Sequential third-order response surface designs

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The use of third-order response surface designs suggests experimental situations involving second-order lack-of-fits. New sequential third-order response surface designs are proposed for use in modeling third-order effects using very simple mathematical principles. The experimental runs admitted into the designs are hat matrix aided and the new designs show high design efficiencies. Grid formation is adopted as a principle of discretizing a continuous design space. For a cuboidal region in k dimensions, five grid levels are utilized and the associated 5^k grid points form the candidate set for consideration in design construction. The new sequential designs are augmentations of the standard central composite designs and are generated using block of points corresponding to some diagonal elements of the hat matrix. All designs studied in two and three variables have very good optimality properties.

Keywords: Sequential designs, Third-order response surfaces, Hat matrix, Cuboidal region, Efficiency.

1 Introduction

Like all Response Surface Methodology (RSM) approximating functions, the third-order model is used for approximating the unknown response function that is assumed to contain cubic effects. Until in recent studies, low-order polynomials (first- and second-order) were considered suitable for modeling and optimization studies involving responses and a number of independent variables. The first-order main effects model represents a linear function. However, when there is a suspected case of interactions between the design factors, interaction terms are added to the first-order main effects model to give a better model fit and adequacy. When there is a curvature in the response function, the first-order model including its interaction is inadequate. In such case, the second-order model becomes imperative (Koukouvinos et al., 2009). The second-order model includes all the first-order terms, its cross product terms and all the pure quadratic terms. Furthermore, when it appears that there is a lack-of-fitin the second-order model, a third-order model must be applied. The third-order model consists of the first-order terms, cross product terms, all the quadratic terms, cross products with the quadratic terms and the cubic terms. Generally, when the d-th-order model appears insufficient to describe the true existing relationship between the response of interest and the predictor variables due to the presence of higher terms or lack-of-fit, then a (d+1)th-order is required to fit the model adequately.

A growing number of researchers are now seeing the need for the third-order response surface designs in the face of failing second-order models and designs. Among authors who have studied third-order response surface designs are Landman et al. (2007) who in an exploratory study involving wind-tunnel testing of high performance aircraft developed a hybrid third-order design called a Nested Face Centered Design (NFCD). The study was to

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adequately characterize an aircraft's aerodynamic behavior while simultaneously reducing the test time. However, in the course of the study it became obvious that the classic second-order Central Composite designs showed inadequacy in prediction qualities over a cuboidal design space. This led to the need for a higher order model thus giving rise to the use of third-order design. The NFCD is a nested fractional factorial design with design points supported at five levels of the control variables and augmented with both axial and center points. This design allowed the use of regression models including pure cubic terms for the characteristic aerodynamic forces and defines moments over a cuboidal design space as a function of model position and control surface deflections.

Practically, third-order models and designs become imperative when it is obvious that there is a lack-of-fit of the second-order polynomial models and designs. A response surface model presents lack-of-fit when it fails to satisfactorily describe the functional relationship existing between the experimental factors and the response variable. Lack-of-fits also occurs if important terms from the model involving interactions, quadratic or higher terms are exempted from the model and/or if several extremely large residuals result from fitting the model (Balasubramanian, 2010). The problem of lack-of-fit of models biases estimation. For better estimation and approximation, there is a mandatory need for a higher model. Although many field problems may be satisfactorily modeled using some second-order models, some show the need for higher models when the lack-of-fit of the second-order model is reported (See Seshubabu et al., 2014). At such point, third-order or even higher-order models are required to overcome the lack-of-fit. The cases of second-order lack-of-fit recorded in literatures reveal the challenges researchers encounter in modeling problems. For second-order lack-of-fitthe reasonable solution is to consider a third-order model or even higher. It is in view of such need that this research is carried out to obtain new third-order response surface designs that are simple to construct and can adequately be used in the presence of second-order lack-of-fit. Unlike many third-order designs requiring rigorous algebraic derivation, construction of the new designs in this research utilizes very simple mathematical principles that can be used by any researcher with fair knowledge of Matrix Algebra.

An advantage of the response surface techniques is that it is sequential in nature where experiments can be performed in different stages. Thus, results obtained from one set of experiments can be employed to successfully prepare the strategy for a next set of experiments (Khuri, 2017). Building a design sequentially is very useful as it enables the efficient estimation of first, second or higher-order terms. By means of some augmentation, previous designs can be used for higher-order models thus researchers do not need to start experimentation from the scratch anytime there is a need for higher order designs. The use of central composite designs in sequential methods was discussed in Derringer (1969) and has great advantage in the sense that most experimental studies requiring second-order designs use the central composite design. These designs permit progressing to higher order surfaces sequentially. The aim of this research is thus to generate new third-order response surface designs that are easy to construct and possess some superior optimality properties when compared with existing designs. In particular, the generation of sequential third-order designs in two or three design variables is the focus and requires augmentation of the standard central composite design. Designs for third-order models have been constructed using a few mathematical and statistical principles some of which are algebraically cumbersome. A simple technique using principles of Hat matrix is adopted in this research and offers sequential third-order designs that are optimally efficient in overcoming lack-of-fit of the second-order models. These designs are practically viable to implement in various fields of study. Unlike some non-sequential designs of Yang (2008) that require starting experiments from the scratch, our new designs accept results of experiments carried out using the central composite designs and are only augmentations of such existing designs. Adopting this procedure saves cost and do not lead to wasteful resources. In the need to revert back to a previous design, one only needs to remove the augmented portion. Yang (2008) presented a sequential third-order design which requires augmenting second-order CCD into the third-order design by I-optimality criterion, we consider augmenting second-order CCD into the third-order design by D-optimality criterion as the D-optimality criterion is most popularly encountered and is readily available in most statistical software. The design points used in the augmentation are selected to maximize the determinant of square information matrix.

