Design Optimality Criteria of Reduced Models for Variations of Central Composite Design

ABSTRACT

This work focuses on the reduced second order model having no quadratic and interaction terms for five variations of Central Composite Design (SCCD, RCCD, OCCD, Slope-R and FCC) using the D-, G- and A- optimality criteria. Results showed that G- and A-optimality criteria are equivalent for models having no quadratic terms and also replication of the axial portion with increase in center points tends to decrease the D-, A- and G-optimality criteria values of the CCDs while for models having no interaction term, showed that replication of the axial portion with increase in center points increases the D-optimality criterion values of SCCD, RCCD and OCCD in all the factors considered

***Key words**: CCDs, FDS, SCCD, RCCD, OCCD, Slope-R, FCC*

1. INTRODUCTION

When modelling an experiment, the researcher's aim is to choose a design which allows for good estimation of relationship between the explanatory factors and the response of interest. This relationship can be written as $y = \eta(x_1, x_2, \ldots, x_k) + \varepsilon$ where y is the response, η is the true unknown function, x_1, x_2, …, x_k are the independent variables, and ε is the error term that represents sources of variability not accounted for in η.

The standard approach in response surface methodology is to model the relationship and approximate it with a low-order polynomial such as a second order model

$$y = \beta_0 + \sum_{i=1}^{k}\beta_i x_i + \sum_{i=1}^{k}\beta_{ii}x_{ii}^2 + \sum_{j=i+1}^{k}\sum_{i=1}^{k-1}\beta_{ij}x_i x_j + \varepsilon_{ij} \quad (1)$$

Where y is the measured response, β's are parameter coefficients; x_i's are the input variables and ε is an error term. Central composite design is among the second order design that utilize this stated model of eqn (1).

Assessment of every design begins with the specification of a model that is proposed for the resulting analysis once the data have been collected. After data collection, and individual effects are tested, some terms may not be significant in the model. In such situation, the experimenter will decide to use a reduced model, which has only a portion of the terms included that were in the original model for which the design was chosen. Design optimality criteria based on the new adopted reduced model are equally or even better than the optimality criteria for the proposed full model. Therefore, a design should be robust over classes of reduced model. The reduced model may only have a fraction of the quadratic terms, or it may be a first order model with some of the interaction terms included. It may be such that the principal of hierarchy may not be appropriate. With this new chosen model, the design may no longer have its desired Properties of the prediction variance. The distribution of the scaled prediction variance (SPV) may change drastically depending on which terms are excluded from the model. The experimenter wants to know how different if any, the SPV curves for each model for a certain design will be. The robustness of the design to model changes is determined by examining the behavior of SPV.

Some authors have studied the design-selection problem when the proposed approximating model is an under parameterized approximation of a true response surface. [1] developed a mean square error design criterion which provides protection against bias error due to model inadequacy. [2] also studied the design-selection problem when the proposed approximating model is an underparameterized approximation of the true response surface. [3] applied a Bayesian approach to reduce the number of possible models through heredity properties. Using the hierarchical nature of different model terms, he developed prior relationships between predictors that were then incorporated into the stochastic search variable selection for any type of linear model. [4] developed a class of model robust designs for estimating main effects and a combination of interactions. After obtaining an upper bound, *g*, on the number of possible two-way interactions from the experimenter, a model robust factorial design was conducted guaranteeing the estimability of any combination of the *g* interactions. [5] did a comparison of design optimality criteria of reduced models for response surface designs (central composite design, computer generated design and small composite design) in the hypercube. They used D-, G-, A- and IV-optimality criteria to evaluate the performance of the designs. They presented some interesting conclusion on how the inclusion or non-inclusion of linear, cross product and quadratic terms affect the behavior of the optimality criteria. Unlike [5], [6] did a comparison of design optimality of reduced models of seven response surface design in a spherical region using only D- and G-optimality criteria to evaluate them. Their results suggest that replication affects different criteria in different ways. That is, what improves one criterion may be detrimental to another. [7] compared optimality criteria of reduced models of split-plot CCD under various ratios of the variance components (or degrees of correlation d). They observed that the optimality criteria for these models strongly depend on the values of d and are robust to changes in the interaction terms. [8] did a comparative study of five variations of the central composite design using the D-, A-, G-, and IV-optimality criteria. The optimal values were estimated under full second order model. Their result show that the replicating the star points tends to decrease the D and G-optimality criterion of CCDs.

