90
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Sequential Robust Response Surface Strategy

by

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(ABSTRACT)

General Response Surface Methodology involves the exploration of some response variable which is a function of other controllable variables. Many criteria exist for selecting an experimental design for the controllable variables. A good choice of a design is one that may not be optimal in a single sense, but rather near optimal with respect to several criteria. This robust approach can lend well to strategies that involve sequential or two stage experimental designs.

An experimenter that fits a first order regression model for the response often fears the presence of curvature in the system. Experimental designs can be chosen such that the experimenter who fits a first order model will have a high degree of protection against potential model bias from the presence of curvature. In addition, designs can also be selected such that the experimenter will have a high chance for detection of curvature in the system. A lack of fit test is usually performed for detection of curvature in the system. Ideally, an experimenter desires good detection capabilities along with good protection capabilities.

An experimental design criterion that incorporates both detection and protection capabilities is the Λ_2^* criterion. This criterion is used to select the designs which maximize the average noncentrality parameter of the lack of fit test among designs with a fixed bias. The first order rotated design class is a new class of designs that offers an improvement in terms of the Λ_2^* criterion over standard first order factorial designs. In conjunction with a sequential experimental strategy, a class of second order rotated designs are easily constructed by augmenting the first order rotated

designs. These designs allow for estimation of second order model terms when a significant lack of fit is observed.

Two other design criteria, that are closely related, and incorporate both detection and protection capabilities are the J_{PCA} and J_{PCMAX} criterion. J_{PCA} considers the average mean squared error of prediction for a first order model over a region where the detection capabilities of the lack of fit test are not strong. J_{PCMAX} considers the maximum mean squared error of prediction over the region where the detection capabilities are not strong. The J_{PCA} and J_{PCMAX} criteria are used within a sequential strategy to select first order experimental designs that perform well in terms of the mean squared error of prediction when it is likely that a first order model will be employed. These two criteria are also adopted for nonsequential experiments for the evaluation of first order model prediction performance. For these nonsequential experiments, second order designs are used and constructed based upon J_{PCA} and J_{PCMAX} for first order model properties and D_s -efficiency and D-efficiency for second order model properties.

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Table of Contents

I. Introduction 1

II. Response Surface Methodology Review 4

2.1 Response Surface Methodology 4

2.2 General Linear Model Representation 6

2.3 The Role of Experimental Design 8

2.4 Design Criteria 10

2.4.1 Design and Region Moments 11

2.4.2 Variance Criteria 12

2.4.3 Bias Criterion 15

2.4.4 Mean Squared Error Criterion 19

2.4.5 Lack of Fit Criteria 20

2.5 Experimental Design Classes 22

2.5.1 Factorial and Fractional Factorial Designs 23

2.5.2 Central Composite Designs 24

2.5.3 Box-Behnken Designs 25

2.5.4 Small Composite Designs 26

2.5.5 Hybrid Designs 27
2.5.6 Notz Designs 28

III. A Lack of Fit Criterion and First Order Designs **30**
3.1 Lack of Fit and Integrated Mean Squared Error Revisited 30
3.1.1 Two Variable Example 33
3.1.2 Λ_2-Optimality - Review 35
3.2 A Lack of Fit/Mean Squared Error Criterion 36
3.3 Factorial Designs 37
3.4 Rotated Designs 39
3.4.1 Effect of Rotation on Bias and Mean Squared Error 44
3.4.2 Effect of Rotation on Lack of Fit 48
3.4.3 Λ_2^* Criterion Applied to the Rotated Design Class 50
3.5 Comparison of Factorial and Rotation Designs 53

IV. Augmentation Of First Order Designs **56**
4.1 Sequential Design Procedure 57
4.2 Second Order Design Criteria 58
4.2.1 Orthogonal Blocking 58
4.2.2 Prediction Properties and Coefficients Estimation 59
4.3 Augmentation of Factorial Designs - Central Composite Designs 59
4.3.1 Orthogonally Blocked Central Composite Designs 60
4.3.2 Rotatable Central Composite Designs 61
4.3.3 D and D_s Efficient Central Composite Designs 61
4.4 Augmentation of Rotated Designs - Second Order Rotated Designs 64
4.4.1 Orthogonally Blocked Second Order Rotated Designs 67
4.4.2 Rotatable Second Order Rotated Designs 69
4.4.3 D and D_s Efficient Second Order Rotated Designs 69

V. A Mean Squared Error Criterion 73
5.1 One Variable Case 74
5.2 Power Conditional Average and Power Conditional Maximum Mean Squared Error 78
5.3 Application of J_{PCA} and J_{PCMAX} to First Order Factorial Designs 80
5.3.1 Factorial Designs with Cuboidal Regions for the Design and Exploration 84
5.3.2 Factorial Designs With Spherical Regions for the Design and Exploration 85
5.3.3 Factorial Designs within a Cuboidal Design Region and Spherical Region of Interest 86
5.4 Robust Second Order Designs 87
5.4.1 Second Order Designs Within a Cuboidal Design Region for a Cuboidal Region of Interest 88
5.4.2 Second Order Designs Within a Spherical Design Region for a Spherical Region of Interest 89
5.4.3 Second Order Designs Within a Cuboidal Design Region for a Spherical Region of Interest 90
5.5 Economical Robust Second Order Designs 91
5.5.1 Economical Second Order Designs Within a Cuboidal Design Region for a Cuboidal Region of Interest 92
5.5.2 Economical Second Order Designs Within a Spherical Design Region for a Spherical Region of Interest 92
5.5.3 Economical Second Order Designs Within a Cuboidal Design Region With a Spherical Region of Interest 93

VI. Summary, Conclusions and Further Research 95
6.1 Λ_2^* and Rotated Designs 96
6.2 J_{PCA} and J_{PCMAX} Design Criteria 98
6.3 Areas of Further Research 100

References 101

Appendix A **103**

Appendix B **110**

Appendix B.1 Development of Λ_2^* 110

Appendix B.2 Development of J_{PCA} 112

Appendix B.3 Development of J_{PCMAX} 113

Appendix C **115**

Vita **152**

List of Tables

Table 2.1 Values of J for Optimal, Minimum Bias and Minimum Variance Designs for $k = 1$ First Order Model 18

Table 3.1 Evaluation of Factorial Designs in Terms of Λ_2^* Criterion 38

Table 3.2 Evaluation of Rotated Designs in Terms of Λ_2^* Criterion 52

Table 4.1 D-efficiency and D_s-efficiency for Central Composite Designs Created by Augmentation of Mean Squared Error Efficient Factorial Designs . . 63

Table 4.2 D-efficiency and D_s-efficiency for Second Order Rotated Designs Created by Augmentation of Mean Squared Error Efficient First Order Rotated Designs 71

Table C.1 Factorial Designs - Minimum J_{PCA} For Designs With Given Sample Size and Power < 0.90 for $\alpha = 0.05$ Test
Design Region: Cuboidal Region of Interest: Cuboidal 116

Table C.2 Factorial Designs - Minimum J_{PCA} For Designs With Given Sample Size and Power < 0.90 for $\alpha = 0.05$ Test
Design Region: Spherical Region of Interest: Spherical 117

Table C.3 Factorial Designs - Minimum J_{PCA} For Designs With Given Sample Size and Power < 0.90 for $\alpha = 0.05$ Test
Design Region: Cuboidal Region of Interest: Spherical 118

Table C.4 Factorial Designs - Minimum J_{PCMAX} For Designs With Given Sample Size and Power < 0.90 for $\alpha = 0.05$ Test
Design Region: Cuboidal Region of Interest: Cuboidal 119

Table C.5 Factorial Designs - Minimum J_{PCMAX} For Designs With Given Sample Size and Power < 0.90 for $\alpha = 0.05$ Test
Design Region: Spherical Region of Interest: Spherical 120

Table C.6 Factorial Designs - Minimum J_{PCMAX} For Designs With Given Sample Size and Power < 0.90 for $\alpha = 0.05$ Test
Design Region: Cuboidal Region of Interest: Spherical 121

Table C.7 Central Composite Designs - Minimum J_{PCA} and J_{PCMAX} For Designs With Given Sample Size and Power < 0.90 for $\alpha = 0.05$ Test Design Region: Cuboidal Region of Interest: Cuboidal 122

Table C.8 Central Composite Designs - Minimum J_{PCA} and J_{PCMAX} For Designs With Given Sample Size and Power < 0.90 for $\alpha = 0.05$ Test Design Region: Spherical Region of Interest: Spherical 125

Table C.9 Central Composite Designs - Minimum J_{PCA} and J_{PCMAX} For Designs With Given Sample Size and Power < 0.90 for $\alpha = 0.05$ Test Design Region: Cuboidal Region of Interest: Spherical 128

Table C.10 Box-Behnken Designs - Minimum J_{PCA} and J_{PCMAX} For Designs With Given Sample Size and Power < 0.90 for $\alpha = 0.05$ Test Design Region: Cuboidal Region of Interest: Cuboidal 131

Table C.11 Box-Behnken Designs - Minimum J_{PCA} and J_{PCMAX} For Designs With Given Sample Size and Power < 0.90 for $\alpha = 0.05$ Test Design Region: Spherical Region of Interest: Spherical 133

Table C.12 Box-Behnken Designs - Minimum J_{PCA} and J_{PCMAX} For Designs With Given Sample Size and Power < 0.90 for $\alpha = 0.05$ Test Design Region: Cuboidal Region of Interest: Spherical 135

Table C.13 Small Composite Designs - Minimum J_{PCA} and J_{PCMAX} For Designs With Given Sample Size and Power < 0.90 for $\alpha = 0.05$ Test Design Region: Cuboidal Region of Interest: Cuboidal 137

Table C.14 Small Composite Designs - Minimum J_{PCA} and J_{PCMAX} For Designs With Given Sample Size and Power < 0.90 for $\alpha = 0.05$ Test Design Region: Spherical Region of Interest: Spherical 138

Table C.15 Small Composite Designs - Minimum J_{PCA} and J_{PCMAX} For Designs With Given Sample Size and Power < 0.90 for $\alpha = 0.05$ Test Design Region: Cuboidal Region of Interest: Spherical 139

Table C.16 Notz Type Designs - Minimum J_{PCA} and J_{PCMAX} For Designs With Given Sample Size and Power < 0.90 for $\alpha = 0.05$ Test Design Region: Cuboidal Region of Interest: Cuboidal 140

Table C.17 Notz Type Designs - Minimum J_{PCA} and J_{PCMAX} For Designs With Given Sample Size and Power < 0.90 for $\alpha = 0.05$ Test Design Region: Spherical Region of Interest: Spherical 141

Table C.18 Notz Type Designs - Minimum J_{PCA} and J_{PCMAX} For Designs With Given Sample Size and Power < 0.90 for $\alpha = 0.05$ Test Design Region: Cuboidal Region of Interest: Spherical 142

Table C.19 Hybrid Designs - Minimum J_{PCA} and J_{PCMAX} For Designs With Given Sample Size and Power < 0.90 for $\alpha = 0.05$ Test Design Region: Cuboidal Region of Interest: Cuboidal 143

Table C.20 Hybrid Designs - Minimum J_{PCA} and J_{PCMAX} For Designs With Given Sample Size and Power < 0.90 for $\alpha = 0.05$ Test Design Region: Spherical Region of Interest: Spherical 146

Table C.21 Hybrid Designs - Minimum J_{PCA} and J_{PCMAX} For Designs With Given Sample Size and Power < 0.90 for $\alpha = 0.05$ Test Design Region: Cuboidal Region of Interest: Spherical 149

List of Figures

Figure 3.1 Two Variable Factorial Design and Corresponding Rotation Design 40

Figure 5.1 Integrated Mean Squared Error of Prediction as a Function of the Second Order Coefficient 76

Figure 5.2 Power of the Lack of Fit Test as a Function of the Second Order Coefficient 77

Chapter I

I. Introduction

Many experimental problems can be characterized as an investigation of some response variable of interest that can be expressed as a mathematical function, f, of k other independent variables. The goals of such an investigation include determining an appropriate functional model representation for the response and then utilizing this model to predict, explore and optimize the response within a region in the independent variables. The procedures of modeling, predicting, exploring and optimizing a response variable are generally referred to as Response Surface Methodology (RSM).

For these experimental investigations, the response variable, η , can be written as

$$\eta = f(x_1, x_2, \ldots, x_k)$$

where $x_1, x_2, \ldots, x_k$ represent the independent variables. In general, the true form of the response function, f, is unknown. The usual assumption is that f, although unknown, can be well approximated by a low order polynomial function. Typically, either a multiple linear regression model or a quadratic regression model is employed as an approximating form for f. Empirical linear or quadratic regression models based upon sample data of the observed response are used to predict, explore and optimize the response variable.

Since the true form of the response function is unknown, the experimenter is typically uncertain of the best characterization for the response function. Employing either a linear or quadratic model will influence the prediction, exploration and optimization. Also, since any empirical model is only an approximation, choosing the best characterization is of great importance. Therefore, in addition to the goals of general RSM procedures, the experimenter also needs good capabilities for the selection of an appropriate characterization for the response function. This selection of either a linear or quadratic model will be made based upon observed responses. Once an appropriate model is chosen, prediction, exploration and optimization procedures can be employed.

In performing an experiment, one usually can select the combinations of values for the independent variables at which the response variable is observed. In general, n selected combinations of values comprise what is referred to as an experimental design. Experimental designs are chosen such that an experimenter can achieve specific goals with the best statistical properties. In choosing a design, the experimenter should select the one that allows for him to make the best choice between a linear or quadratic model characterization of the response function. In addition, designs which perform well in terms of prediction, exploration and optimization are desired. The goal for design selection is then to choose a design that will allow for good quality model selection and perform well in terms of prediction, exploration and optimization. Unfortunately, the experimenter is faced with the dilemma of choosing a design that either performs well in terms of model selection or in terms of prediction and exploration. Designs which perform well in both aspects have not been previously examined. Within this work, an experimental design strategy and specific experimental design criteria are developed for use in selecting robust experimental designs which allow for good quality model selection and good prediction and exploration properties.

After a detailed discussion of the methods of RSM and specific experimental design classes in Chapter II, a new experimental design criterion that incorporates both model selection and prediction is developed in Chapter III. This criterion is applied to standard factorial designs to select the designs that will provide for good model selection and also provide good prediction properties for a linear regression model. In addition, a new design class is proposed that will provide for better model selection properties than factorial designs with equivalent prediction properties for a linear regression model.

Due to the uncertainty of the best response function characterization, if a quadratic regression model is chosen based upon the model selection procedure, then the designs of Chapter III will need to be augmented to allow for quadratic model terms to be estimated. Chapter IV discusses the augmentation of these designs to create designs that will perform well when a quadratic regression model is employed.

Finally, two other closely related design criteria that evaluate the prediction performance and account for the model selection performance are developed in Chapter V. These two criteria are applied to standard design classes to select designs that will perform well in terms of prediction and model selection.

Chapter II

II. Response Surface Methodology Review

2.1 Response Surface Methodology

The origin of Response Surface Methodology (RSM) is usually credited to Box and Wilson (1951). Within their work, they define a sequential framework for experimentation and statistical analysis. This sequential framework is summarized by the following:

1) Employ a model of order d for the response variable.

2) Perform a check of the adequacy of the model.

3) If the model of order d is adequate, use it for exploration.
If the model of order d is inadequate, employ a model of order d + 1.

The work that is presented here corresponds to an experimental philosophy that is consistent with this sequential framework.

In general, RSM combines experimental design and regression techniques to develop a model for a response variable, η , expressed as a function of k other independent variables, $\xi_1, \xi_2, ..., \xi_k$

$$\eta = f(\xi_1, \xi_2, ..., \xi_k) \tag{2.1}$$

The experimenter usually has control over the values of the independent variables and will observe a response at particular combinations of values for the independent variables. In general, experimental design methods are employed to obtain a set of n values at which the response variable is observed.

When considering an experimental design in a response surface problem, it is common to transform the k independent variables into design variables of the form

$$x_{iu} = \frac{\xi_{iu} - \bar{\xi}_i}{s_i}, \quad \begin{array}{l} i = 1, 2, ..., k \\ u = 1, 2, ..., n \end{array} \tag{2.2}$$

where $\bar{\xi}_i = \frac{\sum_{u=1}^{n} \xi_{iu}}{n}$ and s_i is the appropriate scale factor such that $-1 \le x_i \le 1$. Design variables will be used throughout this work, but the values of the independent variables can always be obtained using the above transformation.

The observed data obtained from employing a particular experimental design is then used to estimate the response function, f, usually with a low order polynomial. These low order polynomials are representative of first or second order Taylor series expansions of the response function f.

Response Surface Methods use the estimated response function to predict response values and to locate optimal response values within a specified region of interest in the design variables, R.

The simple polynomial functions that are commonly used to estimate the response functions are low order polynomials in the design variables. First (d = 1) and second (d = 2) order polynomials are frequently adopted. The simplest model is a first order polynomial model of the form

$$y = \beta_0 + \sum_{i=1}^{k} \beta_i x_i + \varepsilon \tag{2.3}$$

where y is the observed response, the β_i are constant coefficients and ε is the model error. An alternative polynomial model used when the first order model is inadequate, is the second order polynomial model of the form

$$y = \beta_0 + \sum_{i=1}^{k} \beta_i x_i + \sum_{i=1}^{k} \beta_{ii} x_i^2 + \sum_{i<j} \beta_{ij} x_i x_j + \varepsilon \tag{2.4}$$

where y is the observed response, the β_i, β_{ii} and β_{ij} are constant coefficients and ε is the random error component.

2.2 General Linear Model Representation

The first and second order polynomial models belong to the class of general linear models of the form

$$\underline{y} = X\underline{\beta} + \underline{\varepsilon} \tag{2.5}$$

where $\underline{y}$ is an $n \times 1$ vector of observed responses, X is an $n \times p$ matrix of the design variables which accounts for the model under consideration, $\underline{\beta}$ is a $p \times 1$ vector of constant coefficients and $\underline{\varepsilon}$ is an $n \times 1$ vector of random errors. The usual assumptions corresponding to the general linear model are,

$$E(\underline{\varepsilon}) = \underline{0} \text{ and } Var(\underline{\varepsilon}) = \sigma^2 I \quad . \tag{2.6}$$

In the general linear model form, an estimate of the model is obtained by estimation of the coefficients of $\underline{\beta}$. Several methods exist for obtaining these estimates. The method of least squares will be used here throughout to obtain estimates of $\underline{\beta}$ based on the sample data. The least squares estimator of $\underline{\beta}$, obtained from sample data is given by

$$\hat{\underline{\beta}} = (X'X)^{-1}X'\underline{y} \quad . \tag{2.7}$$

Based upon the least squares estimates, $\hat{\underline{\beta}}$, the estimated responses are given by

$$\hat{\underline{y}} = X\hat{\underline{\beta}} \quad . \tag{2.8}$$

Properties of the coefficient estimates, $\hat{\underline{\beta}}$ and the response estimates, $\hat{\underline{y}}$ are given by

$$E(\hat{\underline{\beta}}) = \underline{\beta} \quad , \tag{2.9}$$

$$Var(\hat{\underline{\beta}}) = \sigma^2(X'X)^{-1} \quad , \tag{2.10}$$

$$E(\hat{\underline{y}}) = X\underline{\beta} \quad , \tag{2.11}$$

$$Var(\hat{\underline{y}}) = \sigma^2 X(X'X)^{-1}X' \quad . \tag{2.12}$$

Also, it is often of interest to predict values of the response at any specific combination of values of the design variables, that is, at the point $\underline{x}'_0 = [1 \;\; x_{01} \;\; x_{02} \ldots x_{0k}]$. The predicted response based upon least squares estimation is given by

$$\hat{y} = \underline{x}'_0\hat{\underline{\beta}} \tag{2.13}$$

with the variance of this predicted response given by

$$Var(\hat{y}) = \sigma^2\underline{x}'_0(X'X)^{-1}\underline{x}_0 \quad . \tag{2.14}$$

The least squares response function estimate is also used in optimizing the response variable by identifying the values of the design variables which provide for the optimal predicted response. A detailed explanation of optimization methods is given by Myers (1976). In the case of a first order polynomial model, the method of steepest ascent is used for optimization. Canonical analysis and ridge analysis are used for optimizing second order polynomial models.

Throughout this work a partitioning of the general linear model often will be used. First and second order models can be represented by partitioning the X matrix and $\underset{\sim}{\beta}$ vector as follows

$$\underset{\sim}{y} = X_1\underset{\sim}{\beta}_1 + X_2\underset{\sim}{\beta}_2 + \underset{\sim}{\varepsilon} \tag{2.15}$$

where

X_1 contains first order variables $(1, x_i)$,

$\underset{\sim}{\beta}_1$ contains first order regression coefficients (β_0, β_i),

X_2 contains second order variables $(x_i^2,\ x_i x_j)$,

$\underset{\sim}{\beta}_2$ contains second order regression coefficients (β_{ii}, β_{ij}).

2.3 The Role of Experimental Design

An experimental design is a set of values for the design variables $x_1, x_2, \ldots, x_k$ at which the response variable, y, is observed. The choice of an experimental design is an important aspect of RSM. Previous results given in section 2.2 show that properties of the least squares estimators are a function of the values of the design variables which are represented in the general linear model by the X matrix. Since many statistical properties depend upon the experimental design, a specific design can be selected to achieve optimality in terms of some of these properties. Properties related to an experimental design are also dependent upon the model under consideration via the X matrix.

RSM procedures usually follow in a sequential manner. To begin, an experimental design is usually chosen to achieve certain first order model properties and to fit a first order model. Orthogonality among the design variables is a frequently desired property for a first order model. Orthogonality allows for estimation of the model coefficients without the undesirable effect of collinearity. Other properties which will be discussed later can also be achieved for a first order model.

Once an appropriate design is selected and the responses are observed, least squares procedures are used to obtain a first order model estimate. The first order model is then judged for its adequacy as an estimate of the true response function by performing a lack of fit test. If the first order model is adequate then it will be used for prediction and exploration of the response. If the first order model is determined to be inadequate, a second order model is usually adopted. In some instances, a second order model cannot be fit using the data points from the existing design. In such cases, one may supplement the existing design with addition points such that a second order model can be fit. This sequential framework of experimentation is commonly used in RSM when an experimenter is uncertain as to the model form to be used for an estimated response function.