2 Some Review on Response Surface Methodology

Response Surface Methodology (RSM), which adopts techniques in statistical and mathematical field, has over the years become a tool used for process development, optimization and design construction in various fields of human endeavor. It was initially proposed by Box and Wilson (1951) and made more desirable and profitable by Box (1952, 1954). Box and Behnken (1959) believed that the objective of many experimental programs is to find a way to interpret the relationship between a quantifiable characteristic of a study process. This objective is readily achieved by the use of response surface methods (Myers et al., 2009). The relationship is given by the function that relates the response variable to some set of independent variables. As in a great number of literatures on optimal design of experiments, it is worthy to note that the pattern of the relationship is usually unknown in most practical situations. This leads to the understanding that response surface designs come in varying order, usually referred to as d-th order designs. According to Box and Behnken (1959), d-th order designs are designs that allow the experimenter to estimate all model coefficients associated with a d-th-order model. The choice of the d-th-order of the design is very much dependent on its ability to realistically and satisfactorily interpret the relationship between the response of interest and the set of independent variables (Arshad et al., 2020).

Empirically, the order relating response surface design is more encountered in some subject areas. For example, the second-order response surface designs have applications in biological science, agricultural science, pharmaceutical and industrial fields. Aanchal et al. (2016) listed several authors who applied the second-order response surface designs in optimization of cellulase produced by microorganisms. Morshedi and Akbarian (2014) noted the application of second-order response surface designs in production of snap bean yield and in greenhouse experiments. Peasura (2015) applied second-order response surface designs to the modeling of postweld heat treatment process under Industrial Technology. Khuri (2017) applied the second-order response surface designs in Food Sciences. As documented in Arshad et al. (2012), several authors have done extensive studies on practical situations where the second-order lack-of-fit arises in experimental situations and include the works of Castillo et al. (2004), Gao et al. (2009), Norulaini et al. (2009).

For the rising need of higher order designs, Seshubabu et al. (2014) considered the use of third-order response surface and noted the wide applicability of third-order models and designs in Chemical, Physical, Meteorological, and Industrial fields particularly when considering the rates of changes of the response surface, such as rates of changes in the yields of processes. They constructed Third-Order Slope Rotatable Designs (TOSRD) using Balanced Incomplete Block Designs (BIBD). A lot of researches requiring the use of third-order models and designs due to lack-of-fits of the second-order models and designs have been documented in SeshuBabu et al. (2014).

Constructed third-order designs are either sequential or non-sequential. The general concept of sequential designs in the study of response surface methods was considered by Box and Wilson (1951). Their approach to sequential experimentation required that experimental points are moved in a sequential manner along the gradient-based direction using a 2^k factorial design or its fractions, and axial points are added when curvature is detected in the system by the lack-of-fit test. Sequential approach of this nature was utilized in the construction of the widely known second-order class of design called the Central Composite Design (CCD). Hence, the CCD is a sequential design in that it allows experimentation to be carried out in a sequential manner. The 2^k factorial or fractional factorial design points are useful in estimation of first-order effects. With the addition of center runs, pure error can be estimated and model lack-of-fit can be determined. The addition of 2k axial points allows estimation of pure quadratic effects.

Foremost researches on response surfaces were concerned with the rotatable classes of second- and third-order designs as can be seen in Box (1954), Box and Hunter (1957), Draper (1960) and Gardiner et al. (1959). For instance, Gardiner et al. (1959), obtained rotatable designs that were of third-order without giving attention to designs orthogonality. Many techniques have been employed in constructing third-order designs and include the use of Balanced Incomplete Block Designs (BIBDs), Partially Balanced Incomplete Block Designs (PBIBDs), Doubly Balanced Incomplete Block Designs (DBIBDs), Simplex Designs, Split Plot Designs etc. Some useful references specifying these techniques include Das and Narasumham (1962), Baker and Bargmann (1985), Yang (2008), Koske et al. (2011), SeshuBabu et al. (2015), Rotich et al. (2017), Arshad et al. (2018) and Oguaghamba and Onyia (2019).

3 Sequential Designs

Building a design sequentially is very useful in the sense that by means of some augmentation, previous designs can be used for higher-order models and so researchers do not need to start experimentation from the scratch anytime there is a need for research. Also, researches can revisit a design for a lower-order model without repeating the experiment. Box and Wilson (1951) considered the general concept of sequential designs in the study of response surface methods. This led to the construction of the widely known second-order class of design, called the Central Composite Design. Over time, many researchers have taken to the use of sequential designs for varying purposes. Huda (1982) constructed some third-order rotatable designs in three dimensions as sequential designs from some available third-order designs in two dimensions. With these designs, the results of the experiments performed according to two-dimensional designs need not be discarded. Bosque-Sendra et al. (2001) utilized sequential design in pararosaniline determination of formaldehyde. Their procedure involved using a second-order design defined over an entire experimental domain. However, the characteristics of the response surface were confirmed using a new design which was obtained by shrinking the initial design. Lam (2008) studied sequential adaptive designs for fitting response surface models in computer experiments. Also, adaptive sequential response surface methodology was considered by Alaeddini et al. (2013a; 2013b) for industrial experiments involving high experimentation cost, limited experimental resources, and high design optimization performance. Their approach combined principles of nonlinear optimization, design of experiments, and response surface optimization. By using the adaptive response surface methodology, portions of the design space that give the worse responses based a given threshold value are eliminated from the design. Others works involving the use of sequential designs include Morshedi and Akbarian (2014), Ginsbourger (2017) and Bader et al. (2018).

