World Academy of Science, Engineering and Technology
International Journal of Mathematical and Computational Sciences
Vol:6, No:5, 2012

Comparison of Response Surface Designs in a Spherical Region

Boonorm Chomtee, John J. Borkowski

***Abstract*—**The objective of the research is to study and compare response surface designs: Central composite designs (CCD), Box-Behnken designs (BBD), Small composite designs (SCD), Hybrid designs, and Uniform shell designs (USD) over sets of reduced models when the design is in a spherical region for 3 and 4 design variables. The two optimality criteria (D and G) are considered which larger values imply a better design. The comparison of design optimality criteria of the response surface designs across the full second order model and sets of reduced models for 3 and 4 factors based on the two criteria are presented.

***Keywords*—**design optimality criteria, reduced models, response surface design, spherical design region

I. Introduction

In real world application of response surface methodology (RSM), the second order model is widely used as an approximating model to the response model because it is easy to estimate parameters (β 's) in the second order model which is, $y=\beta_0+\sum_{i=1}^{k}\beta_i x_i+\sum_{i=1}^{k}\beta_{ii}x_i^2+\sum_{1\le i<j}^{k}\beta_{ij}x_i x_j+\varepsilon$. However, the final response surface model usually ends up with a reduced model. Hence, the aim of this research is to compare 3 and 4 factor response surface designs in a spherical design region by studying design optimality criteria (D , G)over sets of reduced models.

II. Materials and Methods

A. Design Optimality Criteria

Design optimality criteria are primarily concerned with optimality properties of the $\mathbf{X}'\mathbf{X}$ matrix for the design matrix $\mathbf{X}$. By studying the optimality criteria, the adequacy of proposed experimental design can be assessed prior to running it. In addition, if several alternative designs are proposed, their optimality properties can be compared to aid in the choice of design. The D and G design optimality measures used in this research and calculated over the full second order model and sets of reduced models as:

$$D\text{-efficiency}=100\frac{|\mathbf{X}'\mathbf{X}|^{1/p}}{N} \text{ and}$$

$$G\text{-efficiency}=100\frac{p}{N\,\hat{\sigma}^2_{\max}}$$

Where $\mathbf{X}$ is the design matrix, p is the number of model parameters, N is the design size, $\sigma^2_{\max}$ is the maximum of $\mathbf{f}'(\mathrm{x})(\mathbf{X}'\mathbf{X})^{-1}\mathbf{f}(\mathrm{x})$ approximated over the set of candidate points. The values of the two criteria were calculated using Matlab software [1].

B. Reduced Models

The set of reduced models is consistent with the definition of *weak heredity* given in Chipman [2]. That is, (i) a quadratic x_i^2 term is in the model only if the x_i term is also in the model and (ii) an interaction $x_i x_j$ term is in the model only if the x_i or x_j or both terms are also in the model. Let 1's and 0's indicate, respectively, the presence or absence of the term x_i in the reduced model, p indicates the number of model parameters, dv indicates the number of design variables present in the model, and $l, c,$ and q indicate the number of linear, cross-product, and quadratic terms in the model, respectively. Based on *weak heredity* structure, there are 44 and 224 models for $k=3,4$ design variables, respectively. An example of a set of reduced models ($k=3$) is shown in Table I.

TABLE I
REDUCED MODELS ($k=3$)

Model	p	dv	l	c	q	x_1	x_2	x_3
1	10	3	3	3	3	1	1	1
2	9	3	3	2	3	1	1	1
3	9	3	3	3	2	1	1	1
⋮								
44	2	1	1	0	0	0	0	1

TABLE I
CONT'D

Model	x_1x_2	x_1x_3	x_2x_3	x_1^2	x_2^2	x_3^2
1	1	1	1	1	1	1
2	1	1	1	0	1	1
3	0	1	1	1	1	1
⋮						
44	0	0	0	0	0	0

C. Spherical Region

In RSM, there are variety of response surface designs in cuboidal, spherical, and polyhedral region. In this article, response surface designs in a spherical region are studied where $\sum_{i=1}^{k}x_i^2\le k$; x is a design variable and k is the number of input variable. That is, all $x_i; i=1,2,\ldots,k$ values are inside of a sphere of radius k .