This study will examine the design optimality of reduced models for variation of central composite design without consideration of any particular region. The reduced second order model considered in this paper are models having no quadratic and no interaction terms only. The variation of central composite considered are the spherical central composite design (SCCD), rotatable central composite design (RCCD), orthogonal central composite design (OCCD), slope-rotatable central composite design (Slope-R) and face centered cube design (FCC). The basis of variation in these designs are the distance of the axial points from the center of the design. Also the performance of these designs were examined when the star or axial portions are replicated and center points, be one and three times. The optimality criteria that were used for this study are the D-, G- and A- optimality criteria. All these were considered for factors k = 3, 4, 5 and 6. However, because a design may be superior by one optimality criterion but may perform poorly when evaluated by another optimality criterion, fraction of design space (FDS) plot will also be used to evaluate the prediction capabilities of these designs.

2. METHODOLOGY

Reduced second order model is a technique for reducing the computational complexity of mathematical models in numerical simulation. These values are computed for the proposed model in eqn (1) and for "reasonable" reduced models that are formed by removing terms based on hierarchy. The set of reduced models is consistent with the definition of weak heredity given in [3] that is as follows

1. If a model contains an x_i^2 term, then it must contain the corresponding x_i term
2. If a model contains an $x_i x_j$ term, then it must contain the corresponding x_i or x_j or both terms.

Let 1's and 0's in the L, Q, and C columns indicate, respectively the presence or absence of the term x_i in the reduced model, p indicate 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. Tables 1 – 4 displays the number of models and terms in each of the factors *k* considered.

Table 1: Reduced Second Order Models for factor *k* = 3

Model	*P*	*dv*	*L*	*Q*	*C*	*(l, q, c)*
1	7	3	(1, 1, 1)	(0, 0, 0)	(1, 1, 1)	(3, 0, 3)
2	7	3	(1, 1, 1)	(1, 1, 1)	(0, 0, 0)	(3, 3, 0)

Table 2: Reduced Second Order Models for factor *k* = 4

Model	*p*	*dv*	*L*	*Q*	*C*	*(l, q, c)*
1	11	4	(1,1,1,1)	(0,0,0,0)	(1,1,1,1,1,1)	(4, 0, 6)
2	9	4	(1,1,1,1)	(1,1,1,1)	(0,0,0,0,0,0)	(4, 4, 0)

Table 3: Reduced Second Order Models for factor *k* = 5

Model	*p*	*dv*	*L*	*Q*	*C*	*(l, q, c)*
1	16	5	(1,1,1,1,1)	(0,0,0,0,0)	(1,1,1,1,1,1,1,1,1,1)	(5, 0,10)
2	11	5	(1,1,1,1,1)	(1,1,1,1,1)	(0,0,0,0,0,0,0,0,0,0)	(5, 5, 0)

Table 4: Reduced Second Order Models for factor *k* = 6

Model	p	dv	L	Q	C	(l, q, c)
1	22	6	(1,1,1,1,1,1)	(0,0,0,0,0,0)	(1,1,1,1,1,1,1,1,1,1,1,1,1,1,1)	(6, 0, 15)
2	13	6	(1,1,1,1,1,1)	(1,1,1,1,1,1)	(0,0,0,0,0,0,0,0,0,0,0,0,0,0,0)	(6, 6, 0)