3.1 The Hat matrix

The Hat matrix which plays a major role in modeling has its origin linked to John Tukey back in the 1960s as documented in Hoaglin and Welsch (1978). The concept is based on the linear model given by

$$Y = X\beta + \varepsilon \quad (1)$$

where

Y represents vector of the response variables or observed values;
Xrepresents the model matrix;
βrepresents the vector of unknown parameters;
εrepresents the vector of random error assumed to be normally and independently distributed with zero mean and constant variance i.e $\varepsilon \sim N(\mu, \sigma^2)$.
The least squares estimate of β is defined as $\hat{\beta} = (X'X)^{-1}X'$y.
The estimated value is given as

$$\hat{y} = X(X'X)^{-1}X'\text{y} = Hy \quad (2)$$

where $H = X(X'X)^{-1}X'$ is called the Hat Matrix because it places the “hat” on the vector of the estimated values thereby projecting the observed values (y) into the estimated values $(\hat{y})$ in the model space (Iwundu, 2017).

When dealing with modeling problems in regression analysis, the hat matrix plays a major role particularly as it identifies observations that have greater impacts on the estimation of model parameters and fitted values. Dealing with such observations help improve statistical inferences. The hat matrix is likened to leverage measures studied by Kahng (2007) as a basic components of influence in linear regression models. Each diagonal element h_{ii} of the hat matrix gives a measure of the extent to which the estimated regression model $\hat{y}_i$is attracted by the given observed or data point y_i. That is, the i^{th} leverage h_{ii}quantifies the degree of influence that the observation y_i has on its predicted value $\hat{y}_i$. The diagonal elements of the hat matrix takes values from zero to one (i.e $0 \leq h_{ii} \leq 1$) and the sum is equal to p $(i.e\ \sum_{i=1}^{N} h_{ii} = p)$. N represents the number of data points and p is the total number of model parameters including the intercept. Iwundu (2017) observed that in addition to the role of hat matrix in modeling problems, the hat matrix gives a measure of the effect of removal of one or more observations from a response surface design. We can therefore infer, that based on its components, the hat matrix is very valuable in explaining effects of alterations to a complete data set. Several authors have noted its usefulness and importance in measuring the sensitivity to wild and/or missing observations and reference is made to Akhar and Prescot (1986), Myers et al. (2009), Srisuradetchai (2015) and Iwundu (2018) for such details.

3.2 Third-order response surface model

The third-order model shall be employed in this work and is given by the function

$$y = \beta_0 + \sum_{i=1}^{k} \beta_i x_i + \sum_{i<j=2}^{k} \beta_{ij} x_i x_j + \sum_{i=1}^{k} \beta_{ii} x_i^2 + \sum_{i<j=2}^{k} \beta_{ijj} x_i x_j^2 + \sum_{i<j=2}^{k} \beta_{iij} x_{ii}^2 x_j + \sum_{i<j<l=3}^{k} \beta_{ijl} x_i x_j x_l + \sum_{i=1}^{k} \beta_{iii} x_{iii}^3 + \varepsilon \quad (3)$$

with $\binom{k+3}{3}$ model parameters.

y defines the response variable which is assumed to be normally distributed.
x_i, x_j, x_l are dimensionless coded independent variables; $i < j < l = 3, 4, \ldots, k$.
The$\beta's$areunknown parameters of the model and may be estimated using the method of least squares.
ε is the experimental error.
For k = 2, the full parameter response surface model is given as
$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{12} x_1 x_2 + \beta_{11} x_1^2 + \beta_{22} x_2^2 + \beta_{122} x_1 x_2^2 + \beta_{112} x_{11}^2 x_2 + \beta_{111} x_{111}^3 + \beta_{222} x_{222}^3 + \varepsilon$
and contains 10 parameters.
For k = 3, the full parameter response surface model is given as

$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_{12} x_1 x_2 + \beta_{13} x_1 x_3 + \beta_{23} x_2 x_3 + \beta_{11} x_1^2 + \beta_{22} x_2^2 +$

$\beta_{33} x_3^2 + \beta_{122} x_1 x_2^2 + \beta_{133} x_1 x_3^2 + \beta_{112} x_{11}^2 x_2 + \beta_{113} x_{11}^2 x_3 + \beta_{233} x_2 x_3^2 + \beta_{223} x_{22}^2 x_3 + \beta_{123} x_1 x_2 x_3$

$+ \beta_{111} x_1^3 + \beta_{222} x_2^3 + \beta_{333} x_3^3 + \varepsilon$

and contains 20 parameters.

3.3 The research design

Given a response function y that is influenced by several independent variables x_1, x_2, … , x_k. Suppose that a second-order model shows lack-of-fit and hence the second-order model does not satisfactorily express the relationship between the response function and the set of independent variables. We seek a design such that a third-order model can be employed in establishing the relationship between y and the x_i's. If it can be suspected that a third-order model would well represent that relationship, the required design is called a third-order response surface design. The third-order model is then imposed on a space of experimental trials which may be a continuous space having a continuum of points in the space of the independent variables. In this research, we assume that the space of trials is a cuboidal region which may be discretized by grid formation. Specifically, for k = 2 design variables, 25 grid points are formed. For k = 3 design variables, 125 grid points are formed. For k = 4 design variables, 625 grid points are formed and so on. Generally, there would be 5^k grid points for any fixed k value. These grid points represent a 5^k factorial series.

For the purpose of this research work, the Hat matrix will be used to generate blocks of points for the construction of the new third-order sequential designs. This will be done using five grid levels [-1, -½, 0, ½, 1] on each design variable in the design space. The choice of these grid levels is such as gives uniform grids and allows manageable size of candidate points to be used in the design construction. Furthermore, it allows candidate points to spread over the entire design space. For a cuboidal region, this choice does not violet having axial distance α = 1 and the design space contains continuum of $-1 \leq x_i \leq 1$ but is made discrete by the grid formation. For a spherical region, it is necessary to define the grid levels to include the axial distance. The idea of grid formation was popularized in the recommendation of Hebble and Mitchell (1972) for discretizing a space of trials of an experiment. The Hat matrix, which is a function of the model matrix, is expressed mathematically as

$$\text{H} = X(X'X)^{-1}X'$$

The 25 grid points are called candidate set and selection of points into the new designs shall be from them. For a third-order complete model, a model matrix is formed using the grid points and the model. Corresponding to the 5^k grid points, a hat matrix is obtained. Each diagonal element associated with the hat matrix lies between 0 and 1 and the sum of diagonal elements is approximately equal to 1. The i^{th} diagonal element of the hat matrix gives a measure of influence of the i^{th} grid point.

