CSCanada
Studies in Mathematical Sciences
Vol. 4, No. 1, 2012, pp. 22-29
DOI: 10.3968/j.sms.1923845220120401.1522

ISSN 1923-8444 [Print]
ISSN 1923-8452 [Online]
www.cscanada.net
www.cscanada.org

Sensitivity of Design Optimality Criteria to Second-Order Response Surface Model Restrictions and Center Point Replications

Angela U. Chukwu[1,*]; Yisa Yakubu[2]

[1]Department of Statistics, University of Ibadan, Oyo state, Nigeria
[2]Department of Mathematics and Statistics, Federal University of Technology, Minna, Niger State, Nigeria.
[*]Corresponding author.
Address: Department of Statistics, University of Ibadan, Oyo state, Nigeria

Received 17 December, 2011; accepted 16 February, 2012

Abstract
In this work, we investigate the role of several model characteristics and center point replications on the properties of ***A-, D-, G-,*** and***IV***- optimality for four –factor second-order response surface design. It was discovered that*A-, D-, and G-* efficiencies tend to reduce as the center points are replicated while the effect on scaled average prediction variance tends to be very insignificant. Among the restricted models considered, the pure linear model (model1) turns out to be the best in terms of quality of estimation and model prediction.

Key words
Design optimality criteria; Center point replications; Response surface methodology

Angela U. Chukwu, Yisa Yakubu (2012). Sensitivity of Design Optimality Criteria to Second-order Response Surface Model Restrictions and Center Point Replications. *Studies in Mathematical Sciences, 4*(1), 22-29. Available from: URL: http://www.cscanada.net/index.php/sms/article/view/j.sms.1923845220120401.1522 DOI: http://dx.doi.org/10.3968/j.sms.1923845220120401.1522

INTRODUCTION

Experiments are performed in virtually all fields of inquiry usually to discover something about a particular process or system. Designed experiments allow the analyst to control the factors thought to be important in characterizing or explaining the response variable(s) of the experiment. Response surface methodology (RSM) is an area of experimental design which consists of a group of mathematical and statistical techniques used in the development of an adequate functional relationship between a response of interest, y, and a number of associated input variables (Montgomery D. C., 2001).Usually, the form of the relationship is unknown but can be approximated, within the experimental region, by a low degree polynomial such as the second –order response surface model

$$y = \beta_0 + \sum_{i=1}^{k}\beta_i x_i + \sum_{i=1}^{k}\beta_{ii}x_i^2 + \sum_{i=1}^{k-1}\sum_{j=i+1}^{k}\beta_{ij}x_i x_j + e \tag{1}$$

where y represents the measured response, $\hat{\beta}$s are parameter coefficients and e is anterm(independently and normally distributed with mean zero and common variance σ_e^2) that accounts for random error and bias (Khuri, A. I. and Cornell, J. A. 1996).

A popular response surface design that utilizes the above model is the central composite design (CCD), first introduced by Box and Wilson (1951). The k-factor CCD consists of

i. a complete (or a fraction of) 2^k factorial design denoted by f,

ii. an axial portion consisting of $2k$ points arranged so that two points are chosen on the axis of each control variable at a distance ofα from the design center,

iii. n_0 center points.

Thus in a CCD, $n = f + 2k + n_0$.(Khuri and Connell, 1996).

After data are generated from the experiment and a model is fitted, many parameters in the fitted model are deemed insignificant. Therefore, a reduced model retaining only the significant terms is adopted for use, but the researcher is also faced with the problem of selecting a model that gives the desired optimal design.

Design optimality criteria based on the adopted reduced model are equally if not more important than the optimality criteria for the proposed full model (Borkowski and Valereso, 2001). Therefore, a design should be *robust* over classes of reduced models; that is, the design should maintain high optimality criteria over a wide assortment of potential models.