This information matrix is used in calculating the robustness of design optimality criteria of reduced second order models. For each of the design considered, robustness is quantify by calculating the optimality measure over reduced model of the second order model in eqn(1)

D-efficiency $= \quad 100\dfrac{\left|\mathrm{X}^T\mathrm{X}\right|^{\frac{1}{p}}}{\mathrm{N}}$

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

A-efficiency = $\dfrac{100\,p}{trace\left[N\left(\mathrm{X}^T\mathrm{X}\right)^{-1}\right]}$

Where *N* is the design size, p is the number of model parameters, and $\hat{\sigma}^2_{\max}$ is the minimum of the maximum of $f^{T}(x)\left(\mathrm{X}^T\mathrm{X}\right)^{-1} f(x)$ approximated over the set of candidate points.

3. NUMERICAL RESULT

The D-, G- and A-optimality criteria for the reduced second order model comparisons of the five variation of CCD (RCCD, SCCD, OCCD, FCC and Slope-R) for factors *k* = 3, 4, 5 and 6 are summarized in tables below. For the optimality criteria; larger values imply a better design (on a per point basis). Let r_s indicate the replication of axial portion of the design, n_0 is the number of center points, *p* the number of parameters in the model and *N* the number of design runs.

3.1 Reduced Second Order Models having no Quadratic Terms (q = 0)

The reduced second order models having no quadratic terms in all the factors k considered (*k* = 3, 4, 5, and 6) show that G- and A- optimality criteria values of all the CCDs are the same. This implies that G- and A- optimality criteria are equivalent. Increase in the center points when the axial portion are not replicated decreases the D-, A- and G-optimality criteria values of the CCDs. Also replicating the axial portion (increasing r_s) with increase in the center points tend to decrease the D-, A- and G-optimality criteria of the CCDs. See Tables 5 – 8.

Table 5: Summary Statistics of Variation of Central Composite Designs of Reduced Second order model for *K* = 3

			No Quadratic term					No Interaction term			
Design	n_o	r_s	*P*	*N*	*D-eff*	*G-eff*	*A-eff*	*P*	*D-eff*	*G-eff*	*A-eff*

SCCD	1	1	7	15	74.16	71.14	71.14	7	80.47	46.67	27.74
	3	1		17	66.61	63.53	63.53		83.07	66.52	51.88
	1	2		21	64.76	58.21	58.21		85.91	33.33	21.43
	3	2		23	59.90	46.96	53.54		91.76	83.00	45.65
RCCD	1	1	7	15	73.37	70.57	70.57	7	76.58	47.21	27.39
	3	1		17	65.91	63.01	63.01		78.96	67.78	50.35
	1	2		21	63.80	57.68	57.68		81.22	33.89	21.23
	3	2		23	59.01	53.04	53.04		86.63	84.33	44.40
OCCD	1	1	7	15	66.75	65.22	65.22	7	51.49	81.33	33.46
	3	1		17	61.60	59.58	59.58		57.10	74.64	42.27
	1	2		21	61.78	56.50	56.50		53.27	98.77	35.19
	3	2		23	59.12	53.11	53.11		60.49	91.95	41.40
Slope-R	1	1	7	15	86.10	78.71	78.71	7	56.90	59.76	71.40
	3	1		17	69.65	65.11	65.11		69.60	55.51	80.63
	1	2		21	75.53	63.22	63.22		48.80	71.50	50.63
	3	2		23	66.08	56.59	56.59		58.80	75.50	61.46
FCC	1	1	7	15	64.20	62.92	62.92	7	41.46	83.99	26.58
	3	1		17	57.67	56.11	56.11		39.05	79.88	25.69
	1	2		21	52.03	49.56	49.56		42.23	89.65	31.33
	3	2		23	48.12	45.53	45.53		40.00	82.73	30.72

3.2 Reduced Second Order Models with No Interaction Terms(c = 0)

The reduced second order models with no interaction terms show different outcomes in each of the factors k considered.