The origins of the sequential design procedure are credited to Box and Wilson (1951), who discuss the use of a factorial design or fractional factorial design for fitting a first order model and then augmenting this with axial points to form a central composite design for fitting a second order model. Factorial designs and central composite designs will both be discussed in detail later. The important concept generated by Box and Wilson is that experimentation is performed sequentially.

The sequential framework of experimentation is common practice when the experimenter is uncertain about the model form. Unfortunately the sequential idea has received little attention in terms of formal construction of experimental designs. Only two general concepts of experimental design address the idea of sequential experimentation.

The first concept is that of orthogonal blocking. If an experiment is performed sequentially, then it is possible that responses observed during the initial first order stage were subject to different experimental conditions than the responses observed during the augmentation stage. A block effect could exist due to possibly different experimental conditions in such a case. Designs which block orthogonally have block effects that are orthogonal to the model coefficients and therefore any statistical tests performed on the model coefficients will not be confounded with block effects.

The second concept that addresses sequential experimentation is that of augmenting a first order design with points to obtain a second order D-optimal design (D-optimality will be discussed in section 2.4). Mitchell (1974) has developed the DETMAX algorithm for augmenting first order designs with points that allow for D-optimality to be achieved.

Despite the frequent use of sequential experimentation, design procedures which address this concept are restricted to the two mentioned above. This work attempts to consider the sequential framework of experimentation and incorporate it into the design of RSM experiments.

2.4 Design Criteria

The choice of an experimental design is usually based upon one or more statistical properties of interest. One can optimize a design with respect to these properties. Several design optimality criteria are discussed in this section.

2.4.1 Design and Region Moments

It is necessary to define the concepts of design moments and region moments before discussing particular design criteria.

The design moment matrix is given by,

$$M = \frac{(X'X)}{n} \quad . \tag{2.16}$$

The elements of the design moment matrix are individual design moments of the form,

$$[i] = \sum_{u=1}^{n} \frac{x_{iu}}{n}, \quad [ii] = \sum_{u=1}^{n} \frac{x_{iu}^2}{n}, \quad [ij] = \sum_{u=1}^{n} \frac{x_{iu}x_{ju}}{n},$$

$$[iii] = \sum_{u=1}^{n} \frac{x_{iu}^3}{n}, \quad [iiii] = \sum_{u=1}^{n} \frac{x_{iu}^4}{n}, \quad [iijj] = \sum_{u=1}^{n} \frac{x_{iu}^2 x_{ju}^2}{n} \quad . \tag{2.17}$$

The design moment matrix corresponding to a first order model is given by

$$M = \begin{bmatrix} 1 & [1] & [2] & \dots & [k] \\ [1] & [11] & [12] & \dots & [1k] \\ [2] & [12] & [22] & \dots & [2k] \\ . & . & . & & . \\ . & . & . & & . \\ . & . & . & & . \\ [k] & [k1] & [k2] & \dots & [kk] \end{bmatrix} . \tag{2.18}$$

For a partitioned linear model of the form of (2.15) it is useful to define the design moment matrices

$$M_{11} = \frac{(X'_1X_1)}{n} \quad , \quad M_{12} = \frac{(X'_1X_2)}{n} \quad \text{and } M_{22} = \frac{(X'_2X_2)}{n} \quad , \tag{2.19}$$

where X_1 corresponds to first order model terms and X_2 corresponds to second order model terms.

Region moment matrices are dependent upon the region of interest, R, in k-dimensional space. The region moment matrix is given by,

$$\mu = K\int_R \underline{x}\underline{x}'d\underline{x} \quad . \tag{2.20}$$

where K is the inverse of the volume of the region R given by,

$$K = \frac{1}{\int_R d\underline{x}} \quad .$$

The elements of the region moment matrix are individual region moments of the form

$$\begin{aligned} &w_i = K\int_R x_i d\underline{x} \ , \quad w_{\text{ii}} = K\int_R x_i^2 d\underline{x} \ , \quad w_{\text{ij}} = K\int_R x_i x_j d\underline{x} \ , \\ &w_{\text{iii}} = K\int_R x_i^3 d\underline{x} \ , \quad w_{\text{iiii}} = K\int_R x_i^4 d\underline{x} \ , \quad w_{\text{iijj}} = K\int_R x_i^2 x_j^2 d\underline{x} \ . \end{aligned} \tag{2.21}$$

In addition, other region moment matrices of interest are

$$\begin{aligned} \mu_{11} &= K\int_R \underline{x}_1\underline{x}'_1 d\underline{x} \ , \\ \mu_{12} &= K\int_R \underline{x}_1\underline{x}'_2 d\underline{x} \ , \\ \mu_{22} &= K\int_R \underline{x}_2\underline{x}'_2 d\underline{x} \ . \end{aligned} \tag{2.22}$$

2.4.2 Variance Criteria

An experimenter is often interested in the quality of the prediction obtained from fitting a particular model. The importance of good prediction lies in that optimization is a function of the predicted values obtained from a particular model. One measure of the quality of prediction is the variance of predicted values given by (2.14).

Several design criteria exist pertaining to the variance of prediction. One criterion is based upon the concept of rotatability. An experimental design is said to be rotatable if the prediction variance is constant over spheres of constant radius. If a design is rotatable, then the prediction variance at any point is a function only of the distance of that point from the design center. Box and Hunter (1957) developed design moment conditions which assure rotatability of a design. Most designs used in practice are either rotatable or have moment conditions that are near rotatable.

Another criterion related to the prediction variance is the concept of G-optimality. This criterion considers the maximum prediction variance in a region of interest. A G-optimal design is one which achieves the minimum maximum prediction variance.

The maximum prediction variance is also used for comparing experimental designs via an efficiency measure called G-efficiency defined by Atwood (1969) as

$$\text{G-efficiency} = \frac{\sigma^2 p}{\max\limits_{\underline{x} \in R} Var(\hat{y})} \tag{2.23}$$

where $\sigma^2 p$ is the maximum prediction variance for a G-optimal design (p = the number of parameters in the model) and $\max\limits_{x \in R} Var(\hat{y})$ is the maximum prediction variance in a region R for a particular design D.

Finally, another design criterion based upon the prediction variance is the integrated prediction variance, V. This quantity is usually used for design comparison rather than design optimality. The integrated prediction variance is given by

$$\begin{aligned} V &= \frac{nK}{\sigma^2} \int_R Var(\hat{y}) d\underline{x} \\ &= nK \int_R \underline{x}'(X'X)^{-1} \underline{x} d\underline{x} \\ &= tr(\mu M^{-1}) \ . \end{aligned} \tag{2.24}$$

If the fitted model is a first order model then in the notation of the partitioned linear model

$$V = tr(\mu_{11} M_{11}^{-1}) \ . \tag{2.25}$$

In addition to prediction, an experimenter could also be concerned about the quality of the estimated regression coefficients. The quality of the least squares coefficient estimates is reflected by the variance-covariance matrix of $\hat{\underline{\beta}}$. One commonly used norm on the variance-covariance matrix is the determinant. This determinant is called the generalized variance of $\hat{\underline{\beta}}$. Designs that minimize the generalized variance of $\hat{\underline{\beta}}$, apart from σ^2, are called D-optimal designs. Kiefer (1961) introduced the notion of D-optimality for experimental designs. D-optimal designs minimize $|(X'X)^{-1}|$ or equivalently maximize $|X'X|$. These designs perform well in terms of coefficient estimation and give the smallest $(1-\alpha) \times 100\%$ confidence ellipsoid for $\underline{\beta}$

The generalized variance of $\hat{\underline{\beta}}$ can also be used for comparing designs. Atwood (1969) defines the D-efficiency of a design D to be

$$\text{D-efficiency} = \left[\frac{\frac{|X'X|_D}{n}}{\frac{|X'X|_{\text{D-opt}}}{n_D}} \right]^{\frac{1}{p}} \tag{2.26}$$

where $|X'X|_D$ is the generalized variance of $\hat{\underline{\beta}}$,apart from σ^2 for a design D with n points, $|X'X|_{\text{D-opt}}$ is the generalized variance of $\hat{\underline{\beta}}$, apart from σ^2, for the D-optimal design with n_D points and p is the number of coefficients in the fitted model.

The concept of D-optimality and D-efficiency can also be applied to a subset of the coefficients. In particular, optimization methods for second order models depend heavily upon the estimated second order coefficients (β_{ii} and β_{ij}). Therefore, the generalized variance of this subset of coefficients is of importance for second order models. Kiefer (1961) introduced the idea of D_s-optimal design which are D-optimal designs for a subset of coefficients. D_s-optimal designs minimize the variance-covariance matrix of some subset of estimated coefficients, $\hat{\underline{\beta}}_s$. A D_s-efficiency measure for comparing designs is given by

$$D_s\text{-efficiency} = \left[\frac{|\,Var(\hat{\underline{\beta}}_s)^{OPT}\,|\,/n_{OPT}}{|\,Var(\hat{\beta}_s)^{D}\,|\,/n_D} \right]^{1/p_2} \tag{2.27}$$

where $Var(\hat{\beta}_s)^{OPT}$ is the variance-covariance matrix for a D_s-optimal design with n_{OPT} design points, $Var(\hat{\beta}_s)^D$ is the variance-covariance matrix for a design D with n_D design points and p_2 is the number of coefficients in $\underline{\beta}_s$.

2.4.3 Bias Criterion

Another measure of the quality of prediction is the bias in prediction. Since a model that is used for prediction is always an approximation, bias is present in the prediction due to model misspecification. For the general linear model of (2.15) suppose that the fitted model is given by,

$$\hat{\underline{y}} = X_1 \hat{\underline{\beta}}_1 \tag{2.28}$$

while the model that one protects against is of the form

$$\underline{y} = X_1 \underline{\beta}_1 + X_2 \underline{\beta}_2 + \underline{\varepsilon} \ . \tag{2.29}$$

The estimate $\hat{\underline{\beta}}_1$ is no longer an unbiased estimate, as its expected value is given by,

$$E(\hat{\underline{\beta}}_1) = \underline{\beta}_1 + (X'_1 X_1)^{-1} X'_1 X_2 \underline{\beta}_2 \ . \tag{2.30}$$

Also, the expectation of a predicted value at the point $\underline{x}' = [\underline{x}_1 \ \underline{x}_2]$ is

$$\begin{aligned} E(\hat{\underline{y}}) &= \underline{x}'_1 E(\hat{\underline{\beta}}_1) \\ &= \underline{x}'_1 \underline{\beta}_1 + \underline{x}'_1 (X_1' X_1)^{-1} X'_1 X_2 \underline{\beta}_2 \ . \end{aligned} \tag{2.31}$$

The squared bias in a predicted value is then given by

$$
\begin{aligned}
Bias^2(\hat{y}) &= [E(\hat{y}) - y]^2 \\
&= \underline{\beta}'_2(\underline{x}'_2\underline{x}_2 - 2\underline{x}_2\underline{x}'_1(X_1X_1)^{-1}X'_1X_2 + X'_2X_1(X_1X_1)^{-1}\underline{x}_1\underline{x}'_1(X_1X_1)^{-1}X'_1X_2)\underline{\beta}_2.
\end{aligned} \tag{2.32}
$$

A measure of the bias in prediction, in a region of interest, R, in k-dimensional space is given by the integrated squared bias, B , which is due to Box and Draper (1959).

$$
B = \frac{nK}{\sigma^2}\int_R Bias^2(\hat{y})d\underline{x} \ . \tag{2.33}
$$

Using both design and region moment matrices, the integrated squared bias, B, can be written as,

$$
\begin{aligned}
B &= \frac{n}{\sigma^2}\underline{\beta}'_2[\mu_{22} + M'_{12}M_{11}^{-1}\mu_{11}M_{11}^{-1}M_{12} - 2\mu'_{12}M_{11}^{-1}M_{12}]\underline{\beta}_2 \\
&= \frac{n}{\sigma^2}\underline{\beta}'_2 T\underline{\beta}_2
\end{aligned} \tag{2.34}
$$

where T is called the bias matrix. As shown by Box and Draper, a necessary and sufficient condition for minimizing the integrated squared bias in a region R is given by

$$
M_{11}^{-1}M_{12} = \mu_{11}^{-1}\mu_{12}. \tag{2.35}
$$

Experimental designs which satisfy (2.35) are called minimum bias designs.

The importance of the bias was shown by Box and Draper who not only considered bias but also variance together with bias in terms of a mean squared error. Box and Draper showed that designs that are close to minimum bias achieve minimum mean squared error (which is discussed in section 2.4.4). This seems to be an indication that bias considerations due to model underspecification are dominant over variance considerations.

Consider an example for a $k = 1$ variable design. The integrated mean squared error in prediction, denoted by J, can be divided into a variance portion, V, and a bias portion, B, i.e., $J = V + B$. The variance portion, V, for $k = 1$ variable can be expressed as

$$V = 1 + \frac{1}{3[11]} \ .$$

The bias, B, of equation (2.34) simplifies for $k = 1$ variable to

$$B = \frac{n\beta_{11}^2}{\sigma^2}\left[([11] - 1/3)^2 + \frac{4}{45}\right] .$$

Therefore the mean squared error, J is given by

$$J = 1 + \frac{1}{3[11]} + \frac{n\beta_{11}^2}{\sigma^2}\left[([11] - 1/3)^2 + \frac{4}{45}\right] .$$

Unfortunately the mean squared error J cannot be minimized with respect to the design moment [11] without the knowledge of β_{11}. Table 2.1, taken from Myers (1976) evaluates J for certain values of $\frac{\sqrt{n}\,\beta_{11}}{\sigma}$, which represent values of the pure quadratic coefficient β_{11} corresponding to various ratios of variance, V, to bias, B .

Table 2.1 Values of J for Optimal, Minimum Bias and Minimum Variance Designs for a k = 1 First Order Model

$\sqrt{n}\ \beta_{11}/\sigma$	J-optimal [11]	Optimal J	Min. Bias J ([11] = 1/3)	Min. Variance J ([11] = 1)
9.375 (V = ¼B)	0.349	9.777	9.800	48.208
6.540 (V = ½B)	0.363	5.755	5.799	24.145
4.499 (V = B)	0.388	3.718	3.798	12.129
2.994 (V = 2B)	0.433	2.656	2.797	6.114
1.822 (V = 4B)	0.519	2.052	2.296	3.104
1.215 (V = 6B)	0.623	1.790	2.131	2.121
0.501 (V = 10B)	1.000	1.467	2.022	1.467

Table 2.1 displays the importance of integrated bias for experimental designs. Even for cases when variance, V, contributes heavily to J , the minimum bias design (i.e. [11] = 1/3) is close to the minimum mean squared error design. This seems to indicate that control of the integrated bias in the experimental design is more important than the variance. Box and Draper (1959) have examined the extension to $k > 1$ variables and observed similar results pertaining to the importance of bias.

2.4.4 Mean Squared Error Criterion

The previous two sections have discussed the use of prediction variance and prediction bias for selecting experimental designs. The prediction variance and prediction bias can be combined into the mean squared error of prediction. If a model of the form $\hat{\underline{y}} = X_1\hat{\underline{\beta}}_1$ is fit, then the mean squared error of prediction at a point $\underline{x}' = [\underline{x}'_1 | \underline{x}'_2]$ is given by

$$\begin{aligned} MSE(\hat{y}) &= \sigma^2 \underline{x}'_1(X'_1X_1)^{-1}\underline{x}_1 \\ &+ \underline{\beta}'_2[\underline{x}_2\underline{x}'_2 - 2\underline{x}'_2\underline{x}_1(X'_1X_1)^{-1}X'_1X_2 + X'_2X_1(X'_1X_1)^{-1}\underline{x}_1\underline{x}'_1(X'_1X_1)^{-1}X'_1X_2]\underline{\beta}_2 \\ &= Var(\hat{y}) + Bias^2(\hat{y}) \ . \end{aligned} \tag{2.36}$$

A measure of the mean squared error in prediction for all points within the region of interest, R, is given by the integrated mean squared error, J, defined by Box and Draper (1959) as

$$\begin{aligned} J &= V + B \\ &= tr(\mu_{11}M_{11}^{-1}) + \frac{n}{\sigma^2}\underline{\beta}'_2T\underline{\beta}_2 \ . \end{aligned} \tag{2.37}$$

As previously mentioned, the integrated mean squared error cannot be used for selecting experimental designs without the knowledge of the coefficients in $\underline{\beta}_2$.

2.4.5 Lack of Fit Criteria

Another property of an experimental design which is of interest is the quality of the lack of fit test. It is assumed that the fitted model is of the form (2.28). Then it is of interest to detect if this model is an adequate representation of the response function or if a model of the form (2.29) should be adopted. In particular, following the sequential model development procedure, a first order model is fit and a lack of fit test is used to determine if the first order model is adequate for modeling the response. The quality of the lack of fit test is generally measured by the power of the test.

For the partitioned linear model given by (2.15), the model $\hat{\underline{y}} = X_1\hat{\underline{\beta}}_1$ would be an adequate representation of the response function if $\underline{\beta}_2 = 0$. Therefore it is important to test the lack of fit hypothesis

$$H_0 : \underline{\beta}_2 = \underline{0} \ .$$

Under the usual assumption that $\underline{\varepsilon} \sim N(\underline{0}, \sigma^2 I)$ it is possible to test the hypothesis H_0: $\underline{\beta}_2 = \underline{0}$ using an F statistic of the form,

$$F = \frac{n\hat{\underline{\beta}}_2(M_{22} - M'_{12}M_{11}^{-1}M_{12})\hat{\underline{\beta}}_2}{p_2 s^2} \tag{2.38}$$

where p_2 is the number of coefficients in $\underline{\beta}_2$ and s^2 is the pure error mean square. A detailed description of the lack of fit test procedure is given by Myers (1976) and Draper and Herzberg (1971). The sequential model development procedure is to fit a model of the form $\hat{\underline{y}} = X_1\hat{\underline{\beta}}_1$ if the lack of fit test is not significant, or a model of the form $\hat{\underline{y}} = X_1\hat{\underline{\beta}}_1 + X_2\hat{\underline{\beta}}_2$ if the lack of fit test is significant.

It is well known that the power of the lack of fit test is an increasing function of the noncentrality parameter given by,

$$\lambda = \frac{n\underline{\beta}'_2(M_{22} - M'_{12}M_{11}^{-1}M_{12})\underline{\beta}_2}{\sigma^2}. \tag{2.39}$$

A design will have maximum power for the detection of the adequacy of a fitted model if it maximizes the noncentrality parameter, λ . The noncentrality parameter is a function of the experimental design through the matrix of the quadratic form in the $\underline{\beta}_2$,

$$L = M_{22} - M'_{12}M_{11}^{-1}M_{12}. \tag{2.40}$$

L is referred to as the lack of fit matrix. Unfortunately, λ is also a function of the unknown coefficients in $\underline{\beta}_2$. Therefore, the choice of an experimental design that maximizes λ is also a function of the unknown $\underline{\beta}_2$.

One design criterion that addresses the lack of fit test is the determinant of the lack of fit matrix. Designs that maximize this determinant are referred to as $|L|$-optimal design. Atkinson (1972) has investigated $|L|$-optimal design under the name of T-optimal designs. The $|L|$ considers only the design dependent portion of the noncentrality parameter. This criterion is essentially equivalent to D_s-optimality since the variance-covariance matrix of $\hat{\underline{\beta}}_2$ apart from σ^2 is the lack of fit matrix. In addition an $|L|$-efficiency measure can be defined for comparing designs that is equivalent to the D_s-efficiency given in (2.27).

Atkinson points out that designs that are $|L|$-optimal may provide poor estimates of $\underline{\beta}_1$ when the hypothesis of $\underline{\beta}_2 = 0$ is not rejected. He suggests a procedure for maximizing $|L|$ subject to a bound on the D-efficiency of a design for estimating $\underline{\beta}_1$.

The $|L|$ criterion has two shortcomings in attempting to characterize the power of the lack of fit test. First, $|L|$ does not account for an increase in the power of the lack of fit test associated with an increase in the degrees of freedom. Secondly, $|L|$ does not account for the dependency of the noncentrality parameter on the coefficients in $\underline{\beta}_2$.

The Λ criteria address the quality of the lack of fit test accounting for the coefficients in $\underline{\beta}_2$. The Λ criteria were developed by Jones and Mitchell (1978). The Λ_1 criterion selects designs which maximize the minimum noncentrality parameter λ over a specified region of model inadequacy in the coefficients in $\underline{\beta}_2$. The region of model inadequacy used is

$$\Phi = \{\underline{\beta}_2 : \underline{\beta}'_2 P \underline{\beta}_2 > \delta\} \quad \text{where} \quad P = \mu_{22} - \mu'_{12}\mu_{11}^{-1}\mu_{12} \ . \tag{2.41}$$

Jones and Mitchell show that the minimum value of λ will occur on the boundary of Φ and is equal to

$$\lambda_{\min} = \delta(\text{min eigenvalue of } T^{-1}L). \tag{2.42}$$

The Λ_2 criterion is an average analog of Λ_1. The Λ_2-criterion maximizes the average value of the noncentrality parameter, λ, over the boundary of the region Φ. Jones shows that the average value of λ is equal to

$$\delta tr[T^{-1}L]/p_2 \tag{2.43}$$

where p_2 is the number of parameters in $\underline{\beta}_2$. The design criterion reduces to maximizing $tr[T^{-1}L]$. The Λ_2-optimality criterion has an appealing advantage over the Λ_1 criterion in that the lack of fit matrix L need not be of full rank for the Λ_2 criterion. For many first order designs (i.e., factorial designs), the lack of fit matrix is not of full rank.

2.5 Experimental Design Classes

This section provides an introduction to the design classes considered throughout this work. Factorial designs will be the only first order design class discussed (an additional first order class will be considered in Chapter 3). Several classes of second order designs are given. Designs belonging to all of the classes presented here can be chosen according to most of the criteria given in section 2.4.