Many authors (e.g., Box and Draper 1959, 1963; Karson, Manson, and Hader 1969) have studied the design-selection problem when the proposed approximating model is an *underparameterized* approximation of the true response surface. In such cases, use is made of a low-order polynomial when a higher-order polynomial is a better approximating function. With regard to this design problem, some authors (e.g., Box and Draper (1987), Myers, Montgomery and Anderon-Cook (2009), and, Khuri and Cornell (1996)) also have used the integrated mean squared error ($IMSE = V + B$), where

$$B = \frac{N\Omega}{\sigma^2} \int_R [E(\hat{y}(x) - \eta(x)]^2 dx \tag{2}$$

is the systematic (squared) bias resulting from underestimation of the true response surface with the fitted low-order model;

$$V = \frac{N\Omega}{\sigma^2} \int_R Var[(\hat{y}(x))]dx \tag{3}$$

is the prediction variance, and $\Omega^{-1} = \int_R dx$.

The research by Borkowski and Elsie (2001) addresses the problem in a different dimension. These authors provide an evaluation of the robustness properties of some standard response surface designs (CCD, SCD, NHD, and computer- generated algorithmic designs) over a collection of reduced models based on ***D***−,***G***−,***A***−, and ***IV***- optimality criteria. Thesereduced models are formed by removing terms one after the other from the proposed model.

In this article, we investigate the role of several model characteristics and center point replications on the properties of *A*-, *D*-, *G*-, and *IV*- optimal designs for the model (1) above. The impacts of the designs for a pure linear model, a linear model with two-factor interactions, a linear model with squares, and a full quadratic model,on the properties of *A*-, *D*-, *G*-, and *IV*-optimalityfor a k = four-factor, 25-run CCD with one center run are first investigated. Then we investigate the impacts of these same designs under various numbers of experimental runs. Lastly, we investigate the effects on *A*-, *D*-, *G*-, and *IV*- optimality for the k = four-factor, 25-run full quadratic CCD at various numbers of replications of the center points. These measures are quantified by calculating D, A, and G efficiencies and the *IV* criterion.

In this article, designs were generated using *Design expert version 8.0.6* and *Minitab15* packages.The optimality criteria and efficiency values were computed using *Maple13* package.

1. MATERIALS AND METHODS

Four models consisting of three restricted and one unrestricted were studied in this work. The models are

Model 1:

$$y_i = \beta_0 + \beta_1 x_{1i} + \beta_2 x_{2i} + \beta_3 x_{3i} + \beta_4 x_{4i} + \varepsilon_i \tag{4}$$

Model 2:

$$y_i = \beta_0 + \beta_1 x_{1i} + \beta_2 x_{2i} + \beta_3 x_{3i} + \beta_4 x_{4i} + \beta_{12} x_{1i} x_{2i} \beta_{13} x_{1i} x_{3i} + \beta_{14} x_{1i} x_{4i} + \beta_{23} x_{2i} x_{3i} + \beta_{24} x_{2i} x_{4i} \beta_{34} x_{3i} x_{4i} + \varepsilon_i \quad (5)$$

Model 3:

$$y_i = \beta_0 + \beta_1 x_{1i} + \beta_2 x_{2i} + \beta_3 x_{3i} + \beta_4 x_{4i} + \beta_{11} x_{1i}^2 + \beta_{22} x_{2i}^2 + \beta_{33} x_{3i}^2 + \beta_{44} x_{4i}^2 + \varepsilon_i \quad (6)$$

Model 4:

$$\begin{aligned} y_i = & \beta_0 + \beta_1 x_{1i} + \beta_2 x_{2i} + \beta_3 x_{3i} + \beta_4 x_{4i} + \beta_{12} x_{1i} x_{2i} + \beta_{13} x_{1i} x_{3i} + \beta_{14} x_{1i} x_{4i} \\ & + \beta_{23} x_{2i} x_{3i} + \beta_{24} x_{2i} x_{4i} + \beta_{34} x_{3i} x_{4i} + \beta_{11} x_{1i}^2 \beta_{22} x_{2i}^2 + \beta_{33} x_{3i}^2 + \beta_{44} x_{4i}^2 \varepsilon_i \end{aligned} \quad (7)$$

The corresponding designs are investigated for the role of center point replications and the properties of ***A***−,***D***−,***G***-, and ***IV***- optimality criteria under n = 15, 20 and 25 experimental runs.Since each response surface model generally has its own optimal design, the researcher is always faced with the problem of selecting an efficient design at the design stage without knowing which model is the best fitting one.