3.4 Rules for sequential generation of new third-order designs

The rules to be employed in sequential generation of new third-order response surface designs are as follows;

i. Form 5^k grid points on the given region.
ii. Obtain the model matrix X using the grid points and the model.
iii. Select the design points of the k-variable Central Composite Design.
iv. Augment the k-variable CCD with one or two blocks of points associated with the large h_{ii} entries from the remaining candidate sets.
v. An augmentation that results in the maximum determinant value of the information matrix yields the desired Sequential Third-Order Design (STOD).

It is assumed that there are no outliers and that the design is non-singular. The $5^k=\tilde{N}$ candidate points for k design variables were generated based on the combination of all stipulated grid levels in the design space. Using the $\tilde{N}$ candidate points, the elements of the model matrix for the third-order model are as defined in the matrix X.

$$X = \begin{bmatrix} 1 & x_{11} & x_{12}\cdots & x_{1k} & x_{11}x_{12} & x_{11}x_{13} & \cdots & x_{1k-1}x_{1k}\cdots & x_{11}^2 & \cdots & x_{1k}^3 \\ 1 & x_{21} & x_{22}\cdots & x_{2k} & x_{21}x_{22} & x_{21}x_{23} & \cdots & x_{2k-1}x_{2k}\cdots & x_{21}^2 & \cdots & x_{2k}^3 \\ 1 & x_{31} & x_{32}\cdots & x_{3k} & x_{31}x_{32} & x_{31}x_{33} & \cdots & x_{3k-1}x_{3k}\cdots & x_{31}^2 & \cdots & x_{3k}^3 \\ \vdots & \vdots & \vdots\ \vdots & \vdots & \vdots & \vdots & \cdots & \vdots\ \vdots & \vdots & \vdots & \vdots \\ 1 & x_{\tilde{N}1} & x_{\tilde{N}2}\cdots & x_{\tilde{N}k} & x_{\tilde{N}1}x_{\tilde{N}2} & x_{\tilde{N}1}x_{\tilde{N}3} & \cdots & x_{\tilde{N}k-1}x_{\tilde{N}k}\vdots & x_{\tilde{N}1}^2 & \vdots & x_{\tilde{N}k}^3 \end{bmatrix}$$

The associated hat matrix is as follows

$$H = \begin{bmatrix} h_{11} & h_{12} & \cdots & h_{1\tilde{N}} \\ h_{21} & h_{22} & \cdots & h_{2\tilde{N}} \\ \vdots & \vdots & \vdots & \vdots \\ h_{\tilde{N}1} & h_{\tilde{N}2} & \cdots & h_{\tilde{N}\tilde{N}} \end{bmatrix},$$

where 0 < h_{ii} < 1 and $\sum_{i=1}^{N} h_{ii} = p$

The diagonal elements h_{ii} of the hat matrix will be sorted out according to their magnitudes and the unique values will be grouped together to form various blocks from which the new sequential third-order designs will be based. It is worthy to note that under the sequential method, the CCD will be augmented to generate the new designs. This implies that points associated with the full second-order CCD will be chosen first as a single block and then more points from additional blocks will be added to the CCD to obtain a third-order design known as the augmented third-order CCD.

3.5 Design orthogonality

The concept of design orthogonality is very important in design construction. A well designed experiment is orthogonal if the effects of any factor balance out across the effects of the other factors. Design othogonality guarantees that each model coefficient is estimated independently of the other variables in the model. For the columns of the design matrix X to be orthogonal, the following conditions must be satisfied;

i. ${c_i}^T c_j = 0$ for $i \neq j$ and where c_i is the i^{th} column of X.
ii. ${c_i}^T c_i = N$ and the absolute values of the column entries sum to N, where N is the design size.

Each new sequential third-order design constructed in this research satisfies the above conditions and is thus orthogonal with the guarantee that all model coefficients are estimated independently.

4 Construction of Sequential Third-Order Response Surface Designs in k Control Variables

The analysis involved in the construction of sequential third-order response surface designs are presented for each k variables.

4.1 Construction involving two control variables

Reference is made to the 10-parameter model

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{12} x_1 x_2 + \beta_{11} x_1^2 + \beta_{22} x_2^2 + \beta_{122} x_1 x_2^2 + \beta_{112} x_{11}^2 x_2 + \beta_{111} x_{111}^3 + \beta_{222} x_{222}^3 + \varepsilon$$

The model matrix corresponding to the 25 grid points (candidate sets) is the immediate *25*x*10* matrix X. The diagonal elements h_{ii} of the hat matrix associated with the design matrix X as well as the respective candidate points are given in Table 1. The associated candidate points are grouped according to the magnitude of the diagonal elements and are presented in Table 2.