2.5.1 Factorial and Fractional Factorial Designs

2^k factorial designs are generally employed for the purpose of using a first order model estimate for the response. These designs utilize two levels for each of the k variables. The levels of the factorial design are given by $\pm g$, where $0 \leq g \leq 1$. These designs are orthogonal and therefore first order rotatable. In addition, n_0 center points will be added to the basic factorial structure to allow for an error estimate and to obtain pure quadratic information. Center points are defined to be experimental points where all k design variables are set to zero. Factorial designs with center runs can be used to perform a lack of fit test for detecting second order terms. An example of a factorial design in k = 3 variables is given by

$$\begin{bmatrix} -g & -g & -g \\ -g & -g & g \\ -g & g & -g \\ -g & g & g \\ g & -g & -g \\ g & -g & g \\ g & g & -g \\ g & g & g \end{bmatrix} . \tag{2.44}$$

Fractional factorial designs are also considered. These designs have only a fraction of the design points of a full factorial design. Appropriate fractions are chosen such that all linear and interaction coefficients can be estimated.

2.5.2 Central Composite Designs

Central composite designs (ccd) were originally discussed by Box and Wilson (1951). The central composite design is the most commonly used second order design. The designs consist of three parts:

1) A factorial portion or fractional factorial (for $k \geq 5$) with levels $\pm g$, $0 \leq g < 1$.

2) An axial portion consisting of 2k axial points. An axial point has one variable set to some value $\pm \alpha$, $0 < \alpha \leq 1$, and all other variable values set to zero.

3) Center points portion containing n_0 center points used for replication error and to achieve other properties of interest.

A central composite design has the following form,

$$\begin{bmatrix} \pm \underline{g} & \pm \underline{g} & \pm \underline{g} \\ -\alpha & 0 & 0 \\ \alpha & 0 & 0 \\ 0 & -\alpha & 0 \\ 0 & \alpha & 0 \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ 0 & 0 & -\alpha \\ 0 & 0 & \alpha \\ \underline{0} & \underline{0} & \underline{0} \end{bmatrix} . \qquad (2.45)$$

As discussed by Box and Wilson, central composite designs fit nicely into the sequential framework of experimentation. A factorial design can be used for estimating a first order model and performing a lack of fit test. If a significant lack of fit is observed, the existing factorial design can be augmented with axial points to form a central composite design for estimating a second order model.

2.5.3 Box-Behnken Designs

These designs are constructed by combining 2^k factorial designs with balanced incomplete block designs. These designs are special fractions of 3^k factorial designs. Box-Behnken designs were originally constructed as an alternative to central composite designs with less design points. In addition, Box-Behnken designs require only three levels for the variables whereas the central composite design requires five levels. The levels of a Box-Behnken design are denoted by $\pm g$, $0 \leq g \leq 1$. For $k = 3$, 4 and 5 variables, Box-Behnken designs are constructed by using a 2^2 factorial designs in each of the $\binom{k}{2}$ combinations of variable pairs and setting the values of the other k-2 variables to zero. For $k = 6$ variables, a 2^3 factorial design is combined with all possible variable triples. An example of a Box-Behnken design for $k = 3$ variables is given by

$$\begin{bmatrix} -g & -g & 0 \\ -g & g & 0 \\ g & -g & 0 \\ g & g & 0 \\ -g & 0 & -g \\ -g & 0 & g \\ g & 0 & -g \\ g & 0 & g \\ 0 & -g & -g \\ 0 & -g & g \\ 0 & g & -g \\ 0 & g & g \\ \underline{0} & \underline{0} & \underline{0} \end{bmatrix} . \tag{2.46}$$

The performance of Box-Behnken designs will be compared with that of central composite designs.

The next three subsections discuss saturated or near saturated second order design classes. A saturated design is one in which the number of design points is equal to the number of coefficients to be estimated. Near saturated designs contain slightly more design points than coefficients to be estimated. These designs can be useful when cost constraints limit the number of experimental points. The performance of these three classes will be compared amongst each other.

2.5.4 Small Composite Designs

Small composite designs, as originally defined by Hartley (1959), are very similar to central composite designs. Small composite designs consist of a factorial portion, an axial portion and center points. The designs with just the factorial and axial portions are saturated or near saturated. The factorial portion of these designs is always a special fraction. This chosen fraction makes use of the fact that axial points can be used to estimate first order and pure quadratic coefficients and factorial points can be used to estimate interaction coefficients. An example of a k=3 variable small composite design is given by

$$\begin{bmatrix} -g & -g & -g \\ g & g & -g \\ g & -g & g \\ -g & g & g \\ -\alpha & 0 & 0 \\ \alpha & 0 & 0 \\ 0 & -\alpha & 0 \\ 0 & \alpha & 0 \\ 0 & 0 & -\alpha \\ 0 & 0 & \alpha \\ \underline{0} & \underline{0} & \underline{0} \end{bmatrix} . \tag{2.47}$$

2.5.5 Hybrid Designs

Roquemore (1976) developed this class of designs that are saturated or near saturated when considered without the use of center points. The designs consist of a central composite design in k-1 variables with the values of the k^{th} variable chosen to achieve the same degree of orthogonality among the k variables as a central composite design. The general form of Hybrid design is given by

$$
\begin{bmatrix}
\pm g & \pm g & \cdots & \pm g & \underline{a} \\
\pm \alpha & \underline{0} & \cdots & \underline{0} & \underline{b} \\
\underline{0} & \pm \alpha & \cdots & \underline{0} & \underline{b} \\
\cdot & \cdot & & \cdot & \cdot \\
\cdot & \cdot & & \cdot & \cdot \\
\cdot & \cdot & & \cdot & \cdot \\
\underline{0} & \underline{0} & & \pm \alpha & \underline{b} \\
\underline{0} & \underline{0} & \cdots & \underline{0} & \underline{d} \\
\underline{0} & \underline{0} & & \underline{0} & \underline{0}
\end{bmatrix} . \tag{2.48}
$$

One can notice the central composite design for the first k-1 variables. The values of a, b, c and d are chosen such that all odd design moments are equal to zero and all pure second moments are equal.

2.5.6 Notz Designs

Notz (1982) constructed saturated or near saturated designs that perform well in terms of D-efficiency relative to other saturated design classes. Notz designs consist of a 2^k factorial design, or some part of it, augmented with a k dimensional identity matrix. A Notz design for $k = 3$ variables is given by

$$
\begin{bmatrix}
-g & -g & -g \\
-g & -g & g \\
-g & g & -g \\
-g & g & g \\
g & -g & -g \\
g & -g & g \\
g & g & -g \\
g & g & g \\
1 & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & 1
\end{bmatrix} . \tag{2.49}
$$

Notz uses the levels of $\pm$ 1 to achieve good D-efficiencies. The work performed here will allow the factorial levels to vary over the range $0 < g \leq 1$ for designs that are of the identical structure given by Notz. The D-efficiency values for these designs will be less than that achieved by Notz, but other gains in performance of the designs will be shown.

Chapter III

III. A Lack of Fit Criterion and First Order Designs

In this chapter, in conjunction with the sequential strategy, a new class of robust first order experimental designs will be developed using the $\Lambda_2{}^*$ optimality criterion. These designs offer the best power of the lack of fit test for a design with a given integrated bias. The flexibility of this design class will be shown by optimizing the design parameters with respect to several optimality criteria. In addition, the design class will be compared to standard design classes. However, the next section will begin with a brief review of the lack of fit and integrated mean squared error properties of experimental designs.

3.1 Lack of Fit and Integrated Mean Squared Error Revisited

The general design philosophy of accounting for potential bias in the integrated mean squared error criterion appears to contradict that of maximizing the power of the lack of fit test. This can most easily be seen for the case of $k = 1$ variable, where the fitted model is of first order and the model one protects against is of second order. Technically, the fitted model is $\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 x$ and the assumed model is $y = \beta_0 + \beta_1 x + \beta_{11}x^2$. If it is assumed that an orthogonal first order design will be used, then the design moment matrices are given by

$$M_{11} = \begin{bmatrix} 1 & [1] \\ [1] & [11] \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & [11] \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & \frac{\Sigma x^2}{n} \end{bmatrix}, \tag{3.1}$$

$$M_{12} = \begin{bmatrix} [11] \\ [111] \end{bmatrix} = \begin{bmatrix} [11] \\ 0 \end{bmatrix} = \begin{bmatrix} \frac{\Sigma x^2}{n} \\ 0 \end{bmatrix}, \tag{3.2}$$

and

$$M_{22} = [1111] = \frac{\Sigma x^4}{n}. \tag{3.3}$$

Also, for the region of interest given by the interval [-1,1], the region moment matrices are given by

$$\mu_{11} = \begin{bmatrix} 1 & 0 \\ 0 & \frac{1}{3} \end{bmatrix}, \tag{3.4}$$

$$\mu_{12} = \begin{bmatrix} \frac{1}{3} \\ 0 \end{bmatrix}, \tag{3.5}$$

and

$$\mu_{22} = \frac{1}{5}. \tag{3.6}$$

The conditions for a minimum bias design given by (2.35) are satisfied by designing $[11] = \frac{\Sigma x^2}{n} = \frac{1}{3}$. This implies that the data would be chosen such that the points are restricted in their distance from the design center.

A design which maximizes the power of the lack of fit test is constructed such that the noncentrality parameter is a maximum. The noncentrality parameter for k = 1 variable is given by,

$$\lambda = \frac{n\beta_{11}^2}{\sigma^2}([1111] - [11]^2) = \frac{n\beta_{11}^2}{\sigma^2}\left[\Sigma x^4 - \frac{(\Sigma x^2)^2}{n}\right]. \tag{3.7}$$

This would be maximized regardless of β_{11} by spreading out the design points as much as possible (i.e. the design points are at -1, + 1 and 0).

The conflict between the two criteria is obvious since designs which account for bias restrict the spread of the design points whereas designs which maximize the power of the lack of fit test correspond to the maximum attainable spread in the design points (i.e., in the corners of the operability region). Also, it appears that designs which have good bias properties will have poor lack of fit power properties and vice versa. This general conflict extends to the case of $k \geq 2$ variables in a similar fashion to what has been displayed for the $k = 1$ variable case.

Despite this conflict, many times an experimenter is uncertain of how to specify his model. When this uncertainty exists, as it often does, one usually will estimate the response with a simple model (i.e, first order) then perform a lack of fit test for detection of model terms of order one higher (i.e., second order terms). If a significant lack of fit is observed, the higher order model ($d = 2$) is used to estimate the response. If a nonsignificant lack of fit is observed, then the simple model ($d = 1$) is used to estimate the response.

In experimental problems that are described by the above scenario, an experimental design that will provide a high quality lack of fit test and in addition, provide some protection due to potential bias when a nonsignificant lack of fit is observed are desired.

3.1.1 Two Variable Example

Consider the following example in $k = 2$ variables. The design region, where design points can be placed will be characterized by a unit square. The region of interest for prediction, R will also be the unit square. The integrated mean squared error of prediction, J, and the noncentrality parameter of the lack of fit test can be written as,

$$J = 1 + \frac{2w_{ii}}{[ii]} + \frac{1}{\sigma^2}\Big[(\beta_{11}^2 + \beta_{22}^2)([ii]^2 - 2w_{ii}[ii] + w_{iiii}) + 2\beta_{11}\beta_{22}([ii]^2 - 2w_{ii}[ii] + w_{iijj}) + \beta_{12}^2 w_{iijj}\Big] \tag{3.8}$$

$$\lambda = \frac{n}{\sigma^2}\Big[(\beta_{11}^2 + \beta_{22}^2)([iiii] - [ii]^2) + 2\beta_{11}\beta_{22}([iijj] - [ii]^2) + \beta_{12}^2[iijj]\Big] \tag{3.9}$$

for symmetric designs with odd moments through order 4 equal to zero.

If we assume the second order coefficients are known and given by,

$$\frac{\beta_{11}}{\sigma} = -1/2 \quad \frac{\beta_{22}}{\sigma} = 3/2 \quad \frac{\beta_{12}}{\sigma} = 3$$

then choosing a design with pure second moment, [ii], equal to 0.40 will perform well in terms of mean squared error. Recall table 2.1 which indicated that designs with second moments slightly greater than the minimum bias second moment will perform well in terms of mean squared error.

A factorial design with [ii] = 0.4 and with four center points is given by

$$D = \begin{bmatrix} -0.8944 & -0.8944 \\ -0.8944 & 0.8944 \\ 0.8944 & -0.8944 \\ 0.8944 & 0.8944 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{bmatrix}.$$

The four center points included in this design allow for a lack of fit test to be performed with 3 degrees of freedom for an error estimate. The noncentrality parameter for the lack of fit test given by (3.9) will equal 24.317 and this yields a power of 0.7078 at $\alpha = 0.05$ for the detection of second order terms.

The conflict between bias and power discussed above suggests that one needs to decide which criterion is most important and use the design that is optimal with respect to that criterion. Fortunately, a criterion that accounts for both the power of the lack of fit test and the mean squared error will be developed and used to select robust designs with respect to mean squared error and power of the lack of fit. This criterion is used when an experimenter is unsure about the model and begins the investigation in the sequential manner previously described. A first order design allows for a first order model to be fit and a lack of fit test to be performed to check the adequacy of a first order model. The lack of fit test is used to decide upon a first order (nonsignificant lack of fit) or a second order (significant lack of fit) model. Good power of the lack of fit test is desired since the important decision of a model form is dependent upon this test. In addition, if the lack of fit test is nonsignificant and a first order model is used, then good mean squared error of prediction is desired.

3.1.2 Λ_2-Optimality - Review

The Λ_2-optimality criterion maximizes the average value of the noncentrality parameter of the lack of fit test over a region of model inadequacy. The region of model inadequacy is given by,

$$\Phi = \{\underline{\beta}_2 : \frac{\underline{\beta}'_2 P \underline{\beta}_2}{\sigma^2} = \delta, \delta > 0\} \ . \tag{3.10}$$

The Λ_2 criterion maximizes

$$\frac{\int_{\Phi} \lambda d\underline{\beta}_2}{\int_{\Phi} d\underline{\beta}_2} = \frac{\delta tr[P^{-1}L]}{p_2} . \tag{3.11}$$

Choosing a design that maximizes (3.11) is equivalent to choosing a design which maximizes the $tr[P^{-1}L]$ since p_2 and δ are independent of the design. Jones uses the Λ_2 criterion with a model inadequacy measure that is independent of the design, that is, the P matrix is not design dependent.

An alternative approach to design, which accounts for the lack of fit performance and potential bias, is to redefine the measure of model inadequacy to be the integrated bias or the integrated mean squared error.

In the next section, we will develop a new design criterion denoted by Λ_2^*, that represents a modification of the Λ_2 criterion. The Λ_2^* criterion will consider the average noncentrality parameter of the lack of fit test over a region of fixed integrated bias, B, or integrated mean squared error, J. This new criterion will then be applied to ordinary factorial designs to select the factorial designs that perform best in terms of the lack of fit test for a given bias. In addition, the Λ_2^* criterion will be utilized in developing a new class of experimental designs which offer improved lack of fit performance compared to factorial designs.

3.2 A Lack of Fit/Mean Squared Error Criterion

The Λ_2 criterion developed by Jones attempts to consider the noncentrality parameter of the lack of fit test accounting for the unknown second order coefficients. Unfortunately, Jones' approach considers the second order coefficients through some measure of model inadequacy (3.10) that is somewhat artificial. A more reasonable measure of model inadequacy is given by the integrated bias in prediction. Therefore, one can consider the Λ_2 criterion modified such that the region of model inadequacy is determined by the integrated bias of prediction. The $\Lambda_2{}^*$ criterion is a modification of the Λ_2 criterion defined as,

$$\Phi^* = \{\underline{\beta}_2 : \frac{\underline{\beta}'_2 T \underline{\beta}_2}{\sigma^2} = \delta, \delta > 0\}$$

$$\bar{\lambda} = \frac{\int_{\Phi^*} \lambda d\underline{\beta}_2}{\int_{\Phi^*} d\underline{\beta}_2} \tag{3.12}$$

$$= \frac{\delta tr[T^{-1}L]}{p_2} \; .$$

Again, since δ and p_2 are design independent, the $\Lambda_2{}^*$ criterion uses as a basis for design selection, $tr[T^{-1}L]$. This criterion evaluates the performance of the lack of fit test, through the noncentrality parameter, conditional upon the bias properties of a design being fixed. A detailed derivation of this criterion is given in Appendix B.

If the bias properties of a design are fixed, then since T depends only upon second order design moments, the fixed bias condition corresponds to fixing the second order design moment. In addition, one can see from (3.8) that if the second order design moment is fixed, then the prediction properties (i.e., V, B and J) of a design for a first order model are completely determined. The lack of fit properties, given by the noncentrality parameter of (3.9) are a function of second order and fourth order design moments. If the second order moments are fixed, then the $\Lambda_2{}^*$ criterion is used to select the fourth order design moments that achieve the maximum average noncentrality parameter.

This research will involve utilization of the Λ_2^* criterion when the prediction properties for a first order model are fixed. Therefore the second order design moment is chosen according to some prediction property (bias, variance or mean squared error). Empirical optimization of Λ_2^* criterion will be performed in evaluating the parameters of certain design classes and also to compare among the classes. The design region in which data points can be placed will be considered to be a unit cuboidal region.

3.3 Factorial Designs

The Λ_2^* criterion is applied to the class of first order 2^k factorial designs with n_0 center runs. The criterion is used to choose the fourth order design moments for factorial designs with the second moment chosen according to one of three prediction properties of interest (Bias, Variance, Mean Squared Error). Factorial designs for k = 2, 3 and 4 will be investigated. The $k = 4$ design is a one half fraction of a 2^4 design with defining contrast I = ABCD.

Table 3.1 provides a summary of the evaluation of k=2, 3 and 4 variable factorial designs. Minimum bias, minimum variance and mean squared error efficient factorial designs are evaluated in terms of the Λ_2^* criterion for various sample sizes, n. One can use the results of Table 3.1 to select a design of one of the three types (minimum bias, minimum variance or mean squared error efficient) that performs well in terms of the lack of fit test based upon the Λ_2^* criterion.

Table 3.1 - Evaluation of Factorial Designs in Terms of Λ_2^* Criterion

	Minimum Bias			*Minimum Variance*			*Mean Squared Error Efficient*	
***k* = 2**								
n	g	$tr[T^{-1}L]$	n	g	$tr[T^{-1}L]$	n	g	$tr[T^{-1}L]$
7	0.7638	3.6250	7	1.0	7.5643	7	0.8346	4.9746
8	0.8165	4.5000	8	1.0	7.9615	8	0.8944	6.1527
9	0.8660	5.3750	9	1.0	8.3478	9	0.9487	7.3309
10	0.9129	6.2499	10	1.0	8.5091	10	1.0	8.5091
11	0.9574	7.1250	11	1.0	8.3739	11	1.0	8.3739
12	1.0000	8.0000	12	1.0	8.0	12	1.0	8.0
***k* = 3**								
n	g	$tr[T^{-1}L]$	n	g	$tr[T^{-1}L]$	n	g	$tr[T^{-1}L]$
10	0.6455	4.6875	10	1.0	22.2467	10	0.7331	7.4264
11	0.6770	5.5312	11	1.0	20.7096	11	0.7689	8.6435
12	0.7071	6.3750	12	1.0	19.5789	12	0.8031	9.8605
13	0.7360	7.2187	13	1.0	18.7831	13	0.8359	11.0776
14	0.7638	8.0625	14	1.0	18.2657	14	0.8675	12.2947
15	0.7906	8.9063	15	1.0	17.9745	15	0.8979	13.5117
16	0.8165	9.7500	16	1.0	17.8549	16	0.9274	14.7288
17	0.8412	10.5937	17	1.0	17.8460	17	0.9559	15.9458
18	0.8660	11.4375	18	1.0	17.8824	18	0.9836	17.1629
***k* = 4**								
n	g	$tr[T^{-1}L]$	n	g	$tr[T^{-1}L]$	n	g	$tr[T^{-1}L]$
10	0.6455	8.7500	10	1.0	43.8667	10	0.7500	15.0815
11	0.6770	10.1250	11	1.0	40.3907	11	0.7866	17.1548
12	0.7071	11.5000	12	1.0	37.6667	12	0.8216	19.2281
13	0.7360	12.8750	13	1.0	35.5563	13	0.8551	21.3014
14	0.7638	14.2500	14	1.0	33.9606	14	0.8874	23.3746
15	0.7906	15.6250	15	1.0	32.8000	15	0.9186	25.4479
16	0.8165	17.0000	16	1.0	32.0000	16	0.9487	27.5212
17	0.8416	18.3750	17	1.0	31.4792	17	0.9779	29.5944
18	0.8660	19.7500	18	1.0	31.1428	18	1.0000	31.1428

3.4 Rotated Designs

A class of first order designs which outperforms the class of ordinary factorial designs in terms of the Λ_2^* criterion is the class of rotated factorial designs. These rotated factorial designs are fractions of 4-level designs within the experimental region,

$$-1 \le x_i \le 1 \quad for \quad i = 1,2,\ldots,k.$$

These rotated designs can be considered as factorial designs rotated through an angle θ such that the design points are on the boundary of the experimental design region. Figure 3.1 shows a factorial design with level $g = 0.80$ and a corresponding rotation design.