2. DESIGN OPTIMALITY CRITERIA

Limited resources due to time and cost constraints are inherent to most experiments. Therefore the user typically approaches experimentation with a desire to minimize the number of experimental trials while still being able to estimate adequately the underlying model.

Design optimality criteria are single-number summaries for quality properties of the design such as the precision with which the model parameters are estimated or the uncertainty associated with prediction. These criteria address the design's model estimation or prediction quality through the use of variance characteristics. An optimal designselects design points and allocates the required number of subjects to each levelcombination of the independent variables to attain the smallest possible value of $var(\hat{\beta})$ as measured by the optimality criterion of interest.

The four commonly-used optimality criteria are ***A***-, ***D***-, ***G***-, and ***IV***- optimality criteria.

The *D*-optimality criterion minimizes the product of the squaredlengths of the axes of the ellipsoid and is proportional to the volume of theconfidence ellipsoid. It is the determinant of the information matrix $M(\xi)$. That is,

D-criterion ◊ minimize $|M^{-1}(\xi)|$, or equivalently, maximize $|M(\xi)|$

The *A*-optimality criterion minimizes the sum of the squared lengthsof the axes, which indirectly measures the size of the ellipsoid. This is the sameas minimizing the trace of the inverse of the information matrix.

A-criterion goal◊ minimize trace $[M^{-1}(\xi)]$

A*G*-optimal design is a design that minimizes the maximum standardized varianceof the predicted response over the design space *R*.

G-criterion goal ◊ minimize $\max_{x \in R}[N f'(x) M^{-1}(\xi) f(x)]$ and

IV-criterion goal ◊ minimize average $[N f'(x) M^{-1}(\xi) f(x)]$ over $x \in R$,

Where **X** is the design matrix, **x** is any point in the design region *R*, N is the design size and $f(x) = [f_1(x), \ldots, f_p(x)]$ is a vector of *p* real- valued functions based on the *p* model terms.

A and *D* criteria examine the design's estimation quality while ***G*** and *IV* criteria are based on the scaled prediction variance $V(x)$, which is a function of the variance for the above fitted response model (1). The predicted value at a point **x** is

$$\hat{y}(x) = f'(x)\hat{\beta} \quad (8)$$

where $\hat{\beta} = (X'X)^{-1}X'y$ is the OLS estimator of β and $f'(x)$ is the vector corresponding to the model terms in (1). The *scaledprediction variance* at a point **x**(Box and Hunter, 1957) is given by

$$V(x) = \frac{N}{\sigma^2} Var(\hat{y}(x)) = N f'(x)(X'X)^{-1} f(x) \qquad (9)$$

For each of the design sizes considered, the *D*, *A*, *G*, and *IV*optimality measures were calculated over reduced models of the second –order model in (1). These measures quantify the role of the model characteristics. We have

D efficiency = $100\frac{|x'x|^{1/p}}{N}$,
A efficiency = $100\frac{p}{trace[N(X'X)^{-1}]}$,
G efficiency = $100\frac{p}{N\sigma^2_{\max}}$,
IV efficiency = $N\sigma^2_{ave}$,

where N is the design size, p is the number of model parameters, σ^2_{ave} is the average of N**f**'(**x**)(**X'X**)$^{-1}$f(**x**) over the design region, and σ^2_{ave} is the maximum of N**f**'(**x**)(**X'X**)$^{-1}$f(**x**) approximated over the set of points from a 5^k factorial designs (with factor levels 0, ±1.414,±1).