X =

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	0	0	1	0	0	0	1	0
1	-1	0	0	1	0	0	0	-1	0
1	0	1	0	0	1	0	0	0	1
1	0	-1	0	0	1	0	0	0	-1
1	0	0	0	0	0	0	0	0	0
1	-1	0.5	-0.5	1	0.25	-0.25	0.5	-1	0.125
1	-1	-0.5	0.5	1	0.25	-0.25	-0.5	-1	-0.125
1	1	0.5	0.5	1	0.25	0.25	0.5	1	0.125
1	1	-0.5	-0.5	1	0.25	0.25	-0.5	1	-0.125
1	-0.5	1	-0.5	0.25	1	-0.5	0.25	-0.125	1
1	-0.5	-1	0.5	0.25	1	-0.5	-0.25	-0.125	-1
1	0.5	1	0.5	0.25	1	0.5	0.25	0.125	1
1	0.5	-1	-0.5	0.25	1	0.5	-0.25	0.125	-1
1	-0.5	0.5	-0.25	0.25	0.25	-0.125	0.125	-0.125	0.125
1	-0.5	-0.5	0.25	0.25	0.25	-0.125	-0.125	-0.125	-0.125
1	0.5	0.5	0.25	0.25	0.25	0.125	0.125	0.125	0.125
1	0.5	-0.5	-0.25	0.25	0.25	0.125	-0.125	0.125	-0.125
1	-0.5	0	0	0.25	0	0	0	-0.125	0
1	0	0.5	0	0	0.25	0	0	0	0.125
1	0	-0.5	0	0	0.25	0	0	0	-0.125
1	0.5	0	0	0.25	0	0	0	0.125	0

The standard CCD in two design variables comprises the 9 design points in blocks 1, 3 and 6. It is important to mention that the generation of block size is a complete perturbation of elements of a given design tuple. For instance, the block size of 4 associated with Block 3 is obtained using the arrangements [±1, 0] and [0, ±1]. The standard CCD is augmented with two blocks of points namely [±1, ±0.5] and [±0.5, ±1] associated with diagonal elements of the hat matrix h_{ii}= 0.4085714 and h_{ii} = 0.2928571, respectively. The choice of the additional points is tied to the fact that each i^{th} diagonal element h_{ii} of the hat matrix quantifies the extent to which the fitted regression model $\hat{y}_i$ is attracted by the given observation or data point y_i.Since Hoaglin and Welsch (1978) have suggested that a reasonable rule of thumb for large h_{ii} is $h_{ii}>\frac{2n}{p}$ we suppose that in the absence of no outliers in the design $\left(\text{since } h_{ii} < \frac{2n}{p} \text{ for all i,}\right)$ a large value of h_{ii} should indicate an observation with good influence on prediction and would most likely contribute to maximizing the determinant of information matrix, having good distance from the design center. It is on this reasoning that h_{ii} = 0.4085714 and h_{ii} = 0.2928571 are chosen and results in a 21-point design having a determinant value 5.301368 x10^{-8} of the normalized information matrix. The 21-point design measure is given as follows:

Table 1: The h_{ii}Elements of the Hat Matrix for Candidate Points in Two-Variable Case

Candidate points	X_1	X_2	h_{ii}
1	1	1	0.7428571
2	1	-1	0.7428571
3	-1	1	0.7428571
4	-1	-1	0.7428571
5	1	0	0.3685714
6	-1	0	0.3685714
7	0	1	0.3685714
8	0	-1	0.3685714
9	0	0	0.1542857
10	-1	0.5	0.4085714
11	-1	-0.5	0.4085714
12	1	0.5	0.4085714
13	1	-0.5	0.4085714
14	-0.5	1	0.4085714
15	-0.5	-1	0.4085714
16	0.5	1	0.4085714
17	0.5	-1	0.4085714
18	-0.5	0.5	0.2928571
19	-0.5	-0.5	0.2928571
20	0.5	0.5	0.2928571
21	0.5	-0.5	0.2928571
22	-0.5	0	0.24
23	0	0.5	0.24
24	0	-0.5	0.24
25	0.5	0	0.24

Table 2: Summary of Components of h_{ii} and Block Arrangement in Two Variable Case

Blocks	Design points for two variables	h_{ii}	Block size
1	[±1, ±1]	0.7428571	4
2	[±1, ±0.5] , [±0.5, ±1]	0.4085714	8
3	[±1, 0] , [0, ±1]	0.3685714	4
4	[±0.5, ±0.5]	0.2928571	4
5	[±0.5, 0] , [0, ±5]	0.24	4
6	[0, 0]	0.1542857	1

ξ_{21} =

1	1
1	-1
-1	1
-1	-1
1	0
-1	0
0	1
0	-1
0	0
-1	0.5
-1	-0.5
1	0.5
1	-0.5
-0.5	1
-0.5	-1
0.5	1
0.5	-1
-0.5	0.5
-0.5	-0.5
0.5	0.5
0.5	-0.5

Most encountered two-variable third order response surface designs in the literature have design size *N* = 17. To keep the new design as minimal in run-size, the standard CCD is augmented with one block of points [±1, ±0.5] having diagonal elements h_{ii} = 0.4085714 of the hat matrix. As in the 21-point design, the choice of the additional design points with h_{ii} = 0.4085714 is made as it is expected that the associated would have good influence on prediction and would most likely contribute to maximizing the determinant of information matrix. This results in a 17-point design having a determinant value 4.1979×10^{-8} of the normalized information matrix. The 17-point sequential design is as follows:

ξ_{17} =

1	1
1	-1
-1	1
-1	-1
1	0
-1	0
0	1
0	-1
0	0
-1	0.5
-1	-0.5
1	0.5
1	-0.5
-0.5	1
-0.5	-1

0.5	1
0.5	-1

Yang (2008) generated four third-order designs, namely: Full third-order I-optimal design (FTOD), CCD Augmented by I-optimal (CCDA), Latin Hypercube Space Filled Design Augmented by I-optimal (LHDA) and Nested Face Centered Design (NFCD). Each of the designs had 17 experimental runs. The determinant values of normalized information matrices associated with FTOD, CCDA, LHDA and NFCD are, respectively, 4.043583×10^{-8}, 2.133489×10^{-8}, 1.397857×10^{-8} and 1.312652×10^{-8}. The design points for Yang (2008) designs are as follows:

