

Efficient Response Surface Designs with Quantitative and Qualitative Factors

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(Received : July, 2005)

SUMMARY

Response Surface Methodology involving both qualitative and quantitative factors has been discussed by many authors in the literature. In this paper we develop efficient response surface designs involving qualitative and quantitative factors, by using D-optimal designs. We have also applied global dual response surface optimization technique for finding the optimal setting for a set of design variables involving qualitative and quantitative factors.

Key words : Saturated designs, D-optimal designs, Quantitative factors, Qualitative factors, Global dual response surface optimization.

INTRODUCTION

Consider an agricultural experiment conducted for maximizing corn yield, when same type of seed is used. The effect of five variables is studied on the yield of corn (i) soil water at plantation, (ii) rainfall, (iii) temperature, (iv) amount of manure and (v) type of soil. The first four factors are quantitative, while the fifth one is qualitative in nature. The selection of an appropriate design depends on how the qualitative factors interact with quantitative factors in the model. To study the response of such experiments, Draper and John (1988) and Wu and Ding (1998) have given a systematic method for constructing composite designs involving both qualitative and quantitative factors. Response surface designs involving quantitative and qualitative factors have been discussed by Myers and Montgomery (1995), Aggarwal and Bansal (1998), Wu and Hamada (2000), Aggarwal *et al.* (2000) and Montgomery (2005). The significance of this problem has also been discussed by Das *et al.* (1999). Myers *et al.* (2004) have given excellent review on response surface methodology.

Response surface designs involving qualitative and quantitative factors available in the literature are not saturated. Sometimes, in an experiment when the runs are expensive, difficult, or time consuming then there is certainly a need for smaller designs that are either saturated or nearly saturated. In this paper we apply a systematic method for constructing saturated response surface designs involving qualitative and quantitative factors.

The goal of an experimenter in agricultural field or industry is to find operating conditions which can achieve desired target for the expected response with minimum process variability. Vining and Myers (1990) suggested Dual Response Surface as an alternative to Taguchi's (1959, 1987) Robust Parameter Design. It uses separate linear models for the response and its variance. Ankenman and Dean (2003) have given excellent review on Taguchi's robust design and dual response surface optimization. We have used the global dual response surface optimization technique given by Del Castillo *et al.* (1997, 1999) for finding the optimal setting for a set of design variables involving qualitative and quantitative factors.

CONSTRUCTION METHOD FOR EFFICIENT RESPONSE SURFACE DESIGNS

The saturated fractional factorial designs are used when experiment is expensive or time consuming, the

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experimental error is small, an independent estimate of experimental error is available and a second order model is adequate to explain the phenomenon under study. Mitchell (1974), Galil and Kiefer (1980) and Dean and Draper (1999) have given D-optimal mod designs for $n=1,2,3$ and 4. We have constructed efficient response surface designs involving qualitative and quantitative factors by using the technique given by Wu and Ding (1998) and above mentioned D-optimal designs. Consider a product, process or system involving a response y that depends on $m = k + 1$ factors, where x_1, x_2, \dots, x_k are k quantitative factors and z is one qualitative factor at two levels. The form of the true response function is unknown and we approximate it by a polynomial representation over a limited experimental region. We wish to fit a quadratic response surface model, which depends on $m = k + 1$ factors. Then the required second order model is of the form

$$y = \beta_0 + \delta_0 z + \sum_{i=1}^k \beta_i x_i + \sum_{i=1}^k \beta_{ii} x_i^2 + \sum_{i < j=1}^k \beta_{ij} x_i x_j + \sum_{i=1}^k \delta_i x_i z + \epsilon \tag{1}$$

where β_0 is a fixed unknown; δ_0 is the effect due to the qualitative factor z , β_i 's are regression coefficients, δ_i is the interaction effect between qualitative factor z and i^{th} quantitative factor, $z = -1$ or 1 (2 levels of qualitative factor), x_i is the value of the i^{th} quantitative factor. The quadratic model has $p = \frac{(m+1)(m+2)}{2} - 1$ coefficients to be estimated.