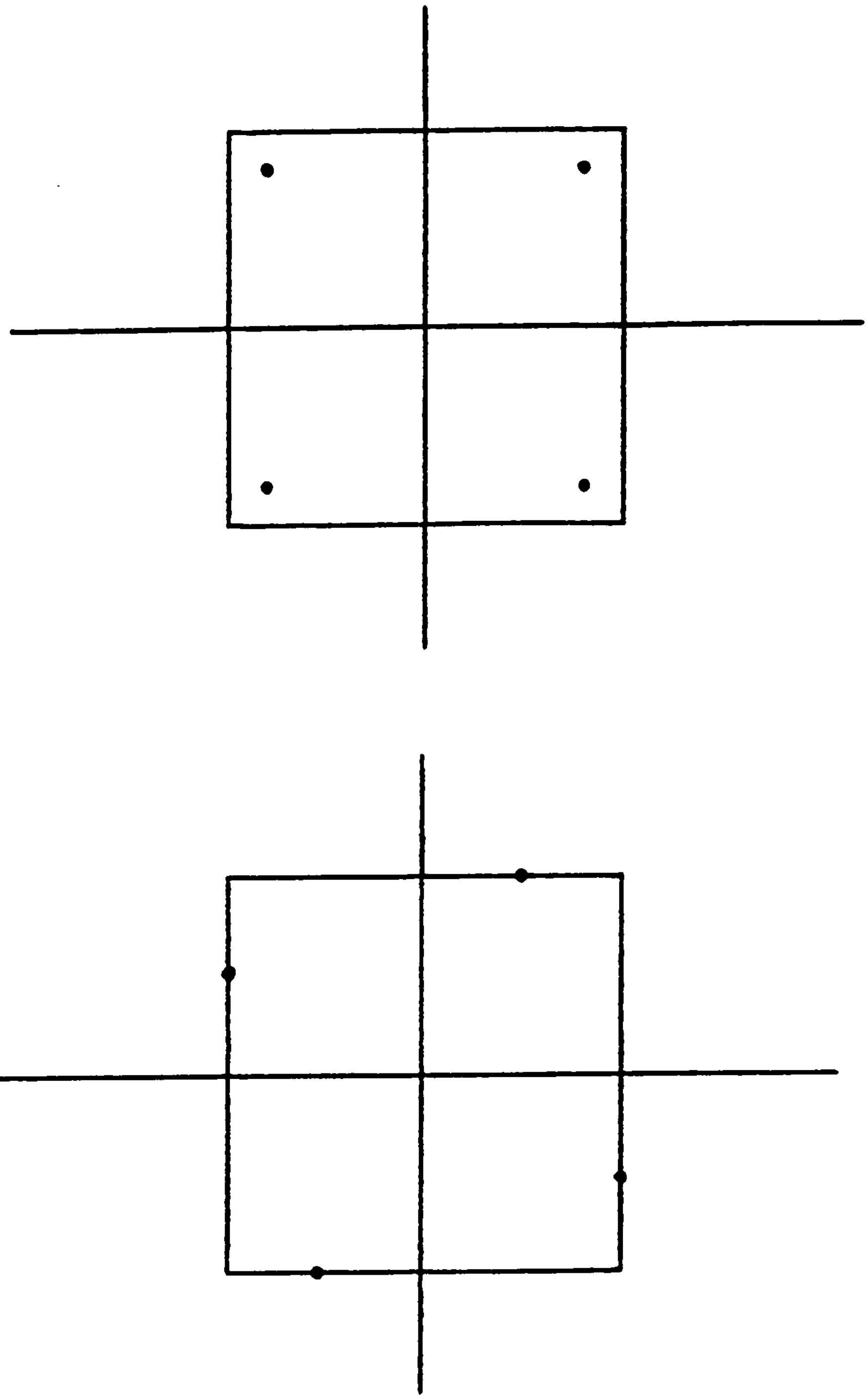

Figure 3.1 - Two Variable Factorial Design and Corresponding Rotation Design

The design matrix corresponding to the factorial design given in Figure 3.1 is given by

$$D = \begin{bmatrix} -g & -g \\ -g & g \\ g & -g \\ g & g \end{bmatrix}. \tag{3.13}$$

If this design is rotated through an angle θ, the transformation matrix is given by,

$$R = \begin{bmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{bmatrix} \tag{3.14}$$

and the new design matrix has the form,

$$RD = \begin{bmatrix} -g(\cos\theta - \sin\theta) & -g(\cos\theta + \sin\theta) \\ -g(\cos\theta + \sin\theta) & g(\cos\theta - \sin\theta) \\ g(\cos\theta + \sin\theta) & -g(\cos\theta - \sin\theta) \\ g(\cos\theta - \sin\theta) & g(\cos\theta - \sin\theta) \end{bmatrix}. \tag{3.15}$$

The four levels of this design can then be appropriately scaled to the values, $1, -1, d$ and $-d$ by reexpressing the transformation matrix as

$$R = \begin{bmatrix} \frac{d+1}{2g} & \frac{-d+1}{2g} \\ \frac{d-1}{2g} & \frac{d+1}{2g} \end{bmatrix} \tag{3.16}$$

and the design matrix as

$$D = \begin{bmatrix} -d & -1 \\ d & 1 \\ -1 & d \\ 1 & -d \end{bmatrix} . \tag{3.17}$$

The design points of (3.17) are all located on the boundary of the experimental design region. The value of d is arbitrary but bounded by $0 \le d \le 1$. ($d = 1$ corresponds to a factorial design with $g = 1$). The value of d can be specified to achieve the desired properties (i.e., bias, variance, etc.) for a design. These properties will be discussed for the rotated design class.

The rotated designs developed for $k = 2$ variables above are easily extended for the case of $k > 2$ variables. The designs are just rotations of the ordinary factorial designs. For $k = 3$ variables the transformation matrix is given by,

$$R = \begin{bmatrix} (d+1)/2g & (-d+1)/2g & 0 \\ (d-1)/2g & (d+1)/2g & 0 \\ 0 & 0 & \sqrt{(d^2+2)/2g} \end{bmatrix} \tag{3.18}$$

yielding the design

$$\begin{bmatrix} -d & -1 & -\sqrt{(d^2+1)/2} \\ -d & -1 & \sqrt{(d^2+1)/2} \\ -1 & d & -\sqrt{(d^2+1)/2} \\ -1 & d & \sqrt{(d^2+1)/2} \\ 1 & -d & -\sqrt{(d^2+1)/2} \\ 1 & -d & \sqrt{(d^2+1)/2} \\ d & 1 & -\sqrt{(d^2+1)/2} \\ d & 1 & \sqrt{(d^2+1)/2} \end{bmatrix} . \tag{3.19}$$

Notice that two variables have been rotated, while the third has just been rescaled to guarantee symmetry.

The transformation matrix for $k = 4$ variables is given by,

$$R = \begin{bmatrix} (d+1)/2g & 0 & (-d+1)/2g & 0 \\ 0 & (d+1)/2g & 0 & (d-1)/2g \\ (-d+1)/2g & 0 & (d+1)/2g & 0 \\ 0 & (d-1)/2g & 0 & (d+1)/2g \end{bmatrix} \tag{3.20}$$

yielding the design

$$\begin{bmatrix} -d & -d & -1 & -1 \\ -d & d & -1 & 1 \\ d & -d & 1 & -1 \\ d & d & 1 & 1 \\ 1 & 1 & -d & -d \\ 1 & -1 & -d & d \\ -1 & 1 & d & -d \\ -1 & -1 & d & d \\ -d & -1 & -1 & d \\ d & 1 & 1 & -d \\ -d & 1 & -1 & -d \\ d & -1 & 1 & d \\ -1 & d & d & 1 \\ 1 & -d & -d & -1 \\ -1 & -d & d & -1 \\ 1 & d & -d & 1 \end{bmatrix}. \tag{3.21}$$

A fractional factorial design for $k = 4$ variables with defining contrast I = ABCD is also often used when the experimenter is limited in the number of allowable experimental runs. The corresponding rotation design of this one-half fraction is given by

$$\begin{bmatrix} -d & -d & -1 & -1 \\ -d & d & -1 & 1 \\ d & d & 1 & -1 \\ d & d & 1 & 1 \\ 1 & 1 & -d & -d \\ 1 & -1 & -d & d \\ -1 & 1 & d & -d \\ -1 & -1 & d & d \end{bmatrix} . \tag{3.22}$$

The general pattern shown in the designs for k = 2, 3 and 4 variables can be extended to construct rotation designs for $k \geq 5$ variables. Only k = 2, 3 and 4 variable designs are studied here, although one would expect similar results to hold for $k \geq 5$ variables.

Consistent with the sequential framework of experimentation, the prediction and lack of fit properties of the rotation designs are now investigated.

3.4.1 Effect of Rotation on Bias and Mean Squared Error

The effect of rotation on the integrated prediction bias, B and the integrated mean squared error of prediction, J is summarized by the following theorems.

Theorem 1:

The integrated bias, B, is invariant to an orthogonal rotation of an orthogonal symmetric first order design when protecting against a second order model.

Proof:

Recall from (2.34)

$$B = \frac{n}{\sigma^2}\underline{\beta}'_2[\mu_{22} - 2\mu'_{12}M_{11}^{-1}M_{12} + M'_{12}M_{11}^{-1}\mu_{11}M_{11}^{-1}M_{12}]\underline{\beta}_2 \ .$$

Only M_{11} and M_{12} are affected by the design, therefore it must be shown that M_{11} and M_{12} are unaffected by rotation.

(i) To show that M_{11} is unaffected by rotation, recall that $M_{11} = X'_1X_1/n$, where $X_1 = [\underline{1}, \underline{x}_1, \underline{x}_2 ... \underline{x}_k]$. The design D is given by $[\underline{x}_1, \underline{x}_2 ... \underline{x}_k]$ therefore $X_1 = [\underline{1} \mid D]$. The orthogonal rotation of D by the transformation matrix R is given by

$$D^* = RD.$$

The rotated X_1 matrix is then of the form,

$$X_1{}^* = [\underline{1} \mid D^*]$$

where X_1 and $X_1{}^*$ are related by the transformation matrix H,

$$H = \begin{bmatrix} 1 & 0 & \dots & 0 \\ 0 & & & \\ . & & & \\ . & & R & \\ . & & & \\ 0 & & & \end{bmatrix}$$

so that

$$X_1{}^* = HX_1.$$

Now,

$$
\begin{aligned}
M_{11}^* &= X_1^{*\prime} X_1^* / n \\
&= X'_1 H' H X_1 / n
\end{aligned}
$$

and since R and therefore also H is an orthogonal rotation,

$$H'H = I$$

which implies that

$$
\begin{aligned}
M_{11}^* &= X'_1 I X_1 / n \\
&= X_1' X_1 / n \\
&= M_{11} \ .
\end{aligned}
$$

(ii) To show that M_{12} is unaffected by rotation, recall that M_{12} consists of the design moments [ii], [iii] and [iij]. [ii] is unaffected by the rotation since the [ii] are the diagonal elements in M_{11}. The moments [iii] = [iij] = 0 for a first order symmetric design. It is assumed that the design center can be centered and scaled to $\underset{\sim}{x} = \underset{\sim}{0}$. For any design point $\underset{\sim}{x}$ of a symmetric design there also exists the design point $-\underset{\sim}{x}$.

Now consider a design point $\underset{\sim}{x}$ from a symmetric experimental design D. Since D is symmetric, the point $-\underset{\sim}{x}$ must also be a design point in D. Consider the orthogonal rotation of D using the transformation matrix R . For the point $\underset{\sim}{x}$, $\underset{\sim}{z}$ corresponds to the rotation of $\underset{\sim}{x}$,

$$\underset{\sim}{z} = R\underset{\sim}{x} \ .$$

For the point $-\underset{\sim}{x}$, the rotation corresponds to

$$R(-\underset{\sim}{x}) = -R\underset{\sim}{x} = -\underset{\sim}{z} \ .$$

Therefore, for any design points $\underset{\sim}{x}$ and $-\underset{\sim}{x}$ in the design D, the corresponding rotated points in D^* will be z and $-\underset{\sim}{z}$. Therefore D^* will also be symmetric, and [iii] = [iij] = 0, which leads to

$$M_{12} = M_{12}^* \ .$$

The integrated bias for a rotated factorial design will be equal to the integrated bias of the corresponding factorial design.

Theorem 2:

The integrated mean squared error, J, is invariant to an orthogonal rotation of an orthogonal symmetric first order design when protecting against a second order model.

Proof:

Recall

$$J = V + B$$

and that B is unaffected from the result of Theorem 1. Also, $V = tr(\mu_{11}M_{11}^{-1})$ is a function of the design only through the matrix M_{11}. It has been shown in the proof of theorem 1 that M_{11} is unaffected by rotation. Therefore V and subsequently J are unaffected by rotation.

Theorem 1 and 2 show that the prediction properties pertaining to a first order model for rotation designs are equivalent to the prediction properties for an ordinary factorial design. Therefore, rotation designs can be used to achieve the same prediction properties as factorial designs.

3.4.2 Effect of Rotation on Lack of Fit

A first order factorial design with the addition of center runs allows for a lack of fit test to be performed on second order coefficients (β_{ij} and β_{ii}). The general linear model form of the test statistic and the noncentrality parameter have been previously given. This test statistic is for testing the general linear hypothesis

$$H_0\colon H\underline{\beta}_2 = \underline{0}$$

which forms the testable hypotheses (i.e., estimable functions) of the second order coefficients contained in $\underline{\beta}_2$. A $k = 2$, first order factorial design with center runs has the testable lack of fit hypothesis in the second order coefficients given by

$$H_0\colon \begin{bmatrix} \beta_{12} \\ \beta_{11} + \beta_{22} \end{bmatrix} = \underline{0} \ . \tag{3.23}$$

The development of these testable hypotheses is given in Myers (1976). A $k = 2$ variable rotated factorial design of the class previously discussed, has the testable lack of fit hypothesis in the second order coefficients given by,

$$H_0\colon \begin{bmatrix} \beta_{12} - \dfrac{(1-d^2)}{d}\beta_{22} \\ \beta_{11} + \beta_{22} \end{bmatrix} = \underline{0} \ . \tag{3.24}$$

The development of these testable hypotheses is given in Appendix A. The rotated factorial design detects additional information based on the pure second order coefficients while sacrificing the detection of some interaction information. The lack of fit testable hypothesis for $k > 2$ variables have a similar structure to the $k = 2$ variable case. For $k = 3$, a factorial design with center runs has the lack of fit testable hypothesis

$$H_0: \begin{bmatrix} \beta_{12} \\ \beta_{13} \\ \beta_{23} \\ \beta_{11} + \beta_{22} + \beta_{33} \end{bmatrix} = \underset{\sim}{0} \ . \tag{3.25}$$

The $k = 3$ rotated design has the testable lack of fit hypothesis,

$$H_0: \begin{bmatrix} \beta_{12} - \frac{1-d^2}{d}\beta_{22} - \frac{1-d^2}{2d}\beta_{33} \\ \beta_{13} \\ \beta_{23} \\ \beta_{11} + \beta_{22} + \beta_{33} \end{bmatrix} = \underset{\sim}{0} \ . \tag{3.26}$$

For $k = 4$, a factorial design with center runs has the testable lack of fit hypothesis

$$H_0: \begin{bmatrix} \beta_{12} \\ \beta_{13} \\ \beta_{14} \\ \beta_{23} \\ \beta_{24} \\ \beta_{34} \\ \beta_{11} + \beta_{22} + \beta_{33} + \beta_{44} \end{bmatrix} = \underset{\sim}{0} \ . \tag{3.27}$$

The $k = 4$ rotated design has the testable lack of fit hypothesis,

$$H_0: \begin{bmatrix} \beta_{12} \\ \beta_{13} + \frac{1-d^2}{2d}\beta_{22} + \frac{1-d^2}{d}\beta_{33} + \frac{1-d^2}{2d}\beta_{44} \\ \beta_{14} \\ \beta_{23} \\ \beta_{24} - \frac{1-d^2}{2d}\beta_{22} + \frac{1-d^2}{2d}\beta_{44} \\ \beta_{34} \\ \beta_{11} + \beta_{22} + \beta_{33} + \beta_{44} \end{bmatrix} = \underline{0} \,. \tag{3.28}$$

The factorial designs allow for testing the interaction coefficients separate from the sum of the pure quadratic coefficients. The rotated factorial designs allow for testing a combination of the interaction and pure quadratic coefficients in addition to the sum of the pure quadratic coefficients.

The power properties can be measured by $tr[T^{-1}L]$ which is the Λ_2^* criterion. A design, D_1, which has larger $tr[T^{-1}L]$ than another design, D_2, will have larger average power than that of D_2. The class of rotated factorial designs consistently provides larger value for $tr[T^{-1}L]$ as compared with the corresponding factorial designs.

3.4.3 Λ_2^* Criterion Applied to the Rotated Design Class

The Λ_2^* criterion is applied to the class of first order rotated factorial designs with n_0 center runs. The criterion is used to choose the fourth order design moments for rotated factorial designs with the second moment chosen according to one of three prediction properties of interest (Bias, Variance, Mean Squared Error). Rotated factorial designs for $k = 2,\ 3$ and 4 are investigated here. The $k = 4$ design is a rotation of a one half fraction of a 2^4 factorial design with defining contrast I = ABCD.

Table 3.2 provides a summary of the evaluation of k = 2, 3 and 4 variable rotated designs. Minimum bias, minimum variance and mean squared error efficient rotated designs are evaluated in terms of the Λ_2^* criterion for various sample sizes, n. One can use the results of Table 3.2 to select a design of one of the three types (minimum bias, minimum variance or mean squared error efficient) that performs well in terms of the lack of fit test based upon the Λ_2^* criterion.

Table 3.2 - Evaluation of Rotated Designs in Terms of Λ_2^* Criterion

	Minimum Bias			Minimum Variance			Mean Squared Error Efficient	
***k* = 2**								
n	d	$tr[T^{-1}L]$	n	d	$tr[T^{-1}L]$	n	d	$tr[T^{-1}L]$
7	0.4082	4.9643	7	1.0	7.5643	7	0.6325	5.6688
8	0.5773	5.2499	8	1.0	7.9615	8	0.7746	6.4227
9	0.7071	5.7499	9	1.0	8.3478	9	0.8944	7.3909
10	0.8165	6.4000	10	1.0	8.5091	10	1.0000	8.5091
11	0.9129	7.1591	11	1.0	8.3739	11	1.0000	8.3739
12	1.0000	8.0000	12	1.0	8.0000	12	1.0000	8.0000
***k* = 3**								
n	d	$tr[T^{-1}L]$	n	d	$tr[T^{-1}L]$	n	d	$tr[T^{-1}L]$
10	*	*	10	1.0	22.2467	10	0.2739	9.7366
11	*	*	11	1.0	20.7096	11	0.4272	10.2839
12	0	8.6250	12	1.0	19.5789	12	0.5385	10.9948
13	0.2887	8.9639	13	1.0	18.7831	13	0.6305	11.8315
14	0.4082	9.4018	14	1.0	18.2657	14	0.7106	12.7672
15	0.5000	9.9187	15	1.0	17.9745	15	0.7826	13.7820
16	0.5774	10.5000	16	1.0	17.8549	16	0.8485	14.8611
17	0.6455	11.1342	17	1.0	17.8460	17	0.9097	15.9937
18	0.7071	11.8125	18	1.0	17.8824	18	0.9670	17.1702
***k* = 4**								
n	d	$tr[T^{-1}L]$	n	d	$tr[T^{-1}L]$	n	d	$tr[T^{-1}L]$
10	*	*	10	1.0	43.8667	10	0.3536	19.2159
11	*	*	11	1.0	40.3907	11	0.4873	20.0000
12	0.0000	16.0000	12	1.0	37.6667	12	0.5916	21.1293
13	0.2887	16.3654	13	1.0	35.5563	13	0.6801	22.5014
14	0.4081	16.9286	14	1.0	33.9606	14	0.7583	24.0713
15	0.5000	16.4500	15	1.0	32.8000	15	0.8292	25.7995
16	0.5774	18.5000	16	1.0	32.0000	16	0.8944	27.6562
17	0.6455	19.4559	17	1.0	31.4792	17	0.9553	29.6188
18	0.7071	20.5000	18	1.0	31.1428	18	1.0	31.1428

* - Minimum Bias Designs do not exist

3.5 Comparison of Factorial and Rotation Designs

Tables 3.1 and 3.2 provide a summary of factorial and rotated designs that achieve minimum bias, minimum variance and efficient mean squared error values. A comparison of factorial designs and rotation designs based upon Tables 3.1 and 3.2 indicates that rotation designs can achieve the same first order prediction properties (minimum bias, minimum variance or mean squared error efficient) but attain better lack of fit properties as measured by the Λ_2^* criterion. Minimum bias and mean squared error efficient designs in Table 3.2 of a given sample size, n, are just rotations of the corresponding designs given with Table 3.1. The minimum variance designs of Tables 3.1 and 3.2 are identical since a rotation design with $d = 1$ is exactly a factorial design with $g = 1$.

Example Revisited

Consider the example of section 3.1.1 in the following context. A chemist is interested in studying the viscosity of star block copolymers. He is interested in how the variables temperature and compression affect the viscosity. The temperature can be set from 130°C to 230°C and the compression as measured by percentage can range from 5 to 25 percent. The cuboidal design region is then given by,

$$\begin{aligned} 130 \;\leq\; &Temp \;\leq\; 230 \\ 5 \;\leq\; &Comp.\% \;\leq\; 25 \;. \end{aligned}$$

This region can then be centered and scaled by defining the design variables,

$$\begin{aligned} x_1 &= \frac{Temp - 180}{50} \\ x_2 &= \frac{Comp.\% - 15}{10} \;. \end{aligned}$$

Therefore the variables x_1 and x_2 are in the region

$$-1 \le x_1 \le 1$$
$$-1 \le x_2 \le 1 \ .$$

The chemist is unsure of how the variables temperature and compression affected viscosity. If a first order model in temperature and compression is inadequate, then a second order model will be adopted. The uncertainty of the model is cause for concern about bias in a first order model and also for concern about the performance of a lack of fit test. A rotated design with 4 center runs will provide a design that attempts to address the integrated mean squared error and power of the lack of fit test. A rotated design in the design variables is given by,

x_1	x_2
−0.7746	−1
0.7746	1
1	−0.7746
−1	0.7746
0	0
0	0
0	0

in terms of the natural variables, temperature and compression percentage, the design is

Temp.	*Comp.%*
141.27	5
218.73	25
230	7.254
130	22.746
180	15
180	15
180	15

The rotated design given above has second order design moment, [ii] equal to 0.4. This design represents a rotation of the factorial design given in the example of section 3.1.1. If we assume the same second order coefficients as previously considered, then the noncentrality parameter for the lack of fit test is equal to 27.2382 which yields the power for detection of second order terms equal to 0.7519 at $\alpha = 0.05$. The rotation design given here allows for approximately a 7% increase in the power of the lack of fit test in comparison to the factorial design given in section 3.1.1. Since the second order moment, [ii], for both designs is 0.40, the prediction properties of both designs are equivalent.