3. RESULTS AND DISCUSSIONS

We first consider the role of model restriction on ***A*-, *D*-, *G*-,** and ***IV***- optimality property of the designs. These optimality criteria values were computed for each design and their corresponding efficiencies are plotted as given in figure 1, (a), (b), (c), and (d) below.

From this figure, we observe that the pure linear model (model1) is the best in terms of $A-$, $D-$,and$G$-efficiencies. That is, in terms of quality of estimation and model prediction, this model is the best among the four models considered here, while models 3 and 4 turn out to be the best in terms of *IV*-efficiency.

Next we consider each of the four models under various numbers of experimental runs. The number of runs we consider here are $n = 15$, 20, and 25. The optimality criteria values were calculated for each design and their corresponding efficiencies plotted. **Figure 2**, (a), (b), (c), and (d) below shows plots of *A*, *D*, *G*, and *IV* efficiencies for each of these models against the number of experimental runs. The following patterns are observed:

1. For ***A:*** this efficiency increases slightly for model1 (pure linear model) as the number of experimental runs increases (indicating less variability of *A*-efficiency for this model to changes in design size). The efficiency decreases with increasing *n* for model2 (linear model with interactions). Models 3 and 4 follow almost the same pattern under this efficiency. The effect of increasing *n* on A-efficiency for these models is inconsistent and depends on the value of n.

2. For ***D***: the *D*-efficiency plot for model 1 is very similar to the *A*-efficiency plot. For model2, this efficiency is also close to that of *A* with slight difference. That of model3 increases slightly with increasing n while that for model4 is similar to the *A* plots.

3. For ***G***: this efficiency increases dramatically for model1 as *n* increases, with a slight bend at n = 20. For models 2 and 4, there is a sharp increase in this efficiency as n moves from 15 to 20 and the same decrease at n = 20. While model3 decreases sharply with increasing n from 15 to 20 and then increases at n = 20.

4. For ***IV:*** models 1 and 2 decreases in this efficiency as n increases, though in a slightly different manner. While model 3 seems to be stationary with increasing n, model4 increases dramatically with slight bend as n increases.

From **figure 2** above, model1 is the best under *A*- and *G*- efficiencies, while models 1 and 3 are the best under *D*-efficiency. These efficiencies increase for this model as the number of experimental runs increases. Under *IV*-efficiency, model4 is the best.

Lastly, we investigate the role of number of center point replications on the *A*-, *D*-, *G*-, and *IV*- optimality property for the four-factor (full quadratic) CCD. The criterion value of each of these optimality properties is computed and the corresponding efficiency plotted, as given below.