B. Chomtee is with the Department of Statistics, Faculty of Science, Kasetsart University, Bangkok, Thailand (phone: 6685-334-4401; fax: 662-942-8384; e-mail: fsciboc@ku.ac.th).

J. J. Borkowski is with the Department of Mathematical Science,Montana State University, Bozeman, MT 59717 USA (e-mail: jobo@ math.montana.edu).

III. Results and Discussions

A. Optimality Criteria for the Full Second Order Model

In this section, the D and G optimality criteria comparisons of the 7 response surface designs for 3 design variables: CCD, BBD, SCD, USD, hybrid 310, 311A, and 311B designs and the 7 response surface designs for 4 design variables: CCD, BBD, SCD, USD, hybrid 416A, 416B, and 416C designs of the full second order model will be summarized in Table II and Table III. For the D and G criteria, larger values imply a better design (on a per point basis). Let r_s indicates the replication of star points of the design, n_0 indicates the number of center points of the design, and N is the design size.

TABLE II
The Optimality Criteria for $k = 3$

Designs	r_s	n_0	N	D	G
CCD	1	1	15	71.12	66.67
	2	1	21	67.31	47.61
	1	3	17	70.04	89.20
	2	3	23	68.59	76.47
BBD	-	1	13	69.58	76.91
	-	3	15	67.31	66.65
SCD	1	1	11	59.07	32.79
	2	1	17	56.66	33.38
	1	3	13	55.79	27.74
	2	3	19	56.58	29.87
USD	-	1	13	69.59	76.92
	-	3	15	67.31	66.67
310	-	0	10	62.17	47.38
	-	1	11	60.63	45.01
	-	3	13	55.01	38.95
311A	-	1	11	67.60	78.62
	-	3	13	63.84	69.01
311B	-	1	11	70.99	90.90
	-	3	13	67.05	77.40

Table II and Table III indicate the following general results:

1. Replicating star points (increasing r_s) tends to reduce the D and G criteria for the CCDs. Similar results are true of the SCDs except for the D criterion when $k = 3$, $n_0 = 3$ and for the G criterion when $k = 4$.
2. Increasing center points (increasing n_0) tends to reduce the D and G criteria except for the G criterion of the CCDs when $k = 3, 4$ whether or not star points are replicated, and for the G criterion of the BBD when $k = 4$.

TABLE III
The Optimality Criteria for $k = 4$

Designs	r_s	n_0	N	D	G
CCD	1	1	25	76.72	60.00
	2	1	33	73.48	45.45
	1	3	27	76.44	95.23
	2	3	35	74.55	81.47
BBD	-	1	25	76.72	60.00
	-	3	27	76.44	95.23
SCD	1	1	17	65.03	29.37
	2	1	25	61.59	32.68
	1	3	19	62.60	26.27
	2	3	27	61.36	30.26
USD	-	1	21	72.40	71.42
	-	3	23	71.13	67.55
416A	-	1	17	70.01	74.30
	-	3	19	67.14	69.10
416B	-	1	17	73.52	70.06
	-	3	19	68.94	62.86
416C	-	1	16	74.94	77.49
	-	3	17	73.86	72.93

The results of these tables suggest replication affects the different criteria in very different ways. That is, what improves one criterion may detrimental to a different criterion. In addition, the results of replicating star and center points for the CCD in a spherical design region are consistent with the results for the CCD in a hypercube design region [3].