FTOD:

-1	-1
1	-1
-1	1
1	1
-1	-0.5
-1	0.5
-0.5	1
0.5	1
1	0
0	-1
-0.5	-0.5
0.5	-0.5
-0.5	0.5
0.5	0.5
0	0.5
-0.5	-0.5
0.5	-0.5

CCDA:

-1	-1
1	-1
-1	1
1	1
-1	0
1	0
0	-1
0	1
0	0
-0.5	-0.5
0.5	-0.5
-0.5	0.5
0.5	0.5
-0.5	-0.5
0.5	-0.5
-0.5	0.5
0.5	0.5

LHDA:

-1	-0.5
0.5	-1
1	0.5
-0.5	1
-0.75	0.25
-0.25	-0.75
0.75	-0.25
0.25	0.75
0	0
-1	-1
1	-1
-1	1
1	1
-0.5	-0.5
0.5	-0.5
-0.5	0.5
0.5	0.5

NFCD:

-1	-1
1	-1
-1	1
1	1
-1	0
1	0
0	-1
0	1
-0.5	-0.5
0.5	-0.5
-0.5	0.5
0.5	0.5
-0.5	0
0.5	0
0	0.5
0	0.5
0	0

The Scaled Prediction Variances (SPVs) of the two-variable designs have been computed and are summarized in Table 3. By definition,

SPV = $N\underline{x}'(\mathrm{X}'\mathrm{X})^{-1}\underline{x} = V[\overline{y}(\underline{x})]$.

For the new 21-point sequential design, the scaled prediction variances at each design points as follows;

$V[\overline{y}(-1,-1)]$ = 15.4956

$V[\overline{y}(1,-1)]$ = 15.4956

$V[\overline{y}(-1,1)]$ = 15.4956

$V[\overline{y}(1,1)]$ = 15.4956

$V[\overline{y}(1,0)]$ = 7.8341
$V[\overline{y}(-1,0)]$ = 7.8341
$V[\overline{y}(0,1)]$ = 7.8341

$V[\overline{y}(0,-1)]$ = 7.8341
$V[\overline{y}(0,0)]$ = 5.2549
$V[\overline{y}(-1,0.5)]$ = 8.5753
$V[\overline{y}(-1,-0.5)]$ = 8.5753
$V[\overline{y}(1,-0.5)]$ = 8.5753
$V[\overline{y}(1,0.5)]$ = 8.5753
$V[\overline{y}(-0.5,1)]$ = 8.5753
$V[\overline{y}(-0.5,-1)]$ = 8.5753
$V[\overline{y}(0.5,-1)]$ = 8.5753
$V[\overline{y}(0.5,1)]$ = 8.5753
$V[\overline{y}(-0.5,-0.5)]$ = 8.20603
$V[\overline{y}(-0.5,0.5)]$ = 8.20603
$V[\overline{y}(0.5,-0.5)]$ = 8.20603
$V[\overline{y}(0.5,0.5)]$ = 8.20603

A close look at each values of the scaled prediction variance for the four reference designs of Yang (2008) and the new sequential designs show that the new 21-point sequential design has minimum maximum scaled prediction variance. By the scaled prediction variances, Yang's sequential design CCDA (CCD Augmented by I-optimality) is not as good as the new sequential designs that were constructed to maximize determinant of the normalized information matrix. Of the four designs due to Yang (2008), three designs are inferior to the new sequential designs in terms of the scaled prediction variance criterion. The augmented Latin hypercubes space filling design (LHDA) whose maximum scaled prediction variance is better than the other three designs of Yang (2008) has nine levels of the design variables. It may be of interest to consider the use of more variable levels against the five used in this research. It is important to note that the order of listing of the design points in Table 3 is as the designs are presented in this research.

4.2 Construction involving three control variables

Reference is made to the 30-parameter model

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_{12} x_1 x_2 + \beta_{13} x_1 x_3 + \beta_{23} x_2 x_3 + \beta_{11} x_1^2 + \beta_{22} x_2^2 + \beta_{33} x_3^2 + \beta_{122} x_1 x_2^2 + \beta_{133} x_1 x_3^2 + \beta_{112} x_{11}^2 x_2 + \beta_{113} x_{11}^2 x_3 + \beta_{233} x_2 x_3^2 + \beta_{223} x_{22}^2 x_3 + \beta_{123} x_1 x_2 x_3 + \beta_{111} x_1^3 + \beta_{222} x_2^3 + \beta_{333} x_3^3 + \varepsilon$$

The diagonal elements h_{ii} associated with the 125x125 hat matrix corresponding to 125 candidate points are presented in Appendix A. The candidate points are grouped according to the magnitude of the diagonal elements and presented in Table 4. As in the two-variable case, these values and respective points will form the bases for the choice of block of points in generating the new sequential designs in three-variables. Also, the generation of block size is a complete perturbation of elements of a given design tuple. For instance, the block size of 24 associated with Block 2 is obtained using the arrangements [±1, ±1, ±0.5], [±1, ±0.5, ±1] and [±0.5, ±1, ±1]. For the new sequential design, the standard CCD will be used as a single block of points. This consists of 15 experimental runs having design points [±1, ±1, ±1], [±1, 0, 0], [0, ±1, 0], [0, 0, ±1] and [0, 0, 0]. The standard CCD is then augmented with one block of points corresponding to [±1, ±1, ±0.5] having h_{ii} value of 0.22628571. The augmenting block of points contains 24 design points. This, together with the 15-point CCD, results in 39-

point design having a determinant value of the normalized information matrix as $1.799756\text{x}10^{-15}$.The 39-point sequential third-order response surface design in three-variables is as follows

Table 3: Summary of the Scaled Prediction Variances for Designs in Two Variables.