For the cube portion of efficient response surface design, we choose m columns from the D-optimal designs having $t = p - 2k - 1$ runs. Next $2k$ points are 'star points' or 'axial points' whose distance from the origin is α . We have considered $\alpha = \sqrt{k}$ for spherical designs. The last two runs: $(t + 2k + 1)^{th}$ and $(t + 2k + 2)^{th}$ are center points. The qualitative factor z can take values ± 1 . For the first t runs the qualitative factor z is one of the columns of the D-optimal designs. For $2k$ star points an overall search has been made over different combinations of ± 1 . Next corresponding to two center runs, we take $z = 1$ and $z = -1$.

Several optimality criterion are proposed for checking design efficiency and D-optimality is one of the most popular as it maximizes $|X'X|$, which means

variance of the individual regression coefficients are minimized. High D-efficiency designs are required for overall good fitting of the model. From all the combinations of ± 1 for z , we select the one which gives maximum D-efficiency $= \frac{|X'X|^{1/p}}{N}$, where 'p' is the number of coefficients to be estimated and 'N' is the run size of the response surface design. Such designs are generically represented in Table 1.

Table 1. Efficient response surface designs for quantitative and qualitative factors

Run	x_1	.	.	.	x_k	z
1	± 1 according to the D-optimal design for $m = k+1$ factors					
2						
.						
.						
t						
t+1	α	.	.	.	0	-1 OR 1
t+2	$-\alpha$.	.	.	0	
.	
.	
t + 2k - 1	0	.	.	.	α	
t + 2k	0	.	.	.	$-\alpha$	
t + 2k + 1	0	.	.	.	0	1
t + 2k + 2	0	.	.	.	0	-1

In this paper we have developed different designs, for $k = 3,4,\dots,8$ quantitative factors and one qualitative factor. We explained the method for $k = 3$ quantitative factors. In the remaining cases we have given number of factors, coefficients to be estimated, the cube portion of the design and different choices of z . We have given two designs for $k = 4$ quantitative factors.

Case 1: Number of quantitative factors = 3: x_1, x_2, x_3

We need at least $N = 15$ runs for the estimation of following 14 coefficients according to model (1)

$$1, x_1, x_2, x_3, x_1 x_2, x_1 x_3, x_1^2, x_2^2, x_3^2, z, z x_1, z x_2, z x_3$$

In order to estimate second order coefficients, we add $2k = 2 \times 3 = 6$ axial points. Further we add two center points corresponding to two levels of z . The minimum possible number of points required for cube portion is $15 - 6 - 2 = 7$. For this case we consider 7-run design of Galil and Kiefer (1980) given in Table 2.

Table 2. D-optimum design for $n = 7$ ($3 \pmod 4$)

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

The above design has 6 columns out of which 4 columns can be chosen in 6C_4 ways. By complete search we observe that column numbers 1, 3, 4 and 6 of this design will give highest efficiency. Therefore, we allocate the factors x_1, x_2, x_3 and z to the column numbers 1, 3, 4 and 6 respectively, and the corresponding coefficient matrix is given below in Table 3.

Table 3. Coefficient matrix

x_1	x_2	x_3	z
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
1.732	0	0	
-1.732	0	0	-1
0	1.732	0	OR
0	-1.732	0	1
0	0	1.732	
0	0	-1.732	
0	0	0	1
0	0	0	-1

Table 4

S. No.	Col. No.'s for cube portion		$z = (z_8, \dots, z_{13})$	D-Eff.
	x_1, x_2, x_3	z		
1	1 3 4	6	-1 -1 -1 -1 -1 -1	70.15
2	1 3 4	6	-1 -1 -1 -1 1 -1	61.67
3	1 3 4	6	-1 -1 -1 -1 -1 1	60.79
4	1 3 4	6	-1 -1 1 -1 1 -1	55.02
5	1 3 4	5	1 1 -1 -1 1 1	56.36
6	1 3 4	5	1 -1 -1 -1 1 1	55.55
7	1 3 4	5	1 1 1 -1 1 1	55.54
8	1 3 4	5	1 1 -1 1 1 1	53.99

Next we choose the level of z for the $2k$ star points. Different choices of z which gives distinct designs with high D-efficiency and allocation of factors are given in Table 4.

Case 2(a): Number of quantitative factors = 4 and

- (i) $m = 4+1 = 5$ factors; x_1, x_2, x_3, x_4, z
- (ii) $N = 21$ runs; $p = 20$ coefficients to be estimated
- (iii) Cube portion: 11-run Galil and Kiefer (1980) design given in Annexure I - Design (a)

In Table 5(a) we give the choices of z which gives distinct designs with high D-efficiency and allocation of factors.