Chapter IV

IV. Augmentation Of First Order Designs

The previous chapter considers the use of factorial designs and rotation designs for estimating a first order response function model. Prediction properties of the first order model estimate (minimum bias, minimum variance, mean squared error efficient) were considered in selecting a specific design within each class. The rotation design class was introduced as a class of experimental designs which possesses first order model prediction properties equivalent to that of the factorial design class. But, the rotation design class was shown to have superior lack of fit properties for the detection of second order model terms.

This chapter examines procedures for augmentation of both factorial and rotation designs that allows for estimation of a second order response function model. These augmentations can be utilized when a significant lack of fit is observed based upon the observed responses corresponding to a first order design.

4.1 Sequential Design Procedure

As previously mentioned in chapter 2, an experimental design strategy that is consistent with the sequential framework given by Box and Wilson is developed throughout this work. When an experimenter is uncertain of the best characterization for the response variable, then a sequential design strategy should be implemented. In such cases, usually the simplest model form, a first order model, is initially considered for the response. An appropriate experimental design plan is chosen and responses observed corresponding to such a plan. Factorial designs or rotation designs are two design classes that can be used for considering first order models. Observed responses corresponding to a first order design are used to obtain a first order model estimate.

The uncertainty on the part of the experimenter in terms of the best model characterization for the response leads to the need for checking for inadequacy of the first order model. The observed responses from a first order design can be used to perform a lack of fit test for checking the adequacy of a first order model. The lack of fit test described in section 2.4.5 is for the detection of second order model terms. If a nonsignificant lack of fit is observed, then the observed data suggests that a first order polynomial model is an adequate approximation of the true response function. A first order model estimate is then employed to predict and explore the response variable within a region of interest in the design variables.

If a significant lack of fit is observed, then the data suggests that a first order model is not an adequate approximation for the response function since second order variable contribution appears to be present in the response system. In such a case, a second order model cannot be estimated using the observations obtained from a first order design. An experimenter could then employ an entirely new second order design to obtain a second order model estimate. Alternatively, the data obtained from the first order design could be augmented with additional experimental points that allow for estimation of a second order model.

Augmentations of both factorial and rotated designs according to various properties of a second order model are considered here. These augmentations are consistent with the sequential framework of experimentation described and are employed when a significant lack of fit is observed.

4.2 *Second Order Design Criteria*

Many criteria exist for evaluating a second order experimental design. Three general concepts which are of great interest within the sequential experimental framework are orthogonal blocking, second order prediction variance properties and variance properties of the estimated regression coefficients.

4.2.1 Orthogonal Blocking

Orthogonal blocking is an important property of experimental designs constructed in a sequential manner when a first order design is augmented with experimental points that allow for estimation of a second order model. These additional points are usually observed at a later time, under possibly different experimental conditions than the original first order design points. A block effect could exist due to the possibly different experimental conditions. Orthogonally blocked designs are of the form such that block effects are orthogonal to the model terms, allowing for estimation and testing of the model terms free of any block effects. Box and Hunter (1957) developed the general conditions for orthogonal blocking of a second order design. These conditions are given by,

(1) Each block must form a first order orthogonal design.

(2) The contribution to the sum of squares of each variable

$(\sum_{u=1}^{n} x_{iu}^2)$ from each block is proportional to the block size. (4.1)

4.2.2 Prediction Properties and Coefficients Estimation

The choice of an experimental design used for prediction purposes with respect to a second order model are generally based upon the prediction variance. Two general prediction variance criteria which are often used in relation to a second order model are rotatability and G-optimality. Both criterion are discussed in general within section 2.4.2 . Rotatability assures that the predicted values of points equal distance from the design center will have equal prediction variances. G-optimality is a design criterion based upon the maximum prediction variance within a region of interest, R. The properties of experimental designs that assure rotatability will be discussed here.

Another often used property for selecting second order experimental designs is based upon the quality of the estimated regression coefficients. D-optimality and D_r-optimality, discussed in section 2.4.2 are frequently adopted criteria for evaluating the quality of estimated coefficients for a second order model.

4.3 Augmentation of Factorial Designs - Central Composite Designs

Central composite designs, introduced by Box and Wilson (1951) are the most commonly used second order designs. These designs are discussed in general in section 2.5.2 . Central composite designs can be partitioned into a factorial section, an axial section and center points. A factorial design used in the initial stage of experimentation can be augmented with axial points and possibly additional center points to form a central composite design. The general structure of a central composite design is given by (2.45). The axial points allow for estimation of the pure quadratic coefficients, β_{ii}, which could not be previously estimated using a factorial design.

The central composite design is a very flexible design that can be made to satisfy several optimality criteria. The flexibility of these designs is a result of the freedom to select the values of g, α and n_0, the number of center points. Initially, the values of g and n_0 are selected to satisfy some criterion of interest pertaining to a first order model. Here, the value of g and n_0 will be chosen according to some first order prediction property. If a significant lack of fit is observed, then the axial points are added with possibly additional center points. The value of α and the number of additional center points are determined by some criterion of interest of a second order model. Orthogonal blocking, rotatability, D-optimality and D_s-optimality are the criteria for selecting α and the number of additional center points investigated within this work.

4.3.1 Orthogonally Blocked Central Composite Designs

The conditions for orthogonal blocking given by (4.1) can easily be attained for central composite designs of the form (2.45). Appropriate selection of g, α and n_0 will guarantee orthogonal blocking. Central composite designs in two blocks can be constructed for all values of k. The first block of n_1 experimental points consists of the initial factorial plus center points design. The augmentation of axial and additional center points to complete the central composite design consists of the second block of n_2 experimental points. The values of g, n_1, α and n_2 are selected to achieve orthogonal blocking. The first condition of orthogonal blocking given in (4.1) will always hold for a central composite design in two blocks. The second condition of (4.1) requires that the following expression in the design parameters holds.

$$\frac{2^{k-1}g^2}{\alpha^2} = \frac{n_1}{n_2} \tag{4.2}$$

The value of g and n_1 are selected based upon some criterion of interest for a first order model (i.e., prediction). If augmentation of the factorial design is necessary, then the possibility of a block effect exists among the factorial block and the axial block. The values of α and n_2 can then be chosen according to (4.2) to obtain orthogonal blocking for the given first block with g and n_1. For the example given in section 3.1, the factorial design with g = 0.8944 and $n_1 = 8$ can be augmented with an axial section with $\alpha = 0.8944$ and zero center points ($n_2 = 4$) or $\alpha = 1.00$ with one center point ($n_2 = 5$) to form an orthogonally blocked central composite design in two blocks.

4.3.2 Rotatable Central Composite Designs

The conditions for rotatability given by Box and Hunter can be satisfied by selecting appropriate values for g and α of a central composite design. Rotatability can be achieved if,

$$\alpha = \sqrt[4]{2^k}\, g \ . \tag{4.3}$$

Again, the value of g is selected based upon some criterion of interest for a first order model. If augmentation of the factorial design is necessary, then prediction properties pertaining to a second order model are of interest. The value of α can be chosen such that the central composite design will be rotatable. Note that the conditions for rotatability are not a function of the number of center runs. Therefore, by choosing an appropriate number of center runs, a rotatable central composite design can be constructed to also block orthogonally.

4.3.3 D and D_s Efficient Central Composite Designs

Central composite designs in general can be constructed to be very efficient with respect to second order coefficient estimation as measured by D-efficiency and D_s-efficiency. These designs which contain few or no center points achieve D-efficiency and D_s-efficiency values of 0.90 and above. In addition, these designs have values of $g = 1$ and $\alpha = 1$. In general, within the sequential experimental framework it has been previously discussed that g is chosen according to some first order model property. Within this work g is chosen according to first order prediction properties.

If the variance of prediction for a first order model is used for selecting g, then g will equal 1.0 and efficient central composite designs can be constructed by augmenting these designs with axial points at $\alpha = 1.0$. If prediction bias or mean squared error for a first order model is used for selection of g, then g will usually be less than one and the central composite design formed by augmenting with axial points at $\alpha = 1.0$ will not be as D-efficient or D_s -efficient as 'variance' designs. Table 4.1 provides some D-efficiency and D_s-efficiency values for designs with factorial sections that are mean squared error efficient as given in Table 3.1 . The designs given in Table 4.1 show that the central composite designs with lower values for g and smaller n perform poorly in terms of the D-efficiency and D_s-efficiency. The better performing central composite designs have higher values of g and larger sample sizes, n.

Table 4.1
D-efficiency and D_s-efficiency for Central Composite Designs Created By Augmentation of Mean Squared Error Efficient Factorial Designs

***k* = 2**

n	g	α	D-efficiency	D_s-efficiency
10	0.77	1.00	0.6065	0.5009
11	0.84	1.00	0.6621	0.6011
12	0.89	1.00	0.7068	0.6890
13	0.95	1.00	0.7454	0.7694
14	1.00	1.00	0.7817	0.8473

***k* = 3**

n	g	α	D-efficiency	D_s-efficiency
16	0.73	1.00	0.4632	0.3869
17	0.77	1.00	0.4988	0.4360
18	0.80	1.00	0.5268	0.4765
19	0.84	1.00	0.5508	0.5126
20	0.87	1.00	0.5732	0.5467
21	0.90	1.00	0.5925	0.5771
22	0.93	1.00	0.6138	0.6104
23	0.96	1.00	0.6306	0.6378
24	0.98	1.00	0.6489	0.6673

***k* = 4**

n	g	α	D-efficiency	D_s-efficiency
25	0.71	1.00	0.3985	0.3322
26	0.75	1.00	0.4428	0.3822
27	0.79	1.00	0.4870	0.4330
28	0.82	1.00	0.5623	0.5229
29	0.86	1.00	0.5623	0.5229
30	0.89	1.00	0.5990	0.5678
31	0.92	1.00	0.6325	0.6096
32	0.95	1.00	0.6610	0.6461
33	0.98	1.00	0.6998	0.6951

4.4 Augmentation of Rotated Designs - Second Order Rotated Designs

The first order rotation designs discussed in section 3.4 can be augmented to form a class of second order rotated designs. These second order rotated designs are essentially rotations of central composite designs. The transformation matrices given by (3.16), (3.18) and (3.20) can be applied to central composite designs to create the second order rotated designs. For k = 2, 3 and 4 variables, second order rotated designs are given by,

$$\begin{bmatrix} -d & -1 \\ d & 1 \\ -1 & d \\ 1 & -d \\ -\alpha & -\alpha(\frac{1-d}{1+d}) \\ \alpha & \alpha(\frac{1-d}{1+d}) \\ -\alpha(\frac{1-d}{1+d}) & \alpha \\ \alpha(\frac{1-d}{1+d}) & -\alpha \\ \underline{0} & \underline{0} \end{bmatrix}, \qquad (4.4)$$

$$
\begin{bmatrix}
d & -1 & -\sqrt{(d^2+1)/2} \\
-d & 1 & -\sqrt{(d^2+1)/2} \\
-1 & -d & \sqrt{(d^2+1)/2} \\
1 & d & \sqrt{(d^2+1)/2} \\
d & -1 & \sqrt{(d^2+1)/2} \\
-d & 1 & \sqrt{(d^2+1)/2} \\
-1 & -d & -\sqrt{(d^2+1)/2} \\
1 & d & -\sqrt{(d^2+1)/2} \\
-\alpha & -\alpha(\frac{1-d}{1+d}) & 0 \\
\alpha & \alpha(\frac{1-d}{1+d}) & 0 \\
\alpha(\frac{1-d}{1+d}) & -\alpha & 0 \\
-\alpha(\frac{1-d}{1+d}) & \alpha & 0 \\
0 & 0 & -\alpha^* \\
0 & 0 & \alpha^* \\
\underline{0} & \underline{0} & \underline{0}
\end{bmatrix}, \tag{4.5}
$$

$$
\begin{bmatrix}
-d & -d & -1 & -1 \\
-d & d & -1 & 1 \\
d & -d & 1 & -1 \\
d & d & 1 & 1 \\
1 & 1 & -d & -d \\
1 & -1 & -d & d \\
-1 & 1 & d & -d \\
-1 & -1 & d & d \\
-d & -1 & -1 & d \\
d & 1 & 1 & -d \\
-d & 1 & -1 & -d \\
d & -1 & 1 & d \\
-1 & d & d & 1 \\
1 & -d & -d & -1 \\
-1 & -d & d & -1 \\
1 & d & -d & 1 \\
-\alpha & 0 & -\alpha(\frac{1-d}{1+d}) & 0 \\
\alpha & 0 & \alpha(\frac{1-d}{1+d}) & 0 \\
0 & -\alpha & 0 & -\alpha(\frac{1-d}{1+d}) \\
0 & \alpha & 0 & \alpha(\frac{1-d}{1+d}) \\
\alpha(\frac{1-d}{1+d}) & 0 & -\alpha & 0 \\
-\alpha(\frac{1-d}{1+d}) & 0 & \alpha & 0 \\
0 & \alpha(\frac{1-d}{1+d}) & 0 & -\alpha \\
0 & -\alpha(\frac{1-d}{1+d}) & 0 & \alpha \\
\underline{0} & \underline{0} & \underline{0} & \underline{0}
\end{bmatrix}, \tag{4.6}
$$

respectively.

The first order rotated designs used during the initial stage of experimentation can be augmented with dual axial points and possibly additional center points to create a second order design. The dual axial points have two variables chosen at specific levels ($\pm\,\alpha$ and $\pm\,\alpha(\frac{1-d}{1+d})$) and the remaining k - 2 variables set to zero. The dual axial points allow for estimation of the second order coefficients, β_{ij} and β_{ii}, free of the effects of aliasing.

The second order rotated designs are very flexible and can be made to satisfy several optimality criteria. This flexibility is the result of the freedom to select the values of d, α and n_0, the number of center points. The values of d and n_0 are initially selected according to some criterion of interest for a first order model. The selection of d and n_0 based upon some prediction property of a first order model has been previously discussed. This choice of d and n_0 is also consistent with the sequential framework of experimentation. If a significant lack of fit is observed based upon the observations of the first order rotated design, then the dual axial points are added along with possibly additional center points. The value of α, $0 \leq \alpha \leq 1$, and the number of additional center points are determined by some criterion of interest pertaining to a second order model.

Orthogonal blocking, rotatability, D-efficiency and D_s-efficiency are the second order criteria investigated here. Where possible, comparisons will be made of the second order rotated designs to central composite designs.

4.4.1 Orthogonally Blocked Second Order Rotated Designs

The conditions for orthogonal blocking given by (4.1) can easily be established for second order rotated designs of the forms (4.4)-(4.6). Appropriate selection of the design parameters, d, α and n_0 can guarantee orthogonal blocking. Second order rotated designs in two blocks can be constructed for all values of k. The first block of n_1 experimental points consists of the initial first order rotated design with center points. The augmentation of dual axial and additional center points to complete the second order rotated design comprise the second block of n_2 experimental points. The values of d, n_1, α. and n_2 are selected to achieve orthogonal blocking. The first condition for orthogonal blocking given in (4.1) will always hold for a second order rotated design in two blocks. Both blocks as described above are first order orthogonal. The second condition in (4.1) requires that the following relationship among the design parameters holds.

$$\frac{1+d^2}{\alpha^2} = \frac{n_1}{n_2} \quad . \tag{4.7}$$

The values of d and n_1 are selected based upon some criterion of interest for a first order model (i.e., prediction). If augmentation of the first order rotated design is necessary, then the possibility of a block effect exists among the initial first order rotated design and the augmented dual axial section. The relationship for orthogonal blocking (4.7) can be used to select values of α and n_2 based upon the d and n_1 used in the first order rotated design.

For the example given in section 3.5, the first order rotated design with d = 0.7746 and n_1 = 8 can be augmented with dual axial points and center points that satisfy (4.7). These values of α and n_2 are given by the following:

n_2	α
4	0.6661
5	0.7447
6	0.8158
7	0.8811
8	0.9420
9	0.9991

Any of the above combinations of α and n_2 will guarantee orthogonal blocking.

4.4.2 Rotatable Second Order Rotated Designs

The conditions for rotatability given by Box and Hunter can be achieved by selecting appropriate values of d and α of a second order rotated design. Rotatability can be achieved for designs of the form (4.4)-(4.6) if,

$$\alpha = \sqrt{\frac{k(1+d)^2}{4}}$$
$$\text{with} \quad \alpha^* = \sqrt{\frac{k(1+d^2)}{2}} \quad \text{for k odd} \tag{4.8}$$

Consistent with the sequential framework, d is chosen according to some criterion of interest for a first order model. If augmentation of the first order rotated design is needed, then prediction properties pertaining to a second order model are addressed by selecting α such that rotatability is achieved. Notice that the conditions for rotatability are not a function of the number of center points. The selection of an appropriate number of center points can be based upon other criterion for a second order model.

4.4.3 D and D_s Efficient Second Order Rotated Designs

Second order rotated designs can be constructed to be very efficient with respect to coefficient estimation for a second order model. These designs which perform well in terms of D-efficiency and D_s-efficiency contain few or no center points with $d = 1$ and $\alpha = 1$. In general, within the sequential experimental framework it has been previously discussed that d is chosen according to some first order model property. Here, first order prediction properties are used for selecting d. If the first order model prediction variance is used, then $d = 1.0$ is chosen and D-efficient and D_s-efficient second order designs can be constructed by augmenting with axial points at $\alpha = 1.0$. If prediction bias or mean squared error for a first order model is used for selecting d, then d will usually be less than one and the second order rotated designs constructed by augmenting with dual axial points at $\alpha = 1.0$ will not be as D-efficient or D_s-efficient as 'variance' designs. Table 4.2 provides some D-efficiency and D_s-efficiency values for designs with first order rotated sections (i.e., d) that are mean squared error efficient as given in Table 3.2. The designs given in Table 4.2 show that second order rotated designs with lower values for d and smaller sample sizes, n, perform poorly in terms of D-efficiency and D_s-efficiency. The better performing designs have larger values for d and n.

Table 4.2
D-efficiency and D_s-efficiency for Second Order Rotated Designs Created By Augmentation of Mean Squared Error Efficient First Order Rotated Designs

$k=2$

n	d	α	D-efficiency	D_s-efficiency
10	0.45	1.00	0.6574	0.5642
11	0.63	1.00	0.6800	0.6252
12	0.77	1.00	0.7128	0.6976
13	0.89	1.00	0.7466	0.7713
14	1.00	1.00	0.7817	0.8473

$k=3$

n	d	α	D-efficiency	D_s-efficiency
16	0.27	1.00	0.5082	0.4368
17	0.43	1.00	0.5226	0.4641
18	0.54	1.00	0.5411	0.4942
19	0.63	1.00	0.5595	0.5238
20	0.71	1.00	0.5782	0.5534
21	0.78	1.00	0.5952	0.5809
22	0.85	1.00	0.6151	0.6121
23	0.91	1.00	0.6311	0.6385
24	0.97	1.00	0.6489	0.6673

$k=4$

n	d	α	D-efficiency	D_s-efficiency
25	0.11	1.00	0.4798	0.4182
26	0.35	1.00	0.4812	0.4258
27	0.49	1.00	0.5096	0.4599
28	0.59	1.00	0.5383	0.4945
29	0.68	1.00	0.5707	0.5335
30	0.76	1.00	0.6036	0.5738
31	0.83	1.00	0.6348	0.6126
32	0.89	1.00	0.6620	0.6474
33	0.96	1.00	0.6999	0.6953

The value of α is chosen to be one for all augmentations since this value will provide for the best D-efficiency and D_s-efficiency. In general, the larger the value of α, the better the two efficiency measures will be.

A comparison of the information provided in Tables 4.1 and 4.2 shows that the second order rotated designs can be made more D-efficient or D_s-efficient than a corresponding central composite design. The values of g and d in both tables are selected such that the second order design moment, [ii], equals 0.43. Designs with second moments slightly greater than 1/3 are generally considered to be mean squared error efficient as discussed in section 2.4.3. In addition, the first order prediction properties for the factorial designs are equivalent to those of the first order rotated designs. But, from Tables 4.1 and 4.2 it is clear that the second order rotated designs will always outperform the central composite designs in terms of second order coefficient efficiencies (D and D_s) if the axial points of both designs are chosen to maximize these efficiencies.

Chapter V

V. A Mean Squared Error Criterion

Experimental designs which perform well in terms of the traditional integrated mean squared error of prediction, J given by (2.1) can be improved in terms of lack of fit performance by utilizing the $\Lambda_2{}^*$ criterion discussed in Chapter III. Conditional upon a second order design moment chosen based upon some prediction property for a first order model, the lack of fit properties for a design are be measured by the $\Lambda_2{}^*$ criterion.

This chapter examines an experimental design criterion that considers the integrated mean squared error of prediction conditional upon the lack of fit properties. Box and Draper (1959, 1963) have discussed experimental designs which perform well in terms of the unconditional mean squared error of prediction. The work here is in the same spirit except that lack of fit properties are incorporated into the evaluation of the integrated mean squared error, J. This conditional integrated mean squared error is consistent with the sequential framework of experimentation.

5.1 One Variable Case

Consider the case of a $k = 1$ variable response model. Within the sequential framework, for a first order response model estimate the integrated mean squared error of prediction is given by,

$$J = 1 + \frac{1}{3[ii]} + \frac{n\beta_{11}^2}{\sigma^2}\left[([ii] - 1/3)^2 + \frac{4}{45}\right] \tag{5.1}$$

and the noncentrality parameter of the lack of fit test for the detection of the quadratic coefficient β_{11} is given by

$$\lambda = \frac{n\beta_{11}^2}{\sigma^2}\left([iiii] - [ii]^2\right) \ . \tag{5.2}$$

The quantity J is used to evaluate the prediction capabilities of a first order response model estimate. The noncentrality parameter, λ , is used to evaluate the lack of fit properties. Notice that both J and λ are functions of the quadratic coefficient β_{11}. For a given experimental design, λ and J can be evaluated in terms of β_{11}.