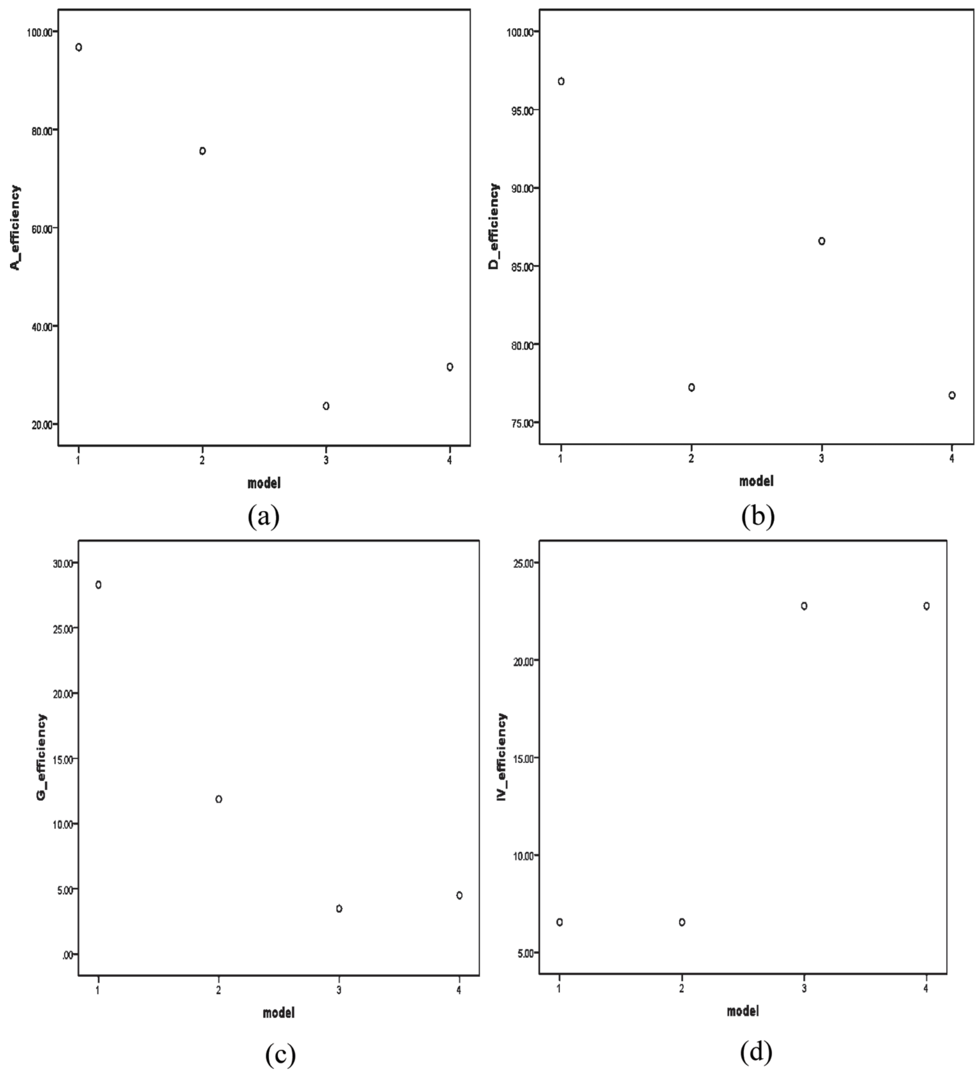

Figure 1
Plots of Model Efficiencies for Four-Factor (25 Run) CCD With One Center Point. The Models are– Pure Linear Model (Model1), Pure Linear Model with Two-Factor Interactions (Model2), Pure Linear Model with Squares (Model3), and Full Quadratic Model (Model4).

Figure3 above shows plots of *A*-, *D*-, *G*-, and *IV*- efficiencies for the four-factor (full quadratic) CCD against various numbers of center point replications. We can see that *A*-, *D*-, *and G*- efficiencies are reduced as the center points are replicated with the *D*-efficiency being the worst. The effect of increasing center point on *IV* tends to be very insignificant. Though the model we consider here is a full quadratic model, these results agree perfectly with those of Borkowski and Valereso, 2001, for their reduced models.

CONCLUSION

From the second-order design model (CCD) we considered in this work, we have shown that optimality criteria are sensitive to center point replications and model restrictions. Therefore when a researcher is faced with a decision of which response surface design to choose, based on one or more optimality criteria, it is important that these criteria be first determined over a subset of restricted models and numbers of