Table 5(a)

S. No.	Col. No.'s for cube portion		$z = (z_{12}, \dots, z_{19})$	D-Eff.
	x_1, x_2, x_3, x_4	z		
1	1 3 4 6	8	-1 -1 -1 -1 -1 -1 -1 -1	71.89
2	1 3 4 6	8	-1 -1 -1 -1 -1 -1 1 -1	65.59
3	1 3 4 6	8	-1 -1 -1 -1 -1 -1 -1 1	65.55
4	1 3 4 6	8	-1 -1 -1 -1 1 -1 1 -1	59.73
5	1 2 3 5	8	-1 -1 -1 -1 -1 -1 -1 -1	69.07
6	1 2 3 5	8	-1 -1 -1 -1 -1 -1 1 -1	63.22
7	1 2 3 5	8	-1 -1 -1 1 -1 -1 -1 -1	63.02
8	1 2 3 5	8	-1 -1 -1 -1 -1 -1 -1 1	62.95

Case 2(b): We have also considered 11-run Galil and Kiefer (1980) design given in Annexure I - Design (b), for cube portion because the earlier design has all its cube points at $z = 1$. We get the following choices of z as shown in Table 5(b) which gives distinct designs with high D-efficiency and allocation of factors.

Table 5(b)

S. No.	Col. No.'s for cube portion		$z = (z_{12}, \dots, z_{19})$	D-Eff.
	x_1, x_2, x_3, x_4	z		
1	1 3 5 8	10	-1 -1 -1 -1 1 1 -1 -1	58.67
2	1 3 5 8	10	1 -1 -1 -1 -1 -1 -1 -1	58.65
3	1 3 5 8	10	-1 1 -1 -1 -1 -1 -1 -1	58.33
4	1 3 5 8	10	-1 -1 -1 -1 -1 -1 -1 -1	57.36
5	1 3 5 8	10	-1 1 -1 -1 -1 1 -1 -1	57.15
6	1 3 5 8	10	-1 -1 1 -1 1 1 -1 -1	56.37

Case 5: Number of quantitative factors = 7 and

- (i) $m = 7 + 1 = 8$; x_1, \dots, x_7, z .
- (ii) $N = 45$ runs; $p = 44$ coefficients to be estimated.
- (iii) Cube portion: 29-run Mitchell (1974) design given in Annexure I

Now the choice of 8 columns out of 27 columns can be done in ${}^{27}C_8$ possible ways. We have chosen columns [7 10 13 15 20 21 26 27] for allocation of factors.

In Table 8 we give the choices of z which gives distinct designs with high D-efficiency and allocation of factors.

Case 6: Number of quantitative factors = 8 and

- (i) $m = 8 + 1 = 9$, x_1, \dots, x_8, z
- (ii) $N = 55$ runs; $p = 54$ coefficients to be estimated
- (iii) Cube portion: 37-run Mitchell (1974) design given in Annexure I

In this case we have to choose 9 columns out of 35. So there are ${}^{35}C_9$ possible choices. We have chosen columns [1 9 12 15 16 24 27 30 33] for allocation of factors.

Table 9 shows the choices of z which gives distinct designs with high D-efficiency and allocation of factors.

Table 8

S. No.	Col. No.'s for cube portion							z	$z = (z_{30}, \dots, z_{43})$	D-Eff.
	x_1, \dots, x_7									
1	7	10	13	15	20	21	26	27	-1 -1 1 1 -1 -1 1 -1 1 -1 -1 -1 -1 -1 -1 -1	48.45
2	7	10	13	15	20	21	26	27	-1 1 1 1 -1 -1 1 -1 1 -1 -1 -1 -1 -1 -1 -1	48.12
3	7	10	13	15	20	21	26	27	-1 1 1 1 -1 -1 -1 -1 1 -1 -1 -1 -1 -1 -1 -1	48.01
4	7	10	13	15	20	21	26	27	-1 -1 1 1 -1 -1 -1 -1 1 -1 -1 -1 -1 -1 -1 -1	47.97
5	7	10	13	15	20	21	26	27	1 -1 1 1 -1 -1 1 -1 1 -1 -1 -1 -1 -1 -1 -1	47.96
6	7	10	13	15	20	21	26	27	-1 1 1 1 -1 1 1 1 1 1 -1 -1 -1 -1 -1 -1	47.93
7	7	10	13	15	20	21	26	27	-1 1 1 1 1 1 1 -1 1 1 -1 -1 -1 -1 -1 -1	47.88
8	7	10	13	15	20	21	26	27	1 1 -1 -1 -1 -1 -1 -1 1 -1 -1 -1 -1 -1 -1 -1	47.86
9	7	10	13	15	20	21	26	27	-1 -1 1 1 -1 -1 -1 1 -1 1 -1 -1 -1 -1 -1 -1	47.85
10	7	10	13	15	20	21	26	27	-1 1 1 1 -1 1 1 1 1 1 -1 1 -1 -1 -1 -1	47.82