For factor k = 3, Table 5 showed that replication of the axial portion with increase in center points increases the D-optimality criterion values of SCCD, RCCD and OCCD. Also replication of the axial portion with increase in center points increases the G-optimality criterion values of SCCD, RCCD and Slope-R. Finally, replication of the axial portion with increase in center points increases the A-optimality criterion values of the CCDs (SCCD, RCCD, OCCD, Slope-R and FCC).

For factor k = 4, Table 6 show that replication of the axial portion with increase in center points increases the D-optimality criterion values of SCCD, RCCD and OCCD. Replication of the axial portion with increase in center points also increases the G-optimality criterion values of SCCD and RCCD. Finally, replication of the axial portion with increase in center points increases the A-optimality criterion values of the CCDs except the FCC.

Table 6: Summary Statistics for Variations of Central Composite Designs of Reduced Second order model for *K* = 4

			No Interaction term					No Quadratic term			
Design	n_o	r_s	*P*	*N*	*D-eff*	*G-eff*	*A-eff*	*P*	*D-eff*	*G-eff*	*A-eff*
SCCD	1	1		25	86.59	36.00	23.67		77.24	75.64	75.64
	3	1		27	90.58	57.15	48.48	11	72.02	70.40	70.40
	1	2	9	33	96.97	27.27	19.08		66.63	62.86	62.86
	3	2		35	92.22	74.82	43.12		63.16	59.46	59.46
RCCD	1	1		25	86.59	36.00	23.67		77.24	75.64	75.64
	3	1		27	90.58	57.15	48.48	11	72.02	70.40	70.40
	1	2	9	33	93.23	52.23	28.95		66.63	62.86	62.86
	3	2		35	97.65	79.96	43.66		63.16	59.46	59.46
OCCD	1	1		25	54.58	64.29	33.96		72.28	71.54	71.54
	3	1		27	60.80	62.02	42.41	11	68.35	67.40	67.40
	1	2	9	33	59.84	84.86	39.50		60.00	58.28	58.28
	3	2		35	67.16	81.53	44.83		58.21	56.12	56.12
Slope-R	1	1		25	92.10	48.97	76.11		85.43	81.29	81.29
	3	1		27	90.97	47.18	83.67	11	78.38	74.88	74.88
	1	2	9	33	97.27	67.98	54.96		74.11	66.85	66.85
	3	2		35	95.00	66.77	63.71		68.31	62.32	62.32
FCC	1	1		25	34.96	67.54	18.19		69.57	69.05	69.05
	3	1		27	33.53	65.85	17.42	11	64.87	64.23	64.23
	1	2	9	33	37.37	92.83	24.64		56.16	55.07	55.07
	3	2		35	35.99	90.35	23.76		53.23	52.07	52.07

For factor k = 5, Table 7 shows that replication of the axial portion with increase in center points increases the D-optimality criterion values of SCCD, RCCD and OCCD. Also replication of the axial portion with increase in center points increases the G-optimality criterion values of the CCDs. Finally, replication of the axial portion with increase in center points increases the A-optimality criterion values of the CCDs except the FCC.

Table 7: Summary Statistics for Variation of Central Composite Designs of Reduced model for K = 5