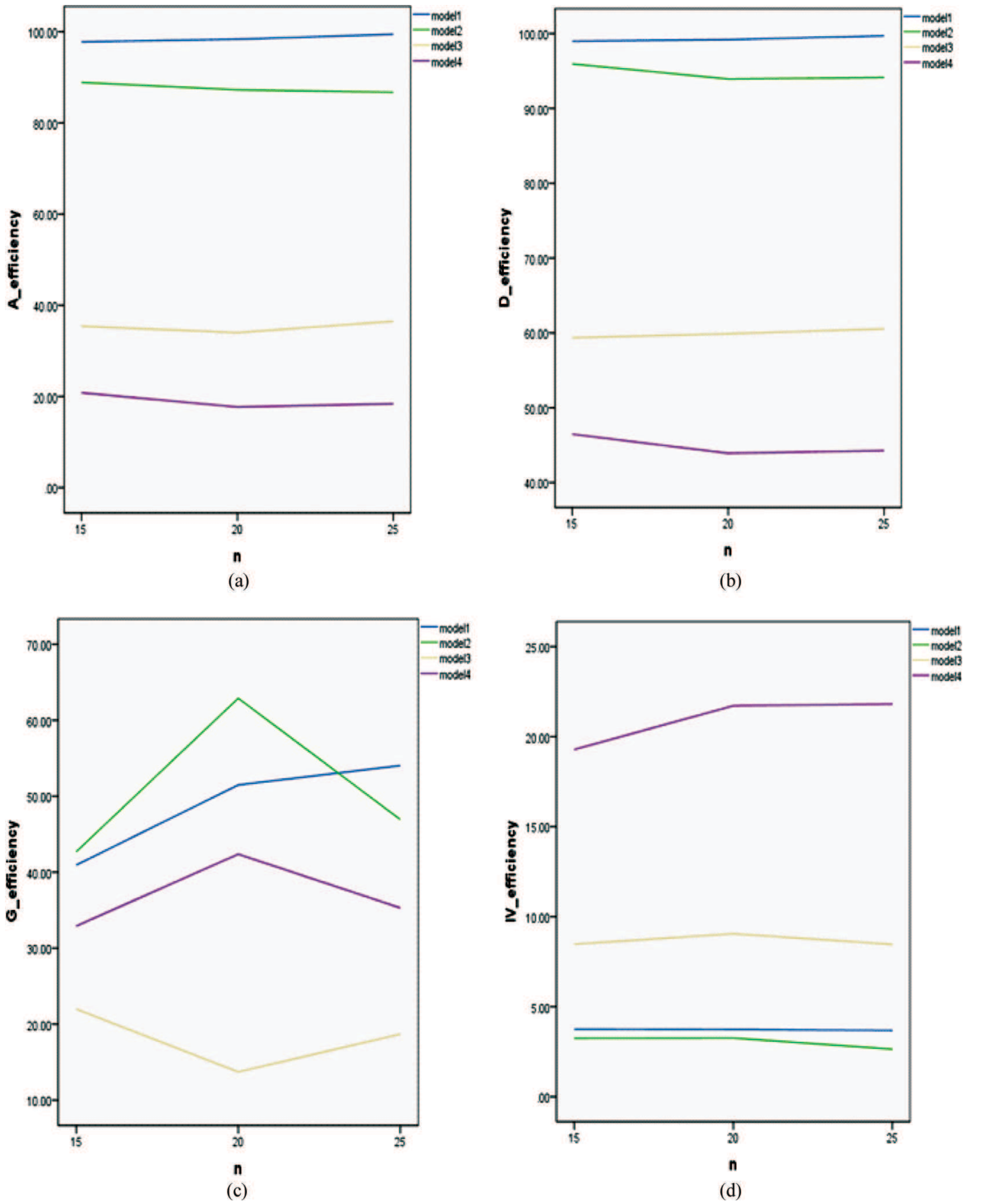

Figure 2

Plots of Model Efficiencies for the Four-Factor (n = 15, 20, and 25) CCD With One Center Point. The Models are–Pure Linear Model (Model1), Pure Linear Model with Two-Factor Interactions (Model2), Pure Linear Model with Squares (Model3), and Full Quadratic Model (Model4).

experimental runs. These criteria are not robust to restricted models and design size.