B. General results for the reduced models

To study the robustness of 3 and 4 factor spherical response designs across the set of reduced models, the 7 response surface designs for 3 design variables: CCD, BBD, SCD, USD, hybrid 310, 311A, and 311B designs and the 7 response surface designs for 4 design variables: CCD, BBD, SCD, USD, hybrid 416A, 416B, and 416C designs are considered. Summaries based on computed values for the D and G criteria for the set of reduced models are as follows:

C. Removing an x_i^2 term from a model

For $k = 3$ with $dv = 3$:

(a) For D: D tends to increase for BBDs and hybrid 310. For other designs, the effects on D vary.

(b) For G: removing an x_i^2 term has varying effects on G.

For $k = 4$ with $dv = 4$:

(a) For D: D tends to decrease for CCDs and BBDs, increase for the hybrid 416C, whereas the effects on D vary for the other designs.

(b) For G: G tends to decrease for SCDs. The effects on G vary for the other designs.

D. Removing an $x_i x_j$ term from a model

For $k = 3$ with $dv = 3$:

(a) For D : D tends to increase except for the hybrid 310.

(b) For G : The effects on G vary for all designs.

For $k = 4$ with $dv = 4$:

(a) For D : D tends to increase for all designs.

(b) For G : G tends to decrease for BBDs and the hybrid 416C. The effects on G vary for the other designs.

Moreover, for $k = 3$, of the 44 reduced models considered, there are 34 models with $dv = 3$ and 10 models with $dv = 1$ or 2. For $k = 4$, of the 224 models considered, there are 170 models with $dv = 4$ and 54 models with $dv = 1, 2$ or 3. Table IV and Table V show the number of models the D and

G criteria values are greater than or smaller than the full second order model criteria values when $k = 3$ and 4 factors, respectively.

TABLE IV
THE NUMBER OF MODELS THE D AND G CRITERIA VALUES ARE GREATER THAN ($dv = 3$) OR SMALLER THAN ($dv = 1, 2$) THE FULL SECOND ORDER MODEL CRITERIA VALUES WHEN $k = 3$

				$dv = 3$ (maximum = 33)		$dv = 1, 2$ (maximum =10)	
Designs	r_s	n_0	N	D	G	D	G
CCD	1	1	15	33	15	9	9
	2	1	21	28	28	8	4
	1	3	17	24	0	10	10
	2	3	23	23	3	9	10
BD	-	1	13	33	4	9	10
	-	3	15	33	4	10	10
CD	1	1	11	26	23	7	0
	2	1	17	26	19	7	3
	1	3	13	24	23	7	0
	2	3	19	23	19	7	3
USD	-	1	13	30	1	9	10
	-	3	15	22	1	10	10
310	-	0	10	32	8	9	8
	-	1	11	31	8	9	8
	-	3	13	32	8	9	8
311A	-	1	11	30	1	9	10
	-	3	13	23	1	10	10
311B	-	1	11	28	1	9	10
	-	3	13	22	1	10	10

E. Comparison of design optimality criteria of reduced models

For the set of reduced models for 3 and 4 factor spherical response surface designs, three comparisons are performed: (i) across the full set of 44 reduced models for $k = 3$ and 224 reduced models for $k = 4$, (ii) across the set of 32 reduced models for $k = 3$ and 181 reduced models for $k = 4$ having at least one squared term, and (iii) across the set of 15 reduced models for $k = 3$ and 109 reduced models for $k = 4$ having at least two squared terms. The results of comparison of design optimality criteria for $k = 3$ are shown in Tables VI-VIII and the results for $k = 4$ are shown in Tables IX-XII.