			No Interaction term	No Quadratic term

Design	n_o	r_s	*P*	*N*	*D-eff*	*G-eff*	*A-eff*	*P*	*D-eff*	*G-eff*	*A-eff*
SCCD	1	1	11	27	95.15	40.74	27.53	16	59.57	69.34	69.34
	3	1		29	92.40	60.13	55.78		55.71	64.48	64.48
	1	2		37	84.80	29.73	21.47		52.59	61.11	61.11
	3	2		39	80.90	76.92	48.26		50.05	58.09	58.09
RCCD	1	1	11	27	87.01	66.67	31.37	16	56.56	68.81	68.81
	3	1		29	88.22	63.07	52.94		52.90	63.50	63.50
	1	2		37	96.27	42.94	27.30		49.69	60.52	60.52
	3	2		39	98.84	80.40	47.99		47.30	57.53	57.53
OCCD	1	1	11	27	42.26	72.58	28.86	16	50.45	65.62	65.62
	3	1		29	47.58	68.74	36.13		48.71	61.85	61.85
	1	2		37	67.06	87.98	47.00		43.88	59.22	59.22
	3	2		39	72.14	84.45	51.75		43.24	56.63	56.63
Slope-R	1	1	11	27	52.30	55.10	65.49	16	67.29	72.62	72.62
	3	1		29	61.90	53.83	75.97		60.97	67.04	67.04
	1	2		37	67.83	29.94	22.20		58.03	62.10	62.10
	3	2		39	51.90	73.22	56.20		52.69	58.59	58.59
FCC	1	1	11	27	31.68	75.15	16.55	16	42.07	63.04	63.04
	3	1		29	30.16	72.40	15.65		39.35	58.80	58.80
	1	2		37	33.03	95.20	21.87		36.13	57.60	57.60
	3	2		39	31.74	90.43	20.95		34.39	54.66	54.66

For factor k = 6, Table 8 shows that replication of the axial portion with increase in center points increases the D-optimality criterion values of SCCD, RCCD and OCCD. Also replication of the axial portion with increase in center points increases the G-optimality criterion values of SCCD and RCCD. Finally, replication of the axial portion with increase in center points increases the A-optimality criterion values of the CCDs.

Table 8: Summary Statistics for Variation of Central Composite Designs of Reduced model for K = 6

			No Interaction term					No Quadratic term			
Design	n_o	r_s	*P*	*N*	*D-eff*	*G-eff*	*A-eff*	*P*	*D-eff*	*G-eff*	*A-eff*
SCCD	1	1		45	98.60	28.89	20.99		78.77	77.94	77.94
	3	1		47	94.70	48.04	46.21		75.57	74.73	74.73
	1	2	13	57	84.10	22.81	17.39	22	67.14	65.05	65.05
	3	2		59	80.00	66.11	41.29		64.96	62.90	62.90
RCCD	1	1		45	96.37	29.75	21.28		78.44	77.66	77.66
	3	1	13	47	99.90	48.64	45.59	22	75.25	74.46	74.46
	1	2		57	81.21	23.89	17.92		66.68	64.75	64.75
	3	2		59	80.11	66.99	41.05		64.52	62.62	62.62
OCCD	1	1		45	61.94	51.61	38.06		75.80	75.45	75.45
	3	1	13	47	68.24	50.80	45.58	22	73.18	72.74	72.74
	1	2		57	71.42	72.70	47.01		63.02	62.11	62.11
	3	2		59	78.85	70.89	51.16		61.65	60.58	60.58
Slope-R	1	1		45	53.90	40.02	70.34		83.01	81.01	81.01
	3	1	13	47	55.50	39.62	77.55	22	79.06	77.29	77.29
	1	2		57	39.60	60.21	53.21		70.94	67.26	67.26
	3	2		59	43.60	60.01	62.12		67.85	64.61	64.61
FCC	1	1		45	25.15	53.14	9.84		73.43	73.25	73.25
	3	1	13	47	24.51	52.29	9.52	22	70.44	70.23	70.23
	1	2		57	29.21	82.81	15.29		59.51	59.11	59.11
	3	2		59	28.46	81.18	14.85		57.59	57.16	57.16

4. CONCLUSION

The reduced second order models having no quadratic terms in all the factors k considered show that G- and A- optimality criteria values of all the CCDs are the same. This implies that G- and A- optimality criteria are equivalent. Increase in the center points when the axial portion are not replicated decreases the D-, A- and G-optimality criteria values of the CCDs

The reduced second order model with no interaction terms the results showed that replication of the axial portion with increase in center points increases the D-optimality criterion values of SCCD, RCCD and OCCD in all the factors considered.

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