Design Points	SD1	SD2	FTOD	CCDA	LHDA	NFCD
1	14.1927	15.4956	14.9616	16.0235	11.9889	16.1656
2	14.1927	15.4956	16.3119	16.0235	11.9889	16.1656
3	14.1927	15.4956	12.946	16.0235	11.9889	16.0761
4	14.1927	15.4956	14.6606	16.0235	11.9889	16.0761
5	7.49354	7.83409	9.70485	13.7585	8.18692	13.4433
6	7.49354	7.83409	10.8978	13.7585	8.18692	13.4433
7	7.49354	7.83409	10.5477	13.7585	8.18692	13.9378
8	7.49354	7.83409	9.92571	13.7585	8.18692	13.2772
9	8.06569	5.2549	13.4651	3.16949	3.65008	8.70347
10	9.39869	8.57526	13.2249	5.96281	15.127	8.70347
11	9.39869	8.57526	5.92433	5.96281	15.127	6.53332
12	9.39869	8.57526	6.23432	5.96281	15.127	6.53332
13	9.39869	8.57526	6.5157	5.96281	15.127	5.13149
14	9.39869	8.57526	6.76892	5.96281	6.28467	5.13149
15	9.39869	8.57526	5.75186	5.96281	6.28467	3.90834
16	9.39869	8.57526	5.92433	5.96281	6.28467	3.90834
17	9.39869	8.57526	6.23432	5.96281	6.28467	2.86195
18		8.20603				
19		8.20603				
20		8.20603				
21		8.20603				

Table 4: Summary of Components of h_{ii} and Block Arrangement in Three-Variable Case

Blocks	Design points for three variables	h_{ii}	Block size
1	[±1, ±1, ±1]	0.39942857	8
2	[±1, ±1, ±0.5] , [±1, ±0.5, ±1] , [±0.5, ±1, ±1]	0.22628571	24
3	[±1, ±1, 0] , [±1, 0, ±1] , [0, ±1, ±1]	0.20571429	12
4	[±1, ±0.5, ±0.5] , [±0.5, ±1, ±0.5] , [±0.5, ±0.5, ±1]	0.13285714	24
5	[±1, ±0.5, 0] , [0, ±1, ±0.5], [±0.5, 0, ±1] [±0.5, ±1, 0] , [0, ±0.5, ±1], [±1, 0, ±0.5]	0.12171429	24
6	[±1, 0, 0] , [0, ±1, 0] , [0, 0, ±1]	0.108	6
7	[±0.5, ±0.5, ±0.5]	0.09214286	8
8	[±0.5, ±0.5, 0] , [±0.5, ±0.5, 0] , [±0.5, ±0.5, 0]	0.08142857	12
9	[±0.5, 0,0] , [0, ±0.5, 0] , [0, 0, ±0.5]	0.06514286	6
10	[0, 0, 0]	0.04228571	1

ξ_{39} =

-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	0	0
1	0	0
0	-1	0
0	1	0
0	0	-1
0	0	1
0	0	0
-1	-1	-0.5
-1	-1	0.5
1	1	-0.5
1	1	0.5
-1	-0.5	-1
-1	-0.5	1
1	0.5	-1
1	0.5	1
-1	0.5	-1
-1	0.5	1
1	-0.5	-1
1	-0.5	1
-1	1	-0.5
-1	1	0.5
1	-1	-0.5
1	-1	0.5
-0.5	-1	-1
-0.5	-1	1
0.5	1	-1
0.5	1	1
-0.5	1	-1
-0.5	1	1
0.5	-1	-1
0.5	-1	1

5 Conclusion

New sequential third-order response surface designs have been obtained as augmentation of the standard central composite designs. All generated designs require blocks of design points from the design space usually a k-dimensional Euclidean space, which in this work is assumed cuboidal. A simple mathematical scheme using grid formation was used in discretizing a continuous design space thereby obtaining admissible candidate points. The hat matrix, which is common in regression problems, served as a vital tool for selection of optimal design points useful in the construction of the new sequential designs. In the course of generating the third-order response surface designs, the importance of the axial points in the estimation of pure quadratic terms was noted as its inclusion provided for superior designs. The new third-order sequentially generated response surface designs possess interesting superior optimality properties. In particular, the determinant values of information matrix were better than those associated with designs due to Yang (2008). These clearly indicate that the new designs offer better estimation of model parameters than those associated with known existing designs. Also, the new designs gained efficiency over existing designs as demonstrated for two-variable cases, having minimum maximum scaled prediction variances. The maximum scaled prediction variance of the new sequential 17-point two-variable third-order design is 14.1927and gives a G-efficiency value of 70.46%. This design has higher G-efficiency value when compared to the four two-variable third-order designs of Yang (2008) cited in this paper. Specifically, the maximum scaled prediction variance and G-efficiency value of Yang's full third-order I-optimal design (FTOD) are 16.3119 and 61.13%, respectively. The maximum scaled prediction variance and G-efficiency value of Yang's CCD augmented design (CCDA)are 16.0235 and 62.41%, respectively. The maximum scaled prediction variance and G-efficiency value of Yang's Latin Hypercube Space-filling Augmented design (LHDA)are 15.127 and 66.11%,respectively. The maximum scaled prediction variance and G-efficiency value of Yang's Nested Face Centered design (NFCD)are 16.1656 and 61.86%, respectively. It is also worth noting that G-efficiency of the new 21-point design as 64.53% having the maximum scaled prediction variance of 15.4956.

In the case of the three-variable design, a constructed third-order design on a cuboidal region was not found in the literature reviewed. Hence the determinant value of information matrix of the new design was not compared with any other design. However, evaluation of scaled prediction variances shows that the new 39-point sequential third-order design in three design variables has a high G-efficiency value. Specifically, the maximum scaled prediction variance of the new 39-point sequential third-order design is 21.83237 and gives a G-efficiency value of 91.61%. While not limiting use to sequential designs, their importance cannot be overlooked as they are mostly applied in constructing optimal designs.