Table 9

S. No.	Col. No.'s for cube portion								z	$z = (z_{38}, \dots, z_{53})$	D-Eff.
	x_1, \dots, x_8										
1	1	9	12	15	16	24	27	30	33	1 -1 1 1 1 1 1 1 -1 1 -1 -1 1 1 1 1	48.76
2	1	9	12	15	16	24	27	30	33	1 1 1 1 1 1 1 -1 -1 1 -1 -1 1 1 1 1	48.58
3	1	9	12	15	16	24	27	30	33	1 1 1 1 1 1 1 1 -1 1 -1 -1 1 1 1 1	48.57
4	1	9	12	15	16	24	27	30	33	1 -1 1 1 1 1 1 -1 -1 1 -1 -1 1 1 1 1	48.55
5	1	9	12	15	16	24	27	30	33	1 -1 1 1 1 1 1 1 -1 1 -1 -1 1 1 -1 1	48.53
6	1	9	12	15	16	24	27	30	33	1 -1 1 1 1 1 1 1 -1 -1 -1 -1 1 1 1 1	48.52
7	1	9	12	15	16	24	27	30	33	1 -1 1 1 1 1 1 1 -1 1 -1 -1 1 -1 1 1	48.44
8	1	9	12	15	16	24	27	30	33	1 1 1 1 1 1 1 1 -1 1 -1 -1 1 1 -1 1	48.42
9	1	9	12	15	16	24	27	30	33	1 -1 1 1 1 1 -1 1 -1 1 -1 -1 1 1 1 1	48.41
10	1	9	12	15	16	24	27	30	33	1 -1 1 1 1 1 1 -1 -1 -1 -1 -1 1 1 1 1	48.40
11	1	9	12	15	16	24	27	30	33	1 -1 1 1 1 1 -1 1 -1 1 -1 -1 1 1 -1 1	48.37

DUAL RESPONSE SURFACE GLOBAL OPTIMIZATION

We have used dual response surface approach given by Del Castillo *et al.* (1997, 1999) for finding global optimal solution to the problem involving both quantitative and qualitative factors. Let us suppose that in an experiment there are N number of design points appropriate for the response model, and further suppose that these N design points are replicated a total of $r \geq 2$ times. Let \bar{y}_m and \bar{y}_s represent the sample mean and sample standard deviation of these design points respectively. The following procedure is adopted to obtain global optimal solution:

- (a) First we fit a second order model for sample mean (\bar{y}_m) and sample standard deviation (\bar{y}_s). The fitted response surfaces in \underline{x} and z are

$$\hat{y}_m(\underline{x}, z) = a_0 + \underline{x}'\underline{b}_0 + z'c_0 + \underline{x}'\underline{B}_0\underline{x} + \underline{x}'\underline{C}_0z \tag{2}$$

$$\hat{y}_s(\underline{x}, z) = a_1 + \underline{x}'\underline{b}_1 + z'c_1 + \underline{x}'\underline{B}_1\underline{x} + \underline{x}'\underline{C}_1z \tag{3}$$

- (b) Next for each level of qualitative factor z, ($z = \pm 1$) we compute the following response and its standard deviation functions

$$\hat{y}_m(\underline{x}, z) = a_{10} + \underline{x}'\underline{b}_{10} + \underline{x}'\underline{B}_0\underline{x} \tag{4}$$

$$\hat{y}_s(\underline{x}, z) = a_{11} + \underline{x}'\underline{b}_{11} + \underline{x}'\underline{B}_1\underline{x} \tag{5}$$

- (c) For each level of z, find the value of \underline{x} such that

- (i) $\hat{y}_s(\underline{x}, z)$ is minimum
- (ii) $\hat{y}_m(\underline{x}, z) = \text{target}$
- (iii) $\underline{x}'\underline{x} \leq \rho^2$, where ρ is the radial bound for the solution \underline{x}

- (d) Optimal solution of the problem is that \underline{x} for which $\hat{y}_s(\underline{x}, z)$ is minimum.