Consider J and λ for the following example with an experimental design.consisting of five experimental points given by

$$\{1, -1, 0, 0, 0\} \ . \tag{5.3}$$

This design in one variable has a second moment equal to 0.4 and the three center runs allow for a lack of fit test to be performed with two degrees of freedom for the pure error term in the denominator. This design is thought to perform well in terms of the integrated mean squared error of prediction, J, as examined by Box and Draper (1959, 1963). Box and Draper suggest that the use of a second moment slightly greater than the minimum bias second moment will perform well in terms of J. Recall from section 2.4.4 that the optimal design in terms of J is a function of the quadratic coefficient, β_{ll}, which is unknown. Figure 5.1 provides a plot of J vs. $\frac{\sqrt{n}\,\beta_{11}}{\sigma}$ for the design given above. In addition, Figure 5.2 provides a plot of the power of the lack of fit test vs. $\frac{\sqrt{n}\,\beta_{11}}{\sigma}$.

Figure 5.2 shows that for large values of $\frac{\sqrt{n}\,\beta_{11}}{\sigma}$, the power of the lack of fit test for this design is quite large. In fact, for $\frac{\sqrt{n}\,\beta_{11}}{\sigma}$ greater than 13.5 the power is greater than 0.9. Therefore, for these large values of $\frac{\sqrt{n}\,\beta_{11}}{\sigma}$, it is highly probable that we will observe a significant lack of fit and subsequently fit a second order response model. When the value of $\frac{\sqrt{n}\,\beta_{11}}{\sigma}$ is not so large, there exists a reasonable chance of observing a nonsignificant lack of fit despite the fact that β_{11} is not zero. For these values of $\frac{\sqrt{n}\,\beta_{11}}{\sigma}$ a first order model estimate would likely be used, and the prediction properties of this model are characterized by J.

The quantity J depends upon the second order coefficient, β_{11}, but for the experimental design given it can be seen from Figures 5.1 and 5.2 that values of J are only important over a range of β_{11} where the power of the lack of fit is not large. Within the sequential framework, when the power of the lack of fit test becomes large, J, which is a prediction measure for a first order model is no longer of great interest since it is highly likely a second order model will be fit when the true β_{11} is in this range.

This example provides the motivation for the next section which discusses a measure that evaluates the integrated mean squared error of prediction (J) over a region of low power for the lack of fit test. This measure is developed in general for any number of variables k and any design class. This measure will be used throughout this chapter for evaluation of first order prediction properties of several design classes.

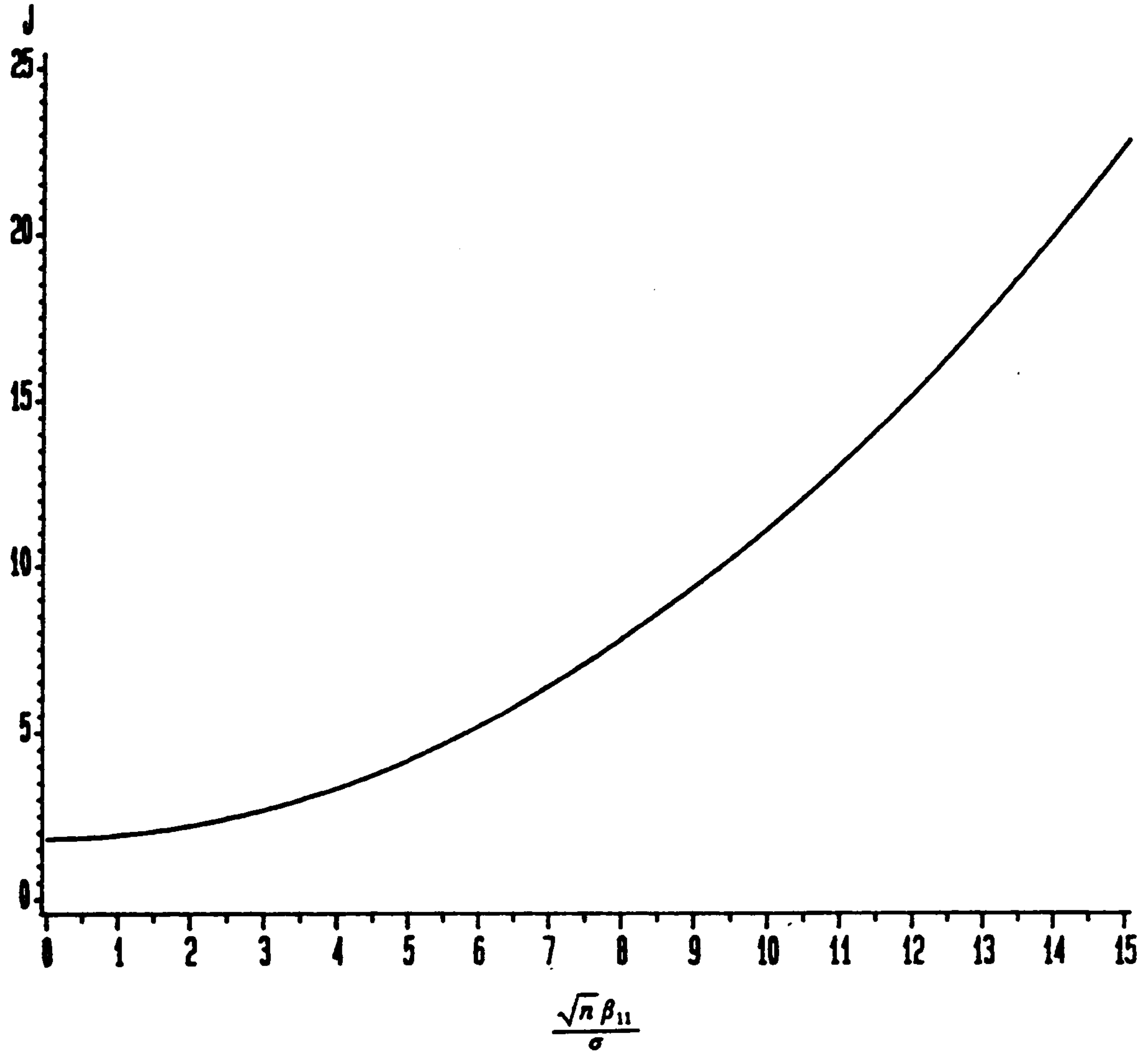

Figure 5.1 - Integrated Mean Squared Error of Prediction vs. The Second Order Coefficient

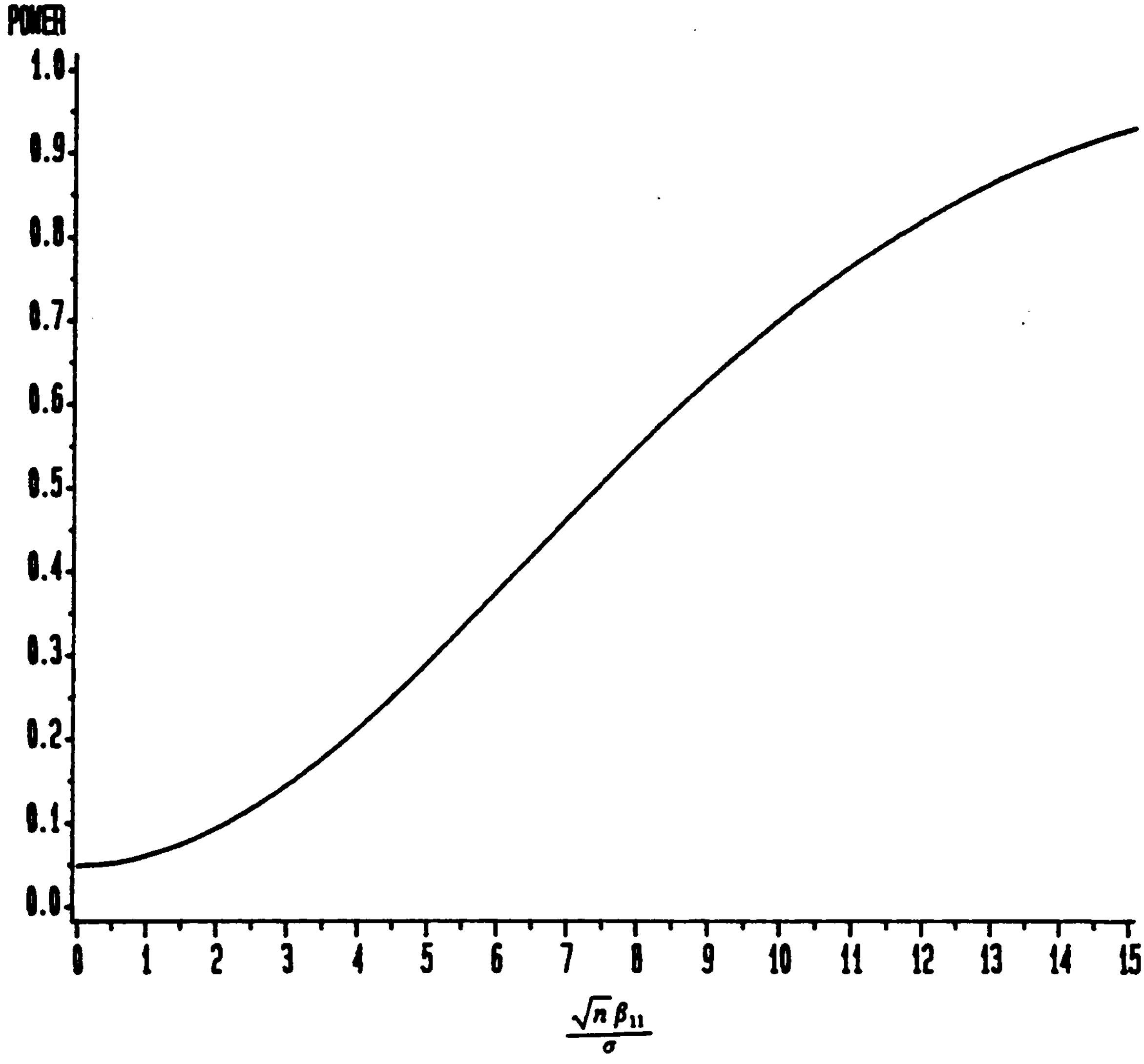

Figure 5.2 - Power of the Lack of Fit Test vs. The Second Order Coefficient

5.2 Power Conditional Average and Power Conditional Maximum Mean Squared Error

As discussed within the context of the one variable example of section 5.1, the mean squared error of prediction for a first order model is of interest only when the first order response model estimate is used for prediction and exploration. When the lack of fit test is significant, indicating that a second order response model is to be used, then J is not of interest. The procedure suggested here is to evaluate the performance of J restricted to a region of second order coefficients such that the power of the lack of fit test is not large. The J-optimal design depends upon the second order coefficients which in general are unknown. Box and Draper (1959, 1963) consider the performance of J over all possible values of the second order coefficients. Their results indicate that designs which perform well in terms of J over many possible values for the second order coefficients have second order design moments that are slightly greater than the minimum bias second moment.

Here within this work, the consideration of J is restricted to values of the second order coefficients that result in low power of the lack of fit test. This evaluation of J is consistent with the sequential experimental framework. A criterion similar to the $\Lambda_2{}^*$ criterion of section 3.2.2 is developed. The $\Lambda_2{}^*$ criterion considers the average noncentrality parameter of the lack of fit test conditional upon the integrated mean squared error of prediction being fixed. The $\Lambda_2{}^*$ criterion can be used to improve upon the lack of fit test performance. If one considers the class of designs with a given integrated mean squared error, J, for a first order model the $\Lambda_2{}^*$ criterion can be used to select the designs of this class that perform best in terms of the lack of fit test.

An idea similar to the $\Lambda_2{}^*$ criterion is to consider the average J over a region of fixed power for the lack of fit test. This criterion is called the power conditional average mean squared error of prediction, denoted by J_{PCA}. Consider for a first order response model estimate the integrated mean squared error of prediction given by,

$$J = tr(\mu_{11} M_{11}^{-1}) + \frac{\beta'_2 T \beta_2}{\sigma^2} \quad . \tag{5.4}$$

Also consider the noncentrality parameter of the lack of fit test for detection of second order model terms given by

$$\lambda = \frac{n\beta'_2 L \beta_2}{\sigma^2} \quad . \tag{5.5}$$

The sequential experimental framework previously discussed specifies that a first order response model estimate is initially considered and based upon the lack of fit test, either a first order or a second order model will be used for prediction and exploration of the response variable. If the lack of fit test is nonsignificant, a measure of the prediction properties for a first order model is given by J. If the lack of fit test is significant, then a second order model is used for estimating the response and J is no longer of interest. Therefore, within the sequential framework, the quantity J is only of interest when a nonsignificant lack of fit is observed, i.e., when the wrong model is being fit. Hence, a measure of the prediction properties of an experimental design pertaining to a first order response model estimate is the average value of J over the values of the second order coefficients that will result in low power for the lack of fit test.

Recall from section 2.4.4 that the optimal integrated mean squared error design when fitting a first order model is a function of the unknown second order coefficients. The J_{PCA} criterion of averaging the integrated mean squared error over a region in the second order coefficients where the power is low accounts for the dependency of J on the second order coefficients. Formally, the J_{PCA} criterion is defined as the following.

Let $\Theta = \{\beta_2 : \frac{n\beta'_2 L \beta_2}{\sigma^2} < \lambda_0\}$ where λ_0 is the noncentrality parameter required to achieve a specified power of the lack of fit test.

$$J_{PCA} = \frac{\int_{\Theta} J d\underline{\beta}_2}{\int_{\Theta} d\underline{\beta}_2}$$
$$= tr(\mu_{11} M_{11}^{-1}) + \frac{\lambda_0 tr[L^{-1}T]}{p_2 + 2} \quad . \tag{5.6}$$

The derivation of J_{PCA} is given in Appendix B. J_{PCA} measures the prediction capabilities of a design pertaining to a first order model.

In addition to the power conditional average mean squared error, J_{PCA}, one may also consider the power conditional maximum mean squared error to evaluate the prediction properties. The maximum J over the region Θ will occur somewhere on the boundary of Θ, therefore a measure associated with this maximum J is given by,

$$J_{PCMAX} = \max_{\Theta} J$$
$$= tr(\mu_{11} M_{11}^{-1}) + \lambda_0(\text{max eigenvalue } (L^{-1}T)) \quad . \tag{5.7}$$

The derivation of J_{PCMAX} is also given in Appendix B.

5.3 Application of J_{PCA} and J_{PCMAX} to First Order Factorial Designs

The J_{PCA} and J_{PCMAX} criteria developed in section 5.2 are used here to evaluate the first order model prediction performance for factorial designs. J_{PCA} and J_{PCMAX} can be used to select the values of the design parameters g and n_0 , the number of center points. Factorial designs with center points often comprise the initial experimental design used to estimate a first order model and to perform a lack of fit test. Within the sequential framework, if a significant lack of fit test is observed, then these factorial designs are supplemented with axial points in order to fit a second order model.

Consider J_{PCA} and J_{PCMAX} given by (5.6) and (5.7). Both are a function of the lack of fit matrix L and the bias matrix T. The L and T matrices for a factorial design with center points can be expressed as the following.

$$L = \begin{bmatrix} (2^k g^4)/nI & 0 \\ 0 & \left[2^k g^4/n - (2^k g^2/n)^2\right] j_k j'_k \end{bmatrix} \tag{5.8}$$

$$T = \begin{bmatrix} w_{iijj} I & 0 \\ 0 & T_Q \end{bmatrix} \tag{5.9}$$

where T_Q is a $k \times k$ matrix with diagonal elements equal to $\left(\frac{2^k g^2}{n}\right)^2 - \frac{2^{k+1} g^2}{n} w_{ii} + w_{iiii}$ and off diagonal elements equal to $\left(\frac{2^k g^2}{n}\right)^2 - \frac{2^{k+1} g^2}{n} w_{ii} + w_{iijj}$. I is an identity matrix of dimension $\binom{k}{2}$.

The L matrix given by (5.8) is not of full rank since all second order coefficients cannot be estimated (or tested) with a factorial design. Since L is not of full rank, it appears that both J_{PCA} and J_{PCMAX} cannot be applied to factorial design since both require the existence of L^{-1}.

For factorial designs, consider the following expressions of the integrated mean squared error, J and the noncentrality parameter, λ :

$$\lambda = \frac{n}{\sigma^2}\left[(\sum \beta_{ii}^2)([iiii] - [ii]^2) + 2(\sum_{i<j} \beta_{ii}\beta_{jj})([iijj] - [ii]^2) + (\sum \beta_{ij}^2)([iijj])\right], \tag{5.10}$$

$$J = 1 + \frac{k w_{ii}}{[ii]} + \frac{1}{\sigma^2}\Big[(\sum \beta_{ii}^2)([ii]^2 - 2w_{ii}[ii] + w_{iiii}) + 2(\sum_{i<j} \beta_{ii}\beta_{jj})([ii]^2 - 2w_{ii}[ii] + w_{iijj}) + (\sum \beta_{ij}^2)(w_{iijj})\Big]. \tag{5.11}$$

Note that both λ and J can be expressed in terms of the same functions of the second order coefficients. Therefore, the form of the second order model can then be reparameterized in terms of the functions of the second order coefficients given in (5.10) and (5.11). These new "parameters" are $\sum\beta_{ii}^2$, $\sum_{i<j}\beta_{ii}\beta_{jj}$ and $\sum\beta_{ij}^2$ and represent the functions of the second order coefficients that are testable hypotheses for a factorial design.

This reparameterized model is given by,

$$\underline{y} = X_1\underline{\beta}_1 + X_2^*\underline{\beta}_2^* + \underline{\varepsilon}$$

$$\text{where } \underline{\beta}_1 = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \cdot \\ \cdot \\ \cdot \\ \beta_k \end{bmatrix} \text{ and } \underline{\beta}_2{}^* = \begin{bmatrix} \sum\beta_{ii}^2 \\ \sum_{i<j}\beta_{ii}\beta_{jj} \\ \sum\beta_{ij}^2 \end{bmatrix} . \tag{5.12}$$

Using this reparameterized model the noncentrality parameter of the lack of fit test can be expressed as

$$\lambda = \frac{\underline{\beta}_2^{*\prime} L^* \underline{\beta}_2^*}{\sigma^2} , \tag{5.13}$$

$$\text{where } L^* = \begin{bmatrix} [iiii] - [ii]^2 & 0 & 0 \\ 0 & [iijj] - [ii]^2 & 0 \\ 0 & 0 & [iijj]I \end{bmatrix} .$$

The expression given by (5.13) is equivalent to that given by (5.10). The advantage of the reparameterized model is that the matrix L^* in the quadratic form of (5.13) is of full rank and its inverse exists.

The mean squared error, J, can also be expressed in the terms of the reparameterized model as

$$J = tr(\mu_{11}M_{11}^{-1}) + \frac{n\beta_2^{*\prime}T^*\beta_2^*}{\sigma^2} \tag{5.14}$$

$$\text{where } T^* = \begin{bmatrix} [ii]^2 - 2w_{ii} + w_{iiii} & 0 & 0 \\ 0 & [ii]^2 - 2w_{ii}[ii] + w_{iijj} & 0 \\ 0 & 0 & w_{iijj}I \end{bmatrix}.$$

Where I is an identity matrix of dimension $\binom{k}{2}$ in both L^* and T^*. The expression given by (5.14) is equivalent to that given by (5.11). This reparameterization of the mean squared error, J, allows for conformability between the lack of fit matrix L^* and the bias matrix T^*.

Based upon this reparameterized model for factorial designs, the J_{PCA} and J_{PCMAX} values can be expressed as the quantities given by (5.6) and (5.7) with L replaced by L^* and T replaced by T^*. The design parameters for a factorial design can then be chosen such that J_{PCA} or J_{PCMAX} is a minimum. These designs would correspond to designs which achieve the minimum average or minimum maximum mean squared error of prediction over the region of low power for the lack of fit test.

The investigation of factorial designs is considered for $k = 2$ to $k = 5$ variables, considering both the full and a one half fraction of the $k = 5$ factorial. In addition both cuboidal and spherical design regions are considered. That is the design points are considered to be within a k-dimensional unit cube or unit sphere. The region of interest in the design variables for exploration, R, is also considered to be a unit cuboidal or unit spherical region. Three combinations of design region and region of interest are examined. These combinations are a cuboidal design region with a cuboidal region of interest, a spherical design region with a spherical region of interest and a cuboidal design region with a spherical region of interest.

Appendix C contains summary tables of factorial designs. The reader is referred to Appendix C for details of comparing factorial designs based upon the J_{PCA} and J_{PCMAX} values. The values of

J_{PCA} calculated in Appendix C are for the average mean squared error over the second order coefficient region such that the power of the lack of fit test is less than or equal to 0.90. J_{PCA} was also examined for regions in which the power was less than 0.75 and 0.50. No substantial differences in terms of conclusions existed among the 0.90, 0.75 and 0.50 regions. Of course the value of J_{PCA} will change, but comparisons of the designs within each of these three regions yielded nearly identical results. The 0.90 "power" region is selected for design comparison throughout this work.

5.3.1 Factorial Designs with Cuboidal Regions for the Design and Exploration

When both the design region and the region of interest are cuboidal the conclusions and recommendations drawn from Appendix C for the J_{PCA} criterion are the following.

(1) The addition of several center points dramatically decreases the values of J_{PCA}. This result is probably due to the fact that the degrees of freedom and hence the power of the lack of fit test will increase when the number of center points increases. Although the optimal values of J_{PCA} are achieved for designs with an extraordinary number of center points, J_{PCA} values fairly close to the optimal values can be obtained with more reasonable numbers of center points. For $k = 2$ variables, 4-7 center points will yield acceptable values for J_{PCA}. For $k = 3$, 5-11 center points will yield acceptable values for J_{PCA}. For $k = 4$ at least 6 center points and for $k = 5$ at least 7 center points will yield acceptable values for J_{PCA} . In addition, for $k = 5$, a one half fractional factorial design achieves consistently smaller values for J_{PCA} than the complete factorial.

(2) The optimal values of g for the recommended number of center points given in (1) are 1.0. The center points allow for a better lack of fit test with more degrees of freedom and also reduce the second order design moments to values which perform well in terms of J for values of g at the extremes of 1.0.

