



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

J. C. Nwanya^{1*}, H. I. Mbachu¹ and K. C. N. Dozie¹

¹*Department of Statistics, Imo State University, Owerri, Imo State, Nigeria.*

Authors' contributions

This work was carried out in collaboration among all authors. Author JCN designed the study, performed the statistical analysis, wrote the protocol and wrote the first draft of the manuscript. Authors HIM and KCND managed the analyses and literature searches of the study. All authors read and approved the final manuscript

Article Information

DOI: 10.9734/ACRI/2019/v19i430164

Editor(s):

(1) Amal Hegazi Ahmed Elrefaei, Division of Radioisotope Production, Hot Laboratory and Waste Management Center, Atomic Energy Authority, Egypt.

Reviewers:

(1) Francisco Bulnes, USA.

(2) Gajendra Sharma, Kathmandu University, Nepal.

Complete Peer review History: <http://www.sdiarticle4.com/review-history/54325>

Received 24 November 2019

Accepted 28 January 2020

Published 11 February 2020

Original Research Article

ABSTRACT

Choosing a response surface design to fit certain kinds of models is a difficult task. This work focuses on the reduced second order models having no quadratic and no 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 show that for models having no quadratic terms that G- and A-optimality criteria are equivalent and 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 terms, 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. Finally, the work have shown that replication of the axial portion reduces the performance of the CCDs with models having no quadratic terms and Slope-R is a better design with respect to D- and A-optimality criteria.

Keywords: CCDs; FDS; SCCD; RCCD; OCCD; Slope-R; FCC.

*Corresponding author: Email: nwjulius@imsu.edu.ng;

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 $y = \eta(x_1, x_2, \dots, x_k) + \varepsilon$ where y is the response, η is the true unknown function, x_1, x_2, \dots, 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.

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

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 Eq. (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. Box and Draper [1] developed a mean square error design criterion which provides protection against bias error due to model inadequacy. Karson, et al. [2] also studied the design-selection problem when the proposed approximating model is an underparameterized approximation of the true response surface. Chipman [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. Li and Nachtsheim [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. Borkowski and Valeroso [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 Borkowski and Valeroso [5], Chomtee and Borkowski [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. Yakubu and Chukwu [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. Iwundu and Jaja [8] did a precision of full polynomial response surface designs on models with missing coefficients using the D- and G-efficiency measures. Their results show that studying the precision of using constructed full model designs on reduced models, the first-order designs had lower loss in D-efficiency as well as

G-efficiency when used on reduced first-order model.

Oyejola and Nwanya [9] 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. Onyeneke and Effanga [10] applied reduced second order model of convex optimization in paper producing industries. They used the rotatable central composite designs (RCCD), and obtained a reduced quadratic model that met our barite and calcite production prerequisites used in favor of improving grinding conditions in paper producing industries.

This study examines the performance of the CCDs under reduced models using the optimality criteria (D, G and A). The variations of central composite design were considered without any particular region of interest. 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 axial portions are replicated twice with one and three center points. All these were considered for factors $k = 3, 4, 5$ and 6 .

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 Eq. (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

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)	(1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1)	(6, 0, 15)
2	13	6	(1,1,1,1,1,1)	(1,1,1,1,1,1)	(0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0)	(6, 6, 0)

models and terms in each of the factors k considered.

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 Eq. (1)

$$D\text{-efficiency} = \frac{100}{N} \frac{|X^T X|^{\frac{1}{p}}}{N}$$

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

$$A\text{-efficiency} = \frac{100p}{\text{trace}[N(X^T X)^{-1}]}$$

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

3. NUMERICAL RESULT AND DISCUSSION

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 5-8. 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.

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.

Table 5. Summary statistics of variation of central composite designs of reduced second order model for $K = 3$

Design	n_0	r_s	P	No Quadratic term				No Interaction term			
				N	D-eff	G-eff	A-eff	P	D-eff	G-eff	A-eff
SCCD	1	1		15	74.16	71.14	71.14		80.47	46.67	27.74
	3	1		17	66.61	63.53	63.53		83.07	66.52	51.88
	1	2	7	21	64.76	58.21	58.21	7	85.91	33.33	21.43
	3	2		23	59.90	46.96	53.54		91.76	83.00	45.65
RCCD	1	1		15	73.37	70.57	70.57		76.58	47.21	27.39
	3	1		17	65.91	63.01	63.01		78.96	67.78	50.35
	1	2	7	21	63.80	57.68	57.68	7	81.22	33.89	21.23
	3	2		23	59.01	53.04	53.04		86.63	84.33	44.40
OCCD	1	1		15	66.75	65.22	65.22		51.49	81.33	33.46
	3	1		17	61.60	59.58	59.58		57.10	74.64	42.27
	1	2	7	21	61.78	56.50	56.50	7	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		15	86.10	78.71	78.71		56.90	59.76	71.40
	3	1		17	69.65	65.11	65.11	7	69.60	55.51	80.63
	1	2	7	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		15	64.20	62.92	62.92		41.46	83.99	26.58
	3	1	7	17	57.67	56.11	56.11	7	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

Table 6. Summary statistics for variations of central composite designs of reduced second order model for $K = 4$

