3	n_4	n_5	N	E	E_1	E_2	E_3
3	4	0	1	0			16	50.00	**100.0**	83.91	87.75
4	8	0	0	1	0		40	60.00	89.99	95.03	**98.63**
	0	4	0	1	0		64	50.00	**100.0**	77.88	82.72
5	16	0	0	0	1	0	96	66.67	76.19	73.52	**99.59**
	16	0	4	0	1	0	256	50.00	**100.0**	73.22	78.30

Notes (i) For the five factor designs the value $n_5 = 1/2$ indicates a half replicate of the full 2^5 factorial.

(ii) Bold face type indicates that the design is most efficient within the class for the given number of trials.

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