The conclusions drawn about the J_{PCMAX} criterion are:

(1) The addition of several center points dramatically decreases the values of J_{PCMAX}. Reasonable number of center points which provide for near optimal values of J_{PCMAX} are

given by 5 to 8 center points for $k = 2$ variables, at least 6 for $k = 3$, at least 8 for $k = 4$ and at least 10 for $k = 5$. In addition, for $k = 5$, a one half fractional factorial design achieves consistently smaller values of J_{PCMAX} than the complete factorial.

(2) The optimal values of g for $k = 2$ and $k = 3$ is 1.0. For $k = 4$ and $k = 5$ smaller values of g will yield the best performing designs in terms of J_{PCMAX}.

5.3.2 Factorial Designs With Spherical Regions for the Design and Exploration

When both the design region and the region of interest are spherical the conclusions and recommendations drawn from Appendix C for the J_{PCA} criterion are the following.

(1) The addition of several center points dramatically decreases the values of J_{PCA}. Again this result is probably due to the gain in performance of the lack of fit test and hence a smaller region in the second order coefficients that J is averaged over. The recommended number of center points that will guarantee optimality or near optimality in terms of J_{PCA} are for $k = 2$, 4 to 6 center points. For $k = 3, 4$ and 5 the recommended number of center points are 5-9, at least 7 and at least 7 respectively. A $k = 5$ one half fractional factorial achieves consistently smaller values of J_{PCA} than the complete factorial.

(2) The optimal values of g for all numbers of center points and all k are the largest possible values within the k-dimensional unit sphere. These values are $g = 1/\sqrt{k}$.

The conclusions drawn about the J_{PCMAX} criterion are:

(1) The addition of several center points dramatically decreases the values of J_{PCMAX}. Again this result is probably due to the gain in performance of the lack of fit test and hence a smaller region in the second order coefficients that J is averaged over. The recommended number of center points that will guarantee optimality or near optimality in terms of J_{PCMAX} are for $k = 2$, 4 to 6 center points. For $k = 3, 4$ and 5 the recommended number of center points are 5-9, at least 7 and at least 7 respectively. A $k = 5$ one half fractional factorial achieves consistently smaller values of J_{PCMAX} than the complete factorial.

(2) The optimal values of g for all number of center points and all k are the largest possible values within the k-dimensional unit sphere. These values are $g = 1/\sqrt{k}$.

5.3.3 Factorial Designs within a Cuboidal Design Region and Spherical Region of Interest

When the design region is represented by a unit cuboidal region and the region of interest is a unit sphere or hypersphere within the design region then the conclusions and recommendations drawn from Appendix C for the J_{PCA} criterion are the following.

(1) The addition of several center points dramatically decreases the values of J_{PCA}. The gain in performance of the lack of fit test through the additional center points is reflected in a decrease in J_{PCA}. The recommended number of center points that will guarantee optimality or near optimality in terms of J_{PCA} for $k = 2$ through 5 variables are 4 to 9, at least 5, at least 6 and at least 7 respectively. A $k = 5$ one half fractional factorial achieves consistently smaller values of J_{PCA} than the complete factorial.

(2) The optimal values of g for designs with the recommended number of center points given in (1) are often less than the maximum allowed of 1.0.

The conclusion drawn about the J_{PCMAX} criterion are:

(1) The addition of several center points dramatically decreases the values of J_{PCMAX}. The recommended number of center points that will guarantee optimality or near optimality in terms of J_{PCMAX} for $k = 2,3,4$ and 5 variables are 5 to 9, at least 7, at least 9 and at least 10 respectively. A $k = 5$ one half fractional factorial achieves consistently small values of J_{PCMAX} than the complete factorial.

(2) The optimal values of g for designs with the recommended number of center points given in (1) are often less than the maximum allowed of 1.0.

5.4 Robust Second Order Designs

The sequential framework utilized throughout this work can be adjusted to the special needs of an experimenter. The framework previously described initially employs a first order design for fitting a first order response model estimate. If a lack of fit test for second order departures is significant then additional sample observations are needed, consisting of either an augmentation of the existing first order design or a new second order design. If additional sample observations cannot be obtained by an experimenter, then the initial design must have the capabilities of fitting a second order model. This is not the case with the first order designs discussed previously (factorial or rotated). This section will consider experimental situations when additional observations cannot be taken after some initial stage.

Specifically, the 'one experiment' framework considered within this section is given by the following. The experimenter is uncertain as to the best characterization for the response variable. Initially, a first order response model estimate will be used, if this model is found to be inadequate based upon a significant lack of fit test, then a second order model will be adopted. Within this framework only one experimental design can be employed to accomplish the objectives mentioned above.

Atkinson (1972, 1973) has previously considered the use of second order designs within the 'one experiment' framework. Atkinson discusses the use of the $|L|$ criterion for evaluating experimental designs in terms of the performance of the lack of fit test and also as a D_s measure to evaluate the quality of the second order coefficient estimates. He points out that experimental designs which perform well in terms of $|L|$, designs with good D_s-efficiency as given in (2.27), may perform poorly in terms of the quality of the first order coefficient estimates. Therefore, Atkinson derives an efficiency measure similar to that of D_s-efficiency for first order model terms. He then constructed experimental designs that will have the largest $|L|$ conditional upon achieving a lower bound for the first order efficiency measure. These designs are considered to perform well in terms of the lack of fit test, $|L|$, and also in terms of estimating a first order model or a second order model depending on the outcome of the lack of fit test. This robust design selection of choosing a design that will perform well in terms of both a first order and second order model based upon the results of the lack of fit test will now be considered using the J_{PCA} criterion to evaluate the performance of a first order response model estimate in terms of prediction capabilities. D_s -efficiency for second order terms and D-efficiency for the full second order model are simultaneously considered for evaluation of second order model performance.

Two often used second order design classes, central composite designs and Box-Behnken designs, are evaluated and compared using the robust selection criteria of J_{PCA} or J_{PCMAX} combined with D_s-efficiency and D-efficiency. The designs discussed here are therefore robust in terms of providing good performance of the lack of fit test and additionally providing good prediction performance for a first order model and good model estimation for a second order model depending upon the result of the lack of fit test.

Appendix C contains summary tables of J_{PCA}, J_{PCMAX}, D_s-efficiency and D-efficiency for central composite designs and Box-Behnken designs. The reader is referred to Appendix C for the details of the evaluation and comparison of central composite and Box-Behnken designs. As with the factorial designs of section 5.3, the values of J_{PCA} and J_{PCMAX} are calculated for the region in the second order coefficients, Θ, such that the power of the lack of fit test is less than or equal to 0.90. Similar results were obtained for other values of the power examined but not presented within this work.

5.4.1 Second Order Designs Within a Cuboidal Design Region for a Cuboidal Region of Interest

When both the design region and the region of interest are best represented by a unit cuboidal region, then the conclusions and recommendations drawn from the tables of Appendix C are the following.

(1) Central composite designs that perform best in terms of all the robust selection criteria, J_{PCA}, J_{PCMAX}, D_s-efficiency and D-efficiency possess the values of g and α to be 1.0. The Box-Behnken designs that perform best possess the value of g equal to 1.0.

(2) The addition of center points at first dramatically decreases the values of J_{PCA} and J_{PCMAX}, but with each additional center point the D_s -efficiency and D-efficiency will also decrease. Therefore to maintain robustness, consideration of all four measures simultaneously yields the following recommendations for the number of center points. For $k = 3, 4$ and 5 variables 6 to 8, 8 to 10 and 9 to 12 center points respectively will provide designs which perform best in terms of the four design criteria.

(3) For $k = 3$ variables, the two design classes are generally equivalent. For $k = 4$ and $k = 5$ variables, the central composite design outperforms the Box-Behnken design. For $k = 5$ a one-half fraction of a 2^5 factorial design used for the factorial portion within the central composite design performs the best.

5.4.2 Second Order Designs Within a Spherical Design Region for a Spherical Region of Interest

When both the design region and the region of interest are best represented by a unit sphere or hypersphere, then the conclusions and recommendations drawn from the tables of Appendix C are the following.

(1) Central composite designs that perform best in terms of all the robust design selection criteria have the values of g equal to $\frac{1}{\sqrt{k}}$ and $\alpha = 1$. These designs are such that all non center points are on the sphere of radius one among the design variables. The Box-Behnken designs that perform best utilize the value of g equal to $\frac{\sqrt{2}}{2}$.

(2) For both design classes the addition of center points at first dramatically decreases the values of J_{PCA} and J_{PCMAX} , but with each additional center point the D-efficiency will also decrease. The following recommendations for the number of center points is based upon simultaneous consideration of J_{PCA} or J_{PCMAX} with the D-efficiency. For $k = 3,4$ and 5

variables, 6 to 10, 7 to 11 and 8 to 12 center points respectively will provide for designs that perform well in a robust sense.

(3) For $k = 3$ variables the central composite design outperforms the Box-Behnken with respect to all four criteria. For $k = 4$, the central composite design and Box-Behnken design are exactly equivalent. This result for $k = 4$ is a consequence of the fact the central composite and Box-Behnken designs are rotations of each other for $k = 4$. The Box-Behnken design is most robust for $k = 5$ although a central composite design containing a one-half fraction performs well in terms of J_{PCA} and J_{PCMAX} but suffers from poor second order model properties, as measured by the D-efficiency.

5.4.3 Second Order Designs Within a Cuboidal Design Region for a Spherical Region of Interest

When the design region is best characterized by a cuboidal region and the region of interest is best characterized by a spherical region the following conclusions and recommendations are drawn from the tables of Appendix C.

(1) Central composite designs that perform best in terms of the robust design selection criteria have the values of g and α equal to 1.0. The Box-Behnken designs that perform best utilize the value of g equal to 1.0.

(2) The addition of center points dramatically decreases the value of J_{PCA} and J_{PCMAX} at first. With each additional center point the D_s-efficiency and D-efficiency simultaneously decrease, resulting in the following recommendations for the number of center points. For $k = 3,4$ and 5 variables, 6 to 9, 8 to 11 and 8 to 11 center points respectively will provide robust designs with respect to all four design criteria.

(3) The central composite and Box-Behnken designs are approximately equivalent for $k = 3$ variables. The central composite designs outperform the Box-Behnken for $k = 4$ and $k = 5$ with a one-half fraction used within the $k = 5$ central composite.

5.5 Economical Robust Second Order Designs

The experimental situation described within section 5.4 is further investigated within this section for second order designs that are more economical than central composite or Box-Behnken designs. These designs are saturated or near saturated with respect to estimation of a second order response model when no center points are used. Without center points, these designs do not possess the capabilities for performing a lack of fit test. Within this section, small composite, Hybrid and Notz type designs which are saturated or near saturated experimental design classes will be examined in a similar fashion as central composite and Box-Behnken designs in section 5.4. These three design classes will be considered in the context of a 'one experiment' sequential framework. The need for a lack of fit test within this framework results in consideration of the three design classes with the addition of center points. These designs with center points are no longer saturated or near saturated for estimation of a second order model, but they provide economical alternatives to central composite and Box-Behnken designs.

The economical designs examined here have the advantage of containing fewer experimental points than central composite or Box-Behnken designs. Unfortunately the performance of the economical designs in terms of the J_{PCA}, J_{PCMAX}, D_s -efficiency and D-efficiency is much worse than the central composite or Box-Behnken. An experimenter should therefore consider using the economical designs only when he or she is limited in the number of experimental points and cannot accommodate the needs for a central composite or Box-Behnken design.

A general examination and comparison of the three economical design classes in terms of J_{PCA}, J_{PCMAX}, D_s-efficiency and D-efficiency is now considered. Appendix C contains summary tables of these four design criteria for the small composite, hybrid and Notz designs with the addition of center points. Consistent with the comparisons for factorial, central composite and Box-

Behnken designs the values of J_{PCA} and J_{PCMAX} calculated in Appendix C are for a region in the second order coefficients, Θ, such that the power of the lack of fit test is less than or equal to 0.90.

5.5.1 Economical Second Order Designs Within a Cuboidal Design Region for a Cuboidal Region of Interest

When both the design region and the region of interest are best represented by a unit cuboidal region, then the conclusions and recommendations drawn from the tables of Appendix C are given by the following.

(1) Small composite and Notz designs that perform best in terms of the J_{PCA}, J_{PCMAX}, D_t-efficiency and D-efficiency possess the values of g and α equal to one. For the hybrid designs, the designs given by Roquemore (1976) with given values for $g, a, b, c,$ and d are scaled such that the largest possible value of these five design parameters is equal to one. This will guarantee that all design points are within the unit cube.

(2) The addition of center points at first dramatically decreases the value of J_{PCA} and J_{PCMAX}, but with each additional center point the D_t-efficiency and D-efficiency will also decrease. In order to maintain robustness in terms of the four design criteria, simultaneous consideration of all four criteria yield the following recommendations for the number of center points. For $k = 3$ and $k = 4$ variables, 6 to 8 and 8 to 10 center points respectively provide for designs which perform well in terms of the four design criteria.

(3) For $k = 3$ variables, the Notz design performs extremely well in terms of the four criteria. It outperforms the other design classes in terms of the criteria by a good margin. The small composite design performs best for $k = 4$ variables.

5.5.2 Economical Second Order Designs Within a Spherical Design Region for a Spherical Region of Interest

When both the design region and the region of interest are best represented by a unit sphere or hypersphere, then the conclusions and recommendations drawn from the tables of Appendix C are given by the following.

(1) The small composite and Notz type designs that perform best possess the values of g and α equal to $\frac{1}{\sqrt{k}}$ and 1.0. The hybrid designs that perform best are such that for the designs given by Roquemore, the experimental point which is the farthest distance from the center of the design is scaled such that it falls on the sphere in the design variables with radius one. All other design points are scaled using the same scaling factor as the farthest point, this will guarantee that all experimental points are within the unit sphere.

(2) The addition of center points dramatically decreases the values of J_{PCA} and J_{PCMAX}, but with each additional center point the D-efficiency will also decrease. For $k = 3$ and $k = 4$ variable designs, 6 to 8 and 7 to 9 center points respectively will result in designs that perform well in terms of the four design criteria.

(3) Among the design classes, the hybrid designs perform best. The hybrid 311B and 416C are the best performing test for $k = 3$ and $k = 4$ variables.

5.5.3 Economical Second Order Designs Within a Cuboidal Design Region With a Spherical Region of Interest

When the design region is best characterized by a cuboidal region and the region of interest is best represented by a spherical region the following conclusions and recommendations are drawn from the tables of Appendix C.

(1) Small composite and Notz type designs that perform best in terms of the four design criteria have the values of g and α equal to one. The hybrid designs of the form given by Roquemore are scaled such that the largest value of g, a, c and d is scaled such that it is equal to one.

(2) The addition of center points dramatically decreases the values of J_{PCA} and J_{PCMAX}, but with each additional center point the D_s-efficiency and D-efficiency will also decrease. The following recommendations for the number of center points will provide robust designs in terms of the four design criteria. For $k = 3$ and $k = 4$ variables, 6 to 9 and 7 to 10 center points respectively will provide for robust design performance.

(3) Among the design classes, the Notz type design performs well for $k = 3$ variables and the small composite performs best for $k = 4$ variables.

Chapter VI

VI. Summary, Conclusions and Further Research

The objective of this research was to investigate sequential response surface design strategies. Due to the nature of the sequential design framework, lack of fit properties and first order response model prediction properties are important features of a first order experimental design. Uncertainty of the best characterization for the response model brings about the need for a lack of fit test. Prediction and exploration goals in a response surface experiment bring about the need for high quality first order prediction properties.

The Λ_2 design criteria which addresses the lack of fit properties of an experimental design was modified to account for the first order mean squared error of prediction. The $\Lambda_2{}^*$ criterion which maximizes the average noncentrality parameter of the lack of fit test for second order coefficients conditioned upon a fixed first order integrated prediction bias, B, was utilized as a design selection criterion for first order designs. Based upon $\Lambda_2{}^*$, the rotation design class was developed and first order model properties of these designs were investigated.

The sequential design framework specifies that if a significant lack of fit is observed then a second order response model estimate is employed. Augmentations of first order designs constructed using the Λ_2^* criterion were investigated using various second order model properties. Augmentations of rotation designs based upon this criterion were given and compared to factorial/central composite designs.

Finally, the J_{PCA} and J_{PCMAX} criteria were developed as methods for evaluating first order prediction properties of experimental designs. The J_{PCA} and J_{PCMAX} criteria incorporate the performance of the lack of fit test into the evaluation of the first order integrated mean squared error of prediction. These two design criteria were used to construct factorial designs for use within the sequential experimental framework. In addition, J_{PCA} and J_{PCMAX} were considered in conjunction with D_s-efficiency and D-efficiency in defining a robust design selection procedure for evaluation of second order designs within the sequential framework limited to the 'one experiment' (no augmentation or redesigning) case.

This chapter summarizes the developments and results of the Λ_2^*, J_{PCA} and J_{PCMAX} criteria. A summary of the results for the construction of various designs applying these three criteria will be given.

6.1 Λ_2^* and Rotated Designs

The Λ_2^* criterion has been used in this work as a design selection criterion for choosing response surface designs that perform well in terms of the lack of fit properties while accounting for first order prediction properties. As formally defined, the Λ_2^* criterion is

$$\bar{\lambda} = \frac{\int_{\frac{\beta'_2 T \beta_2}{\sigma^2} = \delta} \lambda \, d\beta_2}{\int_{\frac{\beta'_2 T \beta_2}{\sigma^2} = \delta} d\beta_2} = \frac{\delta tr[T^{1} L]}{p_2} \; . \tag{6.1}$$

The use of $\bar{\lambda}$ for design selection reduces to evaluating tr[T^{-1}L]. Designs which achieve large values of tr[T^{-1}L] will perform well in terms of the power of the lack of fit test. The evaluation of factorial designs based upon tr[T^{-1}L] resulted in designs with g = 1.0 performing the best for the lack of fit purposes. When incorporating the first order prediction properties (integrated bias, integrated variance or integrated mean squared error) of a factorial design into the evaluation of the design performance, the designs which perform best have g = 1.0 with the number of center points chosen so that the prediction properties are satisfied.

In some cases, i.e., minimum bias and minimum mean squared error efficient, the factorial designs with g = 1.0 required the addition of quite a number of center points. In order to achieve the prediction property of interest (bias or mean squared error) the value of g must be reduced if less center points are to be used. For these designs with fewer center points and $g < 1.0$, the power properties are reduced as measured by tr[T^{-1}L]. Fortunately, for these situations the power properties were improved upon by consideration of the class of first order rotated designs. These designs represent factorial designs with $g < 1.0$ transformed or rotated such that all design points fall on the outer edges of a cuboidal region.

These first order rotated designs were first shown to achieve better lack of fit properties as measured by tr[T^{-1}L] than the corresponding $g < 1.0$ factorial designs. In addition, the prediction properties of the rotation designs as measured by the first order prediction variance, first order prediction bias or the first order prediction mean squared error were shown to be identical to those of the corresponding $g < 1.0$ factorial designs. The rotation design class provides a robust alternative in terms of the lack of fit and prediction properties to ordinary factorial designs.

The first order rotation design class was shown to be easily augmented with dual axial type points for estimation of a second order response model. These designs formed the second order rotated design class. It was shown that second order rotated designs can be constructed to block orthogonally and be rotatable. Also, these designs were shown to be more D-efficient for a full second order model and more D_s-efficient for second order coefficients within a cuboidal design region than central composite designs.

6.2 J_{PCA} and J_{PCMAX} Design Criteria

The J_{PCA} and J_{PCMAX} criteria have been used in this work as design selection criteria for choosing designs that perform well in terms of the first order integrated mean squared error of prediction, J. The evaluation of J is restricted to a region in the second order coefficients where it is somewhat likely that a first order model will be used for prediction based upon the outcome of the lack of fit test. The importance of good prediction for optimization purposes and the lack of fit test for model uncertainty purposes within the sequential experimental framework are addressed by the J_{PCA} and J_{PCMAX} criteria. Formally, J_{PCA} and J_{PCMAX} were defined as,

$$J_{PCA} = \frac{\int_{\frac{\beta'_2 L\beta_2}{\sigma^2} \le \lambda_0} J\,d\beta_2}{\int_{\frac{\beta'_2 L\beta_2}{\sigma^2} \le \lambda_0} d\beta_2} = tr(\mu_{11} M_{11}^{-1}) + \frac{\lambda_0 tr[L^{-1}T]}{p_2 + 2} \tag{6.2}$$

and

$$J_{PCMAX} = \max_{\{\beta_2 : \frac{\beta'_2 L \beta_2}{\sigma^2} \leq \lambda_0\}} J$$

$$= tr(\mu_{11} M_{11}^{-1}) + \lambda_0(\text{ max eigenvalue}(L^{-1}T)) \qquad (6.3)$$

where λ_0 is the noncentrality parameter needed to achieve a specified power for the lack of fit test.

J_{PCA} and J_{PCMAX} were first utilized to evaluate the performance of first order factorial designs. Construction of factorial designs based upon J_{PCA} and J_{PCMAX} was studied in Section 5.3. These factorial designs were examined in both cuboidal and spherical design and interest regions.

J_{PCA} and J_{PCMAX} were also examined along with D_s -efficiency and D-efficiency to construct robust second order experimental designs used within the experimental framework when only one experiment can be performed. These designs can be utilized for testing second order departures from a first order model and for estimating either a first or second order model depending upon the result of the lack of fit test. Central composite and Box-Behnken designs were compared in cuboidal and spherical design and interest regions. The results are presented in Section 5.4. The central composite designs were shown to be more robust with respect to the four criteria except for the case of k = 5 variables for a spherical design region and a spherical region of interest, where the Box-Behnken performs better.

The robust design selection procedure of evaluating J_{PCA}, J_{PCMAX} , D_s-efficiency and D-efficiency was also applied to the construction of economical second order designs. Small composite, hybrid and Notz designs were evaluated and compared for k = 3 and k = 4 variables. Again, cuboidal and spherical design and interest regions were examined in the design evaluation. The results of the evaluations are presented in Section 5.5.

6.3 *Areas of Further Research*

As is common with many types of research work similar to this one, several areas of further research are open for investigation. Some of these areas are listed as follows.