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Appendix

The h_{ii} Elements of the Hat Matrix for Candidate Points in Three Design Variables

Candidate point	x_1	x_2	x_3	h_{ii}
1	-1	-1	-1	0.39942857
2	1	-1	-1	0.39942857
3	-1	1	-1	0.39942857
4	1	1	-1	0.39942857
5	-1	-1	1	0.39942857
6	1	-1	1	0.39942857
7	-1	1	1	0.39942857
8	1	1	1	0.39942857
9	-1	0	0	0.108
10	1	0	0	0.108
11	0	-1	0	0.108
12	0	1	0	0.108
13	0	0	-1	0.108
14	0	0	1	0.108
15	0	0	0	0.04228571
16	-1	-1	-0.5	0.22628571
17	-1	-1	0.5	0.22628571
18	1	1	-0.5	0.22628571
19	1	1	0.5	0.22628571
20	-1	-0.5	-1	0.22628571
21	-1	-0.5	1	0.22628571
22	1	0.5	-1	0.22628571
23	1	0.5	1	0.22628571
24	-1	-1	0	0.20571429
25	1	1	0	0.20571429
26	-1	-0.5	-0.5	0.13285714
27	-1	-0.5	0.5	0.13285714
28	1	0.5	-0.5	0.13285714
29	1	0.5	0.5	0.13285714
30	-1	0	-1	0.20571429
31	-1	0	1	0.20571429
32	1	0	-1	0.20571429
33	1	0	1	0.20571429
34	-1	-0.5	0	0.12171429
35	1	0.5	0	0.12171429
36	-1	0	-0.5	0.12171429
37	-1	0	0.5	0.12171429
38	1	0	-0.5	0.12171429
39	1	0	0.5	0.12171429
40	-1	0.5	-1	0.22628571
41	-1	0.5	1	0.22628571
42	1	-0.5	-1	0.22628571

43	1	-0.5	1	0.22628571
44	-1	0.5	-0.5	0.13285714
45	-1	0.5	0.5	0.13285714
46	1	-0.5	-0.5	0.13285714
47	1	-0.5	0.5	0.13285714
48	-1	0.5	0	0.12171429
49	1	-0.5	0	0.12171429
50	-1	1	-0.5	0.22628571
51	-1	1	0.5	0.22628571
52	1	-1	-0.5	0.22628571
53	1	-1	0.5	0.22628571
54	-1	1	0	0.20571429
55	1	-1	0	0.20571429
56	-0.5	-1	-1	0.22628571
57	-0.5	-1	1	0.22628571
58	0.5	1	-1	0.22628571
59	0.5	1	1	0.22628571
60	-0.5	-1	-0.5	0.13285714
61	-0.5	-1	0.5	0.13285714
62	0.5	1	-0.5	0.13285714
63	0.5	1	0.5	0.13285714
64	-0.5	-0.5	-1	0.13285714
65	-0.5	-0.5	1	0.13285714
66	0.5	0.5	-1	0.13285714
67	0.5	0.5	1	0.13285714
68	-0.5	-1	0	0.12171429
69	0.5	1	0	0.12171429
70	-0.5	-0.5	-0.5	0.09214286
71	-0.5	-0.5	0.5	0.09214286
72	0.5	0.5	-0.5	0.09214286
73	0.5	0.5	0.5	0.09214286
74	-0.5	-0.5	0	0.08142857
75	0.5	0.5	0	0.08142857
76	-0.5	0	-1	0.12171429
77	-0.5	0	1	0.12171429
78	0.5	0	-1	0.12171429
79	0.5	0	1	0.12171429
80	-0.5	0	-0.5	0.08142857
81	-0.5	0	0.5	0.08142857
82	0.5	0	-0.5	0.08142857
83	0.5	0	0.5	0.08142857
84	-0.5	0.5	-1	0.13285714
85	-0.5	0.5	1	0.13285714
86	0.5	-0.5	-1	0.13285714
87	0.5	-0.5	1	0.13285714

88	-0.5	0	0	0.06514286
89	0.5	0	0	0.06514286
90	-0.5	0.5	-0.5	0.09214286
91	-0.5	0.5	0.5	0.09214286
92	0.5	-0.5	-0.5	0.09214286
93	0.5	-0.5	0.5	0.09214286
94	-0.5	0.5	0	0.08142857
95	0.5	-0.5	0	0.08142857
96	-0.5	1	-1	0.22628571
97	-0.5	1	1	0.22628571
98	0.5	-1	-1	0.22628571
99	0.5	-1	1	0.22628571
100	-0.5	1	-0.5	0.13285714
101	-0.5	1	0.5	0.13285714
102	0.5	-1	-0.5	0.13285714
103	0.5	-1	0.5	0.13285714
104	-0.5	1	0	0.12171429
105	0.5	-1	0	0.12171429
106	0	-1	-1	0.20571429
107	0	-1	1	0.20571429
108	0	1	-1	0.20571429
109	0	1	1	0.20571429
110	0	-1	-0.5	0.12171429
111	0	-1	0.5	0.12171429
112	0	1	-0.5	0.12171429
113	0	1	0.5	0.12171429
114	0	-0.5	-1	0.12171429
115	0	-0.5	1	0.12171429
116	0	0.5	-1	0.12171429
117	0	0.5	1	0.12171429
118	0	-0.5	-0.5	0.08142857
119	0	-0.5	0.5	0.08142857
120	0	0.5	-0.5	0.08142857
121	0	0.5	0.5	0.08142857
122	0	-0.5	0	0.06514286
123	0	0.5	0	0.06514286
124	0	0	-0.5	0.06514286
125	0	0	0.5	0.06514286