Design	n_o	r_s	P	No Interaction term				No Quadratic term			
				N	$D\text{-eff}$	$G\text{-eff}$	$A\text{-eff}$	P	$D\text{-eff}$	$G\text{-eff}$	$A\text{-eff}$
SCCD	1	1		25	86.59	36.00	23.67	11	77.24	75.64	75.64
	3	1		27	90.58	57.15	48.48		72.02	70.40	70.40
	1	2	9	33	96.97	27.27	19.08		66.63	62.86	62.86
RCCD	3	2		35	92.22	74.82	43.12		63.16	59.46	59.46
	1	1		25	86.59	36.00	23.67	11	77.24	75.64	75.64
	3	1		27	90.58	57.15	48.48		72.02	70.40	70.40
OCCD	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
	1	1		25	54.58	64.29	33.96	11	72.28	71.54	71.54
Slope-R	3	1		27	60.80	62.02	42.41		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
FCC	1	1		25	92.10	48.97	76.11	11	85.43	81.29	81.29
	3	1		27	90.97	47.18	83.67		78.38	74.88	74.88
	1	2	9	33	97.27	67.98	54.96		74.11	66.85	66.85
FCC	3	2		35	95.00	66.77	63.71		68.31	62.32	62.32
	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
FCC	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

Table 7. Summary statistics for variation of central composite designs of reduced model for $K = 5$

Design	n_o	r_s	P	No Interaction term				No Quadratic term			
				N	$D\text{-eff}$	$G\text{-eff}$	$A\text{-eff}$	P	$D\text{-eff}$	$G\text{-eff}$	$A\text{-eff}$
SCCD	1	1		27	95.15	40.74	27.53		59.57	69.34	69.34
	3	1	11	29	92.40	60.13	55.78	16	55.71	64.48	64.48
	1	2		37	84.80	29.73	21.47		52.59	61.11	61.11
RCCD	3	2		39	80.90	76.92	48.26		50.05	58.09	58.09
	1	1		27	87.01	66.67	31.37		56.56	68.81	68.81
	3	1	11	29	88.22	63.07	52.94	16	52.90	63.50	63.50
OCCD	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
	1	1		27	42.26	72.58	28.86		50.45	65.62	65.62
Slope-R	3	1	11	29	47.58	68.74	36.13	16	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
FCC	1	1		27	52.30	55.10	65.49		67.29	72.62	72.62
	3	1	11	29	61.90	53.83	75.97	16	60.97	67.04	67.04
	1	2		37	67.83	29.94	22.20		58.03	62.10	62.10
FCC	3	2		39	51.90	73.22	56.20		52.69	58.59	58.59
	1	1		27	31.68	75.15	16.55		42.07	63.04	63.04
	3	1	11	29	30.16	72.40	15.65	16	39.35	58.80	58.80
FCC	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 $k = 3$, 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).

Table 8. Summary statistics for variation of central composite designs of reduced model for K = 6

Design	n_o	r_s	P	No Interaction term				No Quadratic term			
				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
RCCD	3	2		59	80.00	66.11	41.29		64.96	62.90	62.90
	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
OCCD	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
	1	1		45	61.94	51.61	38.06		75.80	75.45	75.45
Slope-R	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
FCC	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
	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

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.

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.

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.

4. CONCLUSION

This study have shown that the CCDs in the reduced second order models considered in this work are sensitive when D-, A- and G-optimality criteria are used. 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 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. Finally, the work have showed that replication of the axial portion reduces the performance of the CCDs with models having no quadratic terms and Slope-R is a better design with respect to D- and A-optimality criteria.

COMPETING INTERESTS

Authors have declared that no competing interests exist.

REFERENCES

1. Box GEP, Draper NR. The choice of a second order rotatable design. *Biometrika*. 1963;50:352–335.
2. Karson MJ, Manson AR, Hader RJ. Minimum bias estimation and experimental designs for response surfaces. *Technometrics*. 1969;11:475-461.
3. Chipman HA. Bayesian variable selection with related predictors. *The Canadian Journal of Statistics*. 1996;24:36-17.
4. Li C, Nachtshiem CJ. Model robust factorial designs. *Technometrics*. 2000;42: 352-345.
5. Borkowski JJ, Valeroso ES. Comparison of design optimality criteria of reduced models for response surface designs in the hypercube. *Technometrics*. 2001;43:477-468.
6. Chomtee B, Borkowski JJ. Comparison of response surface designs in spherical region. *World Academy of Science, Engineering and Technology*. 2012;65:4-1.
7. Yakubu Y, Chukwu AU. Comparison of optimality criteria of reduced models for response surface designs with restricted randomization. *Progress in Applied Mathematics*. 2012;4:126-110 .
8. Iwundu MP, Jaja EI. Precision of full polynomial response surface designs on models with missing coefficients. *International Journal of Advanced Statistics and Probability*. 2017;5(1):36-32.
9. Oyejola BA, Nwanya JC. Selecting the right central composite design. *International Journal of Statistics and Application*. 2015;5(1):30-21.
10. Onyeneke CC, Effanga EO. Application of reduced second order response surface model of convex optimization in paper producing industries. *International Journal of Theoretical and Applied Mathematics*. 2016;2(1):23-13.

© 2019 Nwanya et al.; This is an Open Access article distributed under the terms of the Creative Commons Attribution License (<http://creativecommons.org/licenses/by/4.0>), which permits unrestricted use, distribution, and reproduction in any medium, provided the original work is properly cited.

Peer-review history:
The peer review history for this paper can be accessed here:
<http://www.sdiarticle4.com/review-history/54325>