We explain the method with the help of an example.

Example: Consider an experiment involving four quantitative factors x_1, x_2, x_3, x_4 and one qualitative factor z. The purpose of experiment is to find the optimal solution of the problem when we want the desired mean response as 450. We consider the following hypothetical

data set for fitting the response surface design as given in Table 10.

Table 10. Experimental data set

x_1	x_2	x_3	x_4	z	y_1	y_2	y_3	y_m	y_s
-1	1	-1	1	1	134	110	128	124.00	12.49
-1	-1	1	1	1	144	178	188	170.00	23.07
1	-1	1	-1	1	90	122	129	113.67	20.79
1	1	1	1	1	322	350	350	340.67	16.17
-1	-1	1	-1	1	354	345	350	349.67	4.51
-1	1	1	-1	1	311	360	328	333.00	24.88
-1	-1	-1	1	1	234	268	267	256.33	19.35
1	-1	-1	-1	1	290	263	253	268.67	19.14
1	-1	-1	1	1	110	160	192	154.00	41.33
-1	1	-1	-1	1	269	362	392	341.00	64.13
1	1	-1	-1	1	328	294	345	322.33	25.97
2	0	0	0	-1	81	168	78	109.00	51.12
-2	0	0	0	-1	538	489	482	503.00	30.51
0	2	0	0	-1	98	110	105	104.33	6.03
0	-2	0	0	-1	118	117	116	117.00	1.00
0	0	2	0	-1	129	154	131	138.00	13.89
0	0	-2	0	-1	159	155	163	159.00	4.00
0	0	0	2	-1	328	391	394	371.00	37.27
0	0	0	-2	-1	285	217	359	287.00	71.02
0	0	0	0	1	500	459	470	476.33	21.22
0	0	0	0	-1	556	490	525	523.67	33.02

The fitted response equation for mean is

$$\begin{aligned} \hat{Y}_m(X, z) = & 500 - 62.8X_1 + 8.5X_2 - 12.8X_3 - 20.8X_4 \\ & + 13.8Z + 57.5X_1X_2 + 3.2X_1X_3 \\ & + 36.6X_1X_4 + 39.9X_2X_3 + 11.0X_2X_4 \\ & + 20.3X_3X_4 + 35.7ZX_1 + 11.7ZX_2 \\ & - 7.6ZX_3 - 41.8ZX_4 - 43.9X_1^2 \\ & - 92.7X_2^2 - 83.3X_3^2 - 38.1X_4^2 \end{aligned}$$

$$S = 55.8737 \quad R^2 = 99.2\% \quad R^2(\text{adj.}) = 83.1\%$$

Analysis of Variance

Source	DF	SS	MS	F	P
Regression	19	367029	19317	6.19	0.308
Residual Error	1	3122	3122		
Total	20	370151			

The fitted response equation for standard deviation is

$$\hat{Y}_s(X, z) = 27.1 + 3.59X_1 - 1.45X_2 - 0.16X_3 - 4.60X_4 - 1.88Z - 7.53X_1X_2 + 6.08X_1X_3 + 7.51X_1X_4 - 4.14X_2X_3 - 11.0X_2X_4 + 6.60X_3X_4 - 1.56ZX_1 - 2.70ZX_2 - 2.64ZX_3 + 3.84ZX_4 + 3.08X_1^2 - 6.24X_2^2 - 4.89X_3^2 + 6.41X_4^2$$

S = 5.99901 R² = 99.5% R² (adj.) = 89.8%

Analysis of Variance

Source	DF	SS	MS	F	P
Regression	19	7052.96	371.21	10.31	0.241
Residual Error	1	35.99	35.99		
Total	20	7088.95			