We have observed that the pure linear model is the best in terms of $A-$, $D-$,and$G$-efficiencies. That is, in terms of quality of estimation and model prediction, this model is the best among the four models considered here, while models 3 and 4 turn out to be the best in terms of scaled average prediction variance

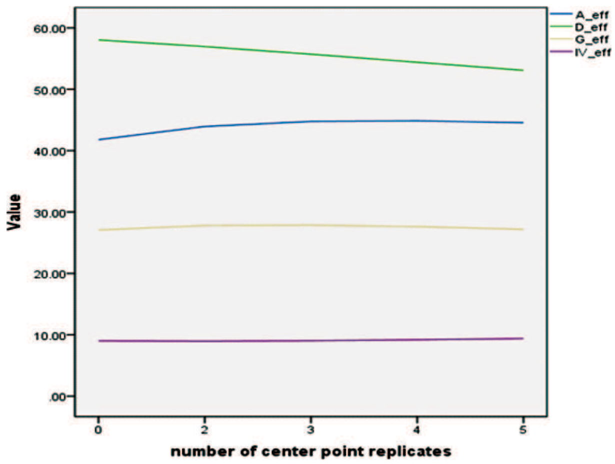

Figure 3

Plots of A-, D-, G-, and IV- Efficiencies for the Four-Factor(Full Quadratic) CCD with Various Numbers of Center Point Replications.

efficiency.

Also, under *A*−, *D*-, and *G*- efficiencies, the pure linear model increases as the number of experimental runs increases.

We see that *A-, D-, and G-* efficiencies are reduced as the center points are replicated with the *D*-efficiency being the worst. The effect of increasing center point on scaled average prediction variance tends to be very insignificant.

Therefore we observed that optimal design selects design points and allocates the required number of subjects to each levelcombination of the independent variables to attain the smallest possible value of $var(\hat{\beta})$ as measured by the optimality criterion of interest.

REFERENCES

[1] Atkinson, A. C., Donev, A. N. Donev & Tobias, R. D. (2007). *Optimum Experimental Designs, with SAS* (1st edition). New York: Oxford University Press.

[2] Box, G. E. P. & Wilson, K.B. (1951). On the Experimental Attainment of Optimum Conditions (with discussions). *Journal of the Royal Statistical Society Series B*, *13*(1), 1-45.

[3] Box, E.P. George, Hunter, J. Stuart & Hunter, G. William (2005). *Statistics forExperimenters*. New Jersey: John Willey and Sons, Inc.

[4] Box, G. E. P. & Drapper N. R. (1975). Robust Designs. *Biometrika*, *62*(2), 347-352.

[5] Box, G. E. P. & Draper, N. R. (1963). The Choice of a Second Order Rotatable Design, *Biometrika*, *50*, 335-352.

[6] Box, G. E. P. & Draper, N. R. (1959). A Basis for the Selection of a Response Surface Design, *Journal of the American Statistical Association*, *54*, 622-654.

[7] Box, G. E. P. & Behnken, D.W. (1960). Some New Three Level Designs for the Study of Quantitative Variables. *Technometrics*, *2*, 455-475.

[8] Box, G. E. P. & Hunter, J. S. (1957). Multi-Factor Experimental Designs for Exploring Response Surfaces, *The Annals of Mathematical Statistics*, *28*, 195-241.

[9] Daniel, C. (1976). *Applications of Statistics to Industrial Experiments.* New York: Wiley.

[10] John J. B. & Valeroso E. S. (2001). Comparison of Design Optimality Criteria of Reduced Models for Response Surface Designs in the Hypercube. *Technometrics, 43*(4), 468-477.

[11] Karson, M. J., Manson, A. R., & Hader, R. J. (1969). Minimum Bias Estimation and Experimental Designs for Response Surfaces, *Technometrics, 11*, 461-475.

[12] Khuri, A. I. & Cornell, J. A. (1996). *Response Surfaces: Design and Analysis.* New York: Marcel Dekker.

[13] Montgomery, D. C. (2001). *Design and Analysis of Statistical Experiments* (5^{th} edition). New York: John Wiley & Sons.

[14] Martijn P. F. Berger & Weng Kee Wong (2009). *An Introduction to Optimal Designs for Social and Biomedical Research* (1^{st} edition). U.K: John Wiley & Sons, Ltd,

[15] Raymond, H. M., Douglas, C. Montgomery & Christine M. Anderson-Cook (2009). *Response Surface Methodology: Process and Product Optimization using Designed Experiments* (3^{rd} ed.). John Wiley and Sons.