TABLE V
THE NUMBER OF MODELS THE D AND G CRITERIA VALUES ARE GREATER THAN ($dv = 4$) OR SMALLER THAN ($dv = 1, 2, 3$) THE FULL SECOND ORDER MODEL CRITERIA VALUES WHEN $k = 4$

				$dv = 4$ (maximum =169)		$dv = 1, 2, 3$ (maximum =54)	
Designs	r_s	n_0	N	D	G	D	G
CCD	1	1	25	164	98	53	50
	2	1	33	142	156	50	30
	1	3	27	130	0	54	54
	2	3	35	111	1	50	54
BBD	-	1	25	164	98	53	50
	-	3	27	130	0	54	54
SCD	1	1	17	146	134	44	2
	2	1	25	130	113	42	17
	1	3	19	123	138	49	2
	2	3	27	117	114	46	16
USD	-	1	21	134	1	51	53
	-	3	23	101	1	53	53
416A	-	1	17	150	1	53	54
	-	3	19	113	1	53	54
416B	-	1	17	163	5	54	53
	-	3	19	139	5	54	53
416C	-	1	16	169	3	53	54
	-	2	17	163	4	54	54

For the comparison ranking tables, each row/column entry contains 3 ranks (r_0, r_1, r_2). Each rank ranges from 1 ('best') to the number of designs to be compared ('worst'). Ranks r_0, r_1, and r_2 represent a design's rank relative to the other designs across the full set of reduced models, across the set of reduced models with having at least one squared term, and across the set of reduced models with at least two squared terms, respectively. In case of ties, average ranks are shown.

TABLE VI
DESIGN CRITERIA COMPARISON RANKING FOR $k = 3$, $N = 11$

	DESIGN			
Design Criterion	SCD	310	311A	311B
D	3, 2.5, 2	4, 4, 4	2, 2.5, 3	1, 1, 1
G	3, 3, 3	4, 4, 4	2, 2, 2	1, 1, 1

TABLE VII
DESIGN CRITERIA COMPARISON RANKING FOR $k = 3$, $N = 13$

	DESIGN					
Design Criterion	SCD	310	311A	311B	BBD	USD
D	5, 5, 4	6, 6, 6	4, 4, 5	3, 3, 2	2, 2, 3	1, 1, 1
G	5, 5, 5	6, 6, 6	4, 4, 4	2, 1, 1	3, 3, 3	1, 2, 2

TABLE VIII
DESIGN CRITERIA COMPARISON RANKING FOR $k = 3$, $N = 15$

	DESIGN		
Design Criterion	CCD	BBD	USD
D	1, 1, 1	2, 2.5, 3	3, 2.5, 2
G	1, 1, 1	3, 3, 3	2, 2, 2

TABLE IX
DESIGN CRITERIA COMPARISON RANKING FOR $k = 4$, $N = 17$

	DESIGN			
Design Criterion	SCD	416A	416B	416C
D	3, 1, 1	4, 4, 4	2, 3, 3	1, 2, 2
G	4, 4, 4	2, 2, 2	3, 3, 3	1, 1, 1

TABLE X
DESIGN CRITERIA COMPARISON RANKING FOR $k = 4$, $N = 19$

	DESIGN		
Design Criterion	SCD	416A	416B
D	2, 1, 1	3, 3, 3	1, 2, 2
G	3, 3, 3	1, 1, 1	2, 2, 2

TABLE XI
DESIGN CRITERIA COMPARISON RANKING FOR $k = 4$, $N = 25$

	DESIGN	
Design Criterion	BBD or CCD	SCD
D	1, 1, 1	2, 2, 2
G	1, 1, 1	2, 2, 2

TABLE XII
DESIGN CRITERIA COMPARISON RANKING FOR $k = 4$, $N = 27$

	DESIGN	
Design Criterion	BBD or CCD	SCD
D	1, 1, 1	2, 2, 2
G	1, 1, 1	2, 2, 2

ACKNOWLEDGMENT

The research was funded by Faculty of Science and Department of Statistics, Kasetsart University, Thailand.

REFERENCES

[1] Mathworks Inc., *Matlab Version 7.1*, 2010.
[2] Chipman, H.A., "Baysian variable selection with related predictors," *The Canadian Journal of Statistics*, vol. 24, pp.17-36, 1996.
[3] Borkowski, J.J. and Valeroso, E.S., "Comparison of design optimality criteria of reduced models for response designs in the hypercube," *Technometrics*, vol. 43, pp. 468-477, 2001.