The fitted mean and standard deviation response function for z = 1 from the above response function is given by

$$\hat{Y}_m(X, z = 1) = 513.81 - 26.3X_1 + 20.24X_2 - 20.43X_3 - 62.6X_4 + 57.5X_1X_2 + 3.2X_1X_3 + 36.6X_1X_4 + 39.9X_2X_3 + 11.0X_2X_4 + 20.3X_3X_4 - 43.9X_1^2 - 92.7X_2^2 - 83.3X_3^2 - 38.1X_4^2$$

$$\hat{Y}_s(X, z = 1) = 25.246 + 2.037X_1 - 4.151X_2 - 2.801X_3 - 0.764X_4 - 7.53X_1X_2 + 6.08X_1X_3 + 7.51X_1X_4 - 4.14X_2X_3 - 11.0X_2X_4 + 6.60X_3X_4 + 3.08X_1^2 - 6.24X_2^2 - 4.89X_3^2 + 6.41X_4^2$$

The fitted mean and standard deviation response function for z = -1 is given by

$$\hat{Y}_m(X, z = -1) = 486.19 - 97.7X_1 - 3.16X_2 - 5.25X_3 + 21.0X_4 + 57.5X_1X_2 + 3.2X_1X_3 + 36.6X_1X_4 + 39.9X_2X_3 + 11.0X_2X_4 + 20.3X_3X_4 - 43.9X_1^2 - 92.7X_2^2 - 83.3X_3^2 - 38.1X_4^2$$

$$\hat{Y}_s(X, z = -1) = 28.996 + 5.151X_1 + 1.257X_2 + 2.473X_3 - 8.438X_4 - 7.53X_1X_2 + 6.08X_1X_3 + 7.51X_1X_4 - 4.14X_2X_3 - 11.0X_2X_4 + 6.60X_3X_4 + 3.08X_1^2 - 6.24X_2^2 - 4.89X_3^2 + 6.41X_4^2$$

We use the technique given by Del Castillo *et al.* (1997) for finding the global optimal solution to the specified problem. We take $\rho = \alpha = \sqrt{k}$ where k is the number of quantitative factors.

For z = 1, $\hat{y}_s(\underline{x}, z) = 13.279590$ is minimum and $\hat{y}_m(\underline{x}, z) = 450$ at $\underline{x} = (-0.404998, 0.701198, 0.562927, -0.059177)$.

For z = -1, $\hat{y}_s(\underline{x}, z) = 11.925140$ is minimum and $\hat{y}_m(\underline{x}, z) = 450$ at $\underline{x} = (-1.126312, 0.505276, 0.334627, 0.745140)$

We observe that $\hat{y}_s(\underline{x}, z)$ is smaller for z = -1, so the optimal setting of factors is $x_1 = -1.126312, x_2 = 0.505276, x_3 = 0.334627, x_4 = 0.745140$ and z = -1

CONCLUDING REMARKS

The response surface designs involving qualitative and quantitative factors developed in this paper are concentrated on economical run size. The saturated designs are used when experiment is expensive or time consuming. The use of such designs has substantial savings on the number of runs. Say, for k = 4 factors, the designs given by Wu and Ding (1998) needs 26 runs and gives maximum D-efficiency of 64% whereas we give 21-run design which has D-efficiency of 58.67%. Similarly, for k = 5 factors, Wu and Ding (1998) needs 44 runs to give maximum D-efficiency of 87.25% and his 28-run design estimates only 24 of the total 27 coefficients with maximum D-efficiency 56.5%. Our design estimates all 27 coefficients in 28 runs with D-efficiency 61.27%. For k = 6, we loose efficiency by less than 7% but we save 10 runs. So, overall we see that we are not loosing too much efficiency but we are reducing the run size as in industries sometimes saving on run size is more important.

We also observe that if a design has all its cube points at z = 1, then it has high D-efficiency. All these designs given in Table 4 to 7 corresponding to

$k = 3, 4, 5$, and 6 are marked bold and italic in the column of qualitative factor.

ACKNOWLEDGEMENT

The authors are grateful to referee for making very useful comments which has helped in improvement of the paper. The first author is grateful to the Department of Mathematical Sciences, University of Memphis, Memphis for providing necessary research facilities. The fourth author is thankful to University Grants Commission, New Delhi for supporting the Research under Teacher's Fellowship Scheme.

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