(1) The first order rotation design class developed within this work was employed within the sequential experimental framework. When a significant lack of fit is observed, augmentation of the first order rotated designs with dual axial type points will allow for estimation of the second order coefficients. The second order rotated design class constructed by the augmentation of a first order rotated design with dual axial points often will consist of an excessive number of design points that an experimenter is unable to obtain. An investigation of more economical augmentations of first order rotated designs is needed when the number of experimental points is limited.

(2) The J_{PCA} and J_{PCMAX} criteria have been applied to several well established experimental design classes. These criteria have not been investigated for the rotated design classes. Preliminary investigations indicate that a reparameterization for first order rotated designs similar to that of a factorial design will not produce conformability among the integrated bias and the noncentrality parameter. A more complete investigation of the possible use of these two criteria within the rotated class is warranted.

(3) The J_{PCA} and J_{PCMAX} criteria present summary or overall norms on the performance of the integrated mean squared error. A possible investigation of the performance of J over all possible values of the noncentrality parameter could display interesting features not obtainable from overall norms such as J_{PCA} and $J_{\max}$. Plots of J vs. λ could provide for an overall description of the mean squared error performance relative to the lack of fit performance.

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Appendix A

Appendix A

The development of the testable hypotheses for the first order rotated design class is given by the following.

Graybill (1976) gives the following results concerning testable hypotheses for the general linear model.

When considering the general linear model of the form $\underline{y} = X\underline{\beta} + \varepsilon$,

(1) Elements of $(X'X)\underline{\beta}$ are testable hypotheses.

(2) Any linear combination of testable hypotheses is a testable hypothesis.

Consider $\underline{\beta}$ to be the vector of all coefficients of a second order model.

$$\underline{\beta} = \begin{bmatrix} \underline{\beta}_i \\ \underline{\beta}_{ij} \\ \underline{\beta}_{ii} \end{bmatrix}$$

where

$\underline{\beta}_i$ is the $1 \times (k+1)$ vector of first order coefficients.

$\underline{\beta}_{ij}$ is the: $1 \times \binom{k}{2}$ vector of interaction coefficients.

$\underline{\beta}_{ii}$ is the $1 \times k$ vector of pure quadratic coefficients.

Also consider the rotated designs of the form (3.17), (3.19) and (3.21). The elements of $(X'X)\underline{\beta}$ for these designs are given by,

k = 2

$$\begin{bmatrix} n\beta_0 + 2(1+d^2)\beta_{11} + 2(1+d^2)\beta_{22} \\ 2(1+d^2)\beta_1 \\ 2(1+d^2)\beta_2 \\ 4d^2\beta_{12} + 2d(1-d^2)\beta_{11} - 2d(1-d^2)\beta_{22} \\ 2(1+d^2)\beta_0 + 2d(1-d^2)\beta_{12} + 2(1+d^4)\beta_{11} + 4d^2\beta_{22} \\ 2(1+d^2)\beta_0 - 2d(1-d^2)\beta_{12} + 4d^2\beta_{11} + 2(1+d^4)\beta_{22} \end{bmatrix} = \begin{bmatrix} T_1 \\ T_2 \\ T_3 \\ T_4 \\ T_5 \\ T_6 \end{bmatrix}$$

k = *3*

$$
\begin{bmatrix}
n\beta_0 + 4(1+d^2)(\beta_{11}+\beta_{22}+\beta_{33}) \\
4(1+d^2)\beta_1 \\
4(1+d^2)\beta_2 \\
4(1+d^2)\beta_3 \\
8d^2\beta_{12} + 4d(1-d^2)(\beta_{22}-\beta_{11}) \\
2(1+d^2)^2\beta_{13} \\
2(1+d^2)^2\beta_{23} \\
4(1+d^2)\beta_0 - 4d(1-d^2)\beta_{12} + 4(1+d^4)\beta_{11} + 8d^2\beta_{22} + 2(1+d^2)^2\beta_{33} \\
4(1+d^2)\beta_0 + 4d(1-d^2)\beta_{12} + 8d^2\beta_{11} - 4(1+d^4)\beta_{22} + 2(1+d^2)^2\beta_{33} \\
4(1+d^2)\beta_0 + 2(1+d^2)^2(\beta_{11}+\beta_{22}+\beta_{33})
\end{bmatrix}
=
\begin{bmatrix}
T_1 \\ T_2 \\ T_3 \\ T_4 \\ T_5 \\ T_6 \\ T_7 \\ T_8 \\ T_9 \\ T_{10}
\end{bmatrix}
$$

$k = 4$

$$\begin{bmatrix}
n\beta_0 + 8(1+d^2)(\beta_{11}+\beta_{22}+\beta_{33}) \\
8(1+d^2)\beta_1 \\
8(1+d^2)\beta_2 \\
8(1+d^2)\beta_3 \\
8(1+d^2)\beta_4 \\
4(1+d^2)^2\beta_{12} \\
16d^2\beta_{13} + 8d(1-d^2)(\beta_{33}-\beta_{11}) \\
4(1+d^2)^2\beta_{14} \\
4(1+d^2)^2\beta_{23} \\
16d^2\beta_{24} + 8d(1-d^2)(\beta_{44}-\beta_{22}) \\
4(1+d^2)^2\beta_{34} \\
8(1+d^2)\beta_0 - 8d(1-d^2)\beta_{13} + 8(1+d^4)\beta_{11} + 16d^2\beta_{33} + 4(1+d^2)^2(\beta_{22}+\beta_{44}) \\
8(1+d^2)\beta_0 - 8d(1-d^2)\beta_{24} + 4(1+d^2)^2(\beta_{11}+\beta_{33}) + 8(1+d^4)\beta_{22} + 16d^2\beta_{44} \\
8(1+d^2)\beta_0 + 8d(1-d^2)\beta_{13} + 16d^2\beta_{11} + 8(1+d^4)\beta_{33} + 4(1+d^2)^2(\beta_{22}+\beta_{44}) \\
8(1+d^2)\beta_0 + 8d(1-d^2)\beta_{24} + 4(1+d^2)^2(\beta_{11}+\beta_{33}) + 16d^2\beta_{22} + 8(1+d^4)\beta_{44}
\end{bmatrix}
=
\begin{bmatrix}
T_1 \\ T_2 \\ T_3 \\ T_4 \\ T_5 \\ T_6 \\ T_7 \\ T_8 \\ T_9 \\ T_{10} \\ T_{11} \\ T_{12} \\ T_{13} \\ T_{14} \\ T_{15}
\end{bmatrix}$$

The testable hypotheses are given by,

***k* = 2**

$X'X$ is of rank 5, therefore there exists 5 independent testable hypotheses.

$$\frac{T_1}{n-4} - \frac{T_5 + T_6}{(n-4)(1+d^2)} = \beta_0$$

$$\frac{T_2}{2(1+d^2)} = \beta_1$$

$$\frac{T_3}{2(1+d^2)} = \beta_2$$

$$\frac{T_1}{n-4} - \frac{n(T_5 + T_6)}{4(n-4)(1+d^2)} = \beta_{11} + \beta_{22}$$

$$\frac{-(1-d^2)T_1}{2d(n-4)} + \frac{T_4}{4d^2} + \frac{n(1-d^2)(T_5+T_6)}{8d(n-4)(1-d^2)} = \beta_{12} - \frac{(1-d^2)}{d}\beta_{22}$$

k = 3

$X'X$ is of rank 8, therefore there exists 8 independent testable hypotheses.

$$\frac{T_1}{n-8}-\frac{2T_{10}}{(1-d^2)(n-8)}=\beta_0$$

$$\frac{T_2}{4(1+d^2)}=\beta_1$$

$$\frac{T_3}{4(1+d^2)}=\beta_2$$

$$\frac{T_4}{4(1+d^2)}\beta_3$$

$$\frac{-(1-d^2)T_1}{d(1+d^2)(n-8)}+\frac{T_5}{8d^2}+\frac{n(1-d^2)}{4d(1+d^2)^2(n-8)}=\beta_{12}-\frac{(1-d^2)}{d}\beta_{22}-\frac{(1-d^2)}{2d}\beta_{33}$$

$$\frac{T_6}{2(1+d^2)^2}=\beta_{13}$$

$$\frac{T_7}{2(1+d^2)^2}=\beta_{23}$$

$$\frac{-2T_1}{(1+d^2)(n-8)}+\frac{((n-8)+4(1+d^2))T_1}{2(n-8)(1+d^2)^2}=\beta_{11}+\beta_{22}+\beta_{33}$$

k = 4

$X'X$ is of rank 12, therefore there exists 12 independent testable hypotheses.

$$\frac{T_1}{n-16} - \frac{T_{12}+T_{13}+T_{14}+T_{15}}{2(n-16)(1+d^2)} = \beta_0$$

$$\frac{T_2}{8(1+d^2)} = \beta_1$$

$$\frac{T_3}{8(1+d^2)} = \beta_2$$

$$\frac{T_4}{8(1+d^2)} = \beta_3$$

$$\frac{T_5}{8(1+d^2)} = \beta_4$$

$$\frac{T_6}{4(1+d^2)^2} = \beta_{12}$$

$$\frac{T_7}{16d^2} = \beta_{13} + \frac{1-d^2}{2d}(\beta_{33}-\beta_{11})$$

$$\frac{T_8}{4(1+d^2)^2} = \beta_{14}$$

$$\frac{T_9}{4(1+d^2)^2} = \beta_{23}$$

$$\frac{T_{10}}{16d^2} = \beta_{24} + \frac{1-d^2}{2d}(\beta_{44}-\beta_{22})$$

$$\frac{T_{11}}{4(1+d^2)^2} = \beta_{34}$$

$$\frac{n(T_{12}+T_{13}+T_{14}+T_{15})}{16(1+d^2)^2(n-16)} - \frac{2T_1}{(1-d^2)(n-16)} = \beta_{11}+\beta_{22}+\beta_{33}+\beta_{44}$$

Appendix B

Appendix B

The development and derivation of the Λ_2^*, J_{PCA} and J_{PCMAX} criteria are given here.

Appendix B.1 Development of Λ_2^*

Recall from (3.12) that the Λ_2^* criterion is given by,

$$\bar{\lambda} = \frac{\displaystyle\int_{\frac{\underline{\beta}'_2 T \underline{\beta}_2}{\sigma^2} = \delta} \lambda \, d\underline{\beta}_2}{\displaystyle\int_{\frac{\underline{\beta}'_2 T \underline{\beta}_2}{\sigma_2} = \delta} d\underline{\beta}_2} .$$

The development here follows closely to that of the Λ_2 criterion given by Jones (1975), the reader is referred there for more details.

Let $p_2 = k + \binom{k}{2}$, the number of coefficients in $\underline{\beta}_2$.

$$\bar{\lambda} = \lim_{\varepsilon \to 0} \frac{\displaystyle\int_{\delta \le \frac{\underline{\beta}'_2 T \underline{\beta}_2}{\sigma^2} \le \delta+\varepsilon} \frac{\underline{\beta}'_2 L \underline{\beta}_2}{\sigma^2}\, d\underline{\beta}_2}{\displaystyle\int_{\delta \le \frac{\underline{\beta}'_2 T \underline{\beta}_2}{\sigma^2} \le \delta+\varepsilon} d\underline{\beta}_2}$$

where

$$\int_{\delta \le \frac{\underline{\beta}'_2 T \underline{\beta}_2}{\sigma^2} \le \delta+\varepsilon} \frac{\underline{\beta}'_2 L \underline{\beta}_2}{\sigma^2}\, d\underline{\beta}_2 = \frac{\pi^{p_2/2}\ tr[T^{-1}L]}{(p_2+2)\Gamma(\frac{p_2}{2}+1)|T|^{1/2}}\left((\delta+\varepsilon)^{(p_2/2+1)} - \delta^{(p_2/2+1)}\right)$$

and

$$\int_{\delta \le \frac{\underline{\beta}'_2 T \underline{\beta}_2}{\sigma^2} \le \delta+\varepsilon} d\underline{\beta}_2 = \frac{\pi^{p_2/2}}{\Gamma(\frac{p_2}{2}+1)|T|^{1/2}}\left((\delta+\varepsilon)^{p_2/2} - \delta^{p_2/2}\right) .$$

Therefore,

$$\bar{\lambda} = \lim_{\varepsilon \to 0} \frac{\dfrac{\pi^{p_2/2} tr[T^{-1}L]}{(p_2+2)\Gamma(p_2/2+1)|T|^{1/2}}\left((\delta+\varepsilon)^{(p_2/2+1)} - \delta^{(p_2/2+1)}\right)}{\dfrac{\pi^{p_2/2}}{\Gamma(p_2/2+1)|T|^{1/2}}\left((\delta+\varepsilon)^{p_2/2} - \delta^{p_2/2}\right)} .$$

Following the form given by Jones, applying L 'Hospital's rule gives,

$$\bar{\lambda} = \lim_{\varepsilon \to 0} tr[T^{-1}L]\frac{\delta+\varepsilon}{p_2}$$

$$= \frac{\delta tr[T^{-1}L]}{p_2} .$$

Appendix B.2 Development of J_{PCA}

Recall from (5.6) that the J_{PCA} criterion is given by,

$$J_{PCA} = \frac{\displaystyle\int_{\frac{\beta'_2 L\beta_2}{\sigma^2} \le \lambda_0} J d\beta_2}{\displaystyle\int_{\frac{\beta'_2 L\beta_2}{\sigma^2} \le \lambda_0} d\beta_2}$$

$$= \frac{\displaystyle\int_{\frac{\beta'_2 L\beta_2}{\sigma^2} \le \lambda_0} V d\beta_2 + \int_{\frac{\beta'_2 L\beta_2}{\sigma^2} \le \lambda_0} B d\beta_2}{\displaystyle\int_{\frac{\beta'_2 L\beta_2}{\sigma^2} \le \lambda_0} d\beta_2}$$

$$= \frac{\displaystyle\int_{\frac{\beta'_2 L\beta_2}{\sigma^2} \le \lambda_0} tr(\mu_{11} M_{11}^{-1}) d\beta_2 + \int_{\frac{\beta'_2 L\beta_2}{\sigma^2} \le \lambda_0} \frac{\beta'_2 T\beta_2}{\sigma^2} d\beta_2}{\displaystyle\int_{\frac{\beta'_2 L\beta_2}{\sigma^2} \le \lambda_0} d\beta_2}$$

$$= \frac{tr(\mu_{11} M_{11}^{-1}) \left[\dfrac{\pi^{p_2/2} \lambda_0^{p_2/2}}{\Gamma(\frac{p_2}{2} + 1) |L|^{1/2}} \right] + \dfrac{\pi^{p_2/2} \lambda_0^{(p_2/2+1)} tr[L^{-1}T]}{(p_2 + 2)\Gamma(\frac{p_2}{2} + 1) |L|^{1/2}}}{\left[\dfrac{\pi^{p_2/2} \lambda_0^{p_2/2}}{\Gamma(\frac{p_2}{2} + 1) |L|^{1/2}} \right]}$$

$$= tr(\mu_{11} M_{11}^{-1}) + \frac{\lambda_0}{p_2 + 2} tr[L^{-1}T] .$$

Appendix B.3 Development of J_{PCMAX}

Recall from (5.7) that the J_{PCMAX} criterion is given by,

$$J_{PCMAX} = \max_{\{\beta_2 : \lambda \le \lambda_0\}} J$$

$$= \max_{\{\beta_2 : \frac{\beta'_2 L \beta_2}{\sigma^2} \le \lambda_0\}} [tr(\mu_{11} M_{11}^{-1}) + \frac{\beta'_2 T \beta_2}{\sigma^2}] \ .$$

The maximum value of J within this ellipsoidal region in β_2 will always occur on the boundary, $\frac{\beta'_2 L \beta_2}{\sigma_2} = \lambda_0$.

Since $tr(\mu_{11} M_{11}^{-1})$ is not dependent upon β_2 this piece is constant with respect to the maximization and the evaluation of $\max_{\{\beta_2 : \frac{\beta'_2 L \beta_2}{\sigma_2} = \lambda_0\}} \frac{\beta'_2 T \beta_2}{\sigma^2}$ is all that is necessary.

Note that $\frac{\beta'_2 L \beta_2}{\sigma^2}$ and $\frac{\beta'_2 T \beta_2}{\sigma^2}$ are both positive definite quadratic forms.

Now, since L is positive definite, it can be expressed as

$$L = P' L_* P$$

where P is an orthogonal matrix and L_* is a diagonal matrix with the eigenvalues of L on the diagonal.

The positive definite symmetric square root of L is given by,

$$L^{1/2} = P' L_*^{1/2} P$$

and

$$\frac{\underline{\beta}'_2 L \underline{\beta}_2}{\sigma^2} \text{ can be expressed as } \frac{\underline{\alpha}'_2 \underline{\alpha}_2}{\sigma^2}$$

where $\underline{\alpha}_2 = L^{1/2}\underline{\beta}_2$.

Therefore,

$$\max_{\{\underline{\beta}_2 : \frac{\underline{\beta}'_2 L \underline{\beta}_2}{\sigma^2} = \lambda_0\}} \frac{\underline{\beta}'_2 T \underline{\beta}_2}{\sigma^2} = \max_{\{\frac{\underline{\alpha}'_2 \underline{\alpha}_2}{\sigma^2} = \lambda_0\}} \frac{\underline{\alpha}'_2 L^{-1/2} T L^{-1/2} \underline{\alpha}'_2}{\sigma^2}$$

$$= \lambda_0 \text{ max eigenvalue } [L^{-1/2} T L^{-1/2}]$$

$$= \lambda_0 \text{ max eigenvalue } [L^{-1} T]$$

and

$$J_{PCMAX} = tr(\mu_{11} M_{11}^{-1}) + \lambda_0 \text{ max eigenvalue } [L^{-1} T] .$$

Appendix C

Appendix C

Table C.1
Factorial Designs - Minimum J_{PCA} For Designs With Given Sample Size and Power < 0.90 For $\alpha = 0.05$ Test
Design Region : Cuboidal   Region of Interest : Cuboidal

k = 2

n	g	[ii]	J_{PCA}
7	0.98	0.5488	20.5020
8	1.00	0.5000	9.1936
9	1.00	0.4444	6.8199
10	1.00	0.4000	6.0974
11	1.00	0.3636	5.9163
12	1.00	0.3333	5.9721

k = 3

n	g	[ii]	J_{PCA}
11	0.92	0.6156	63.2490
12	0.99	0.6534	23.4157
13	1.00	0.6154	14.2405
14	1.00	0.5714	10.8241
15	1.00	0.5333	9.2318
16	1.00	0.5000	8.4112
17	1.00	0.4706	7.9796
18	1.00	0.4444	7.7685
19	1.00	0.4211	7.6931

k = 4

n	g	[ii]	J_{PCA}
19	0.86	0.6228	15.0769
20	0.92	0.6771	54.0690
21	0.98	0.7171	30.3279
22	1.00	0.7273	20.9476
23	1.00	0.6957	16.3396
24	1.00	0.6666	13.7371
25	1.00	0.6400	12.1324
26	1.00	0.6154	11.0806
27	1.00	0.5926	10.3797

k = 5

n	g	[ii]	J_{PCA}
36	0.86	0.6570	112.4210
37	0.90	0.7005	60.9461
38	0.95	0.7600	40.6565
39	0.99	0.8205	30.2894
40	1.00	0.8000	24.1892
41	1.00	0.7805	20.3431
42	1.00	0.7619	17.7503
43	1.00	0.7442	15.9157
44	1.00	0.7273	14.5702

k = 5 (1/2 fraction)

n	g	[ii]	J_{PCA}
20	1.00	0.8000	68.0726
21	1.00	0.7619	37.6649
22	1.00	0.7273	26.1520
23	1.00	0.6957	20.5324
24	1.00	0.6666	17.3695
25	1.00	0.6400	15.4270
26	1.00	0.6154	14.1662
27	1.00	0.5926	13.3196
28	1.00	0.5714	12.7413

Table C.2
Factorial Designs - Minimum J_{PCA} For Designs With Given Sample Size and Power < 0.90 For $\alpha = 0.05$ Test
Design Region : Spherical Region of Interest : Spherical

k = 2

n	g	[ii]	J_{PCA}
7	0.70	0.2800	21.5691
8	0.70	0.2450	11.9769
9	0.70	0.2177	10.1611
10	0.70	0.1960	9.8506
11	0.70	0.1780	10.0499
12	0.70	0.1633	10.4772

k = 3

n	g	[ii]	J_{PCA}
11	0.57	0.2363	76.6960
12	0.57	0.2166	33.5343
13	0.57	0.1999	23.6721
14	0.57	0.1857	20.0628
15	0.57	0.1733	18.5157
16	0.57	0.1625	17.8690
17	0.57	0.1529	17.6877
18	0.57	0.1444	17.7756

k = 4

n	g	[ii]	J_{PCA}
19	0.50	0.2105	195.4490
20	0.50	0.2000	74.5790
21	0.50	0.1905	46.6494
22	0.50	0.1818	35.7541
23	0.50	0.1739	30.3752
24	0.50	0.1666	27.3690
25	0.50	0.1600	25.5736
26	0.50	0.1538	24.4711
27	0.50	0.1481	23.7986

k = 5

n	g	[ii]	J_{PCA}
36	0.447	0.1777	155.7200
37	0.447	0.1730	90.3990
38	0.447	0.1684	64.7790
39	0.447	0.1641	51.8560
40	0.447	0.1600	44.3380
41	0.447	0.1560	39.5540
42	0.447	0.1524	36.3220
43	0.447	0.1488	34.0470
44	0.447	0.1455	32.4010

k = 5 (1/2 fraction)

n	g	[ii]	J_{PCA}
20	0.447	0.1600	125.1640
21	0.447	0.1524	78.2140
22	0.447	0.1455	59.6030
23	0.447	0.1391	50.2500
24	0.447	0.1333	44.9080
25	0.447	0.1280	41.6220
26	0.447	0.1231	39.5190
27	0.447	0.1185	38.1530
28	0.447	0.1143	37.2750

Table C.3
Factorial Designs - Minimum J_{PCA} For Designs With Given Sample Size and Power < 0.90 For $\alpha = 0.05$ Test
Design Region : Cuboidal Region of Interest : Spherical

k=2

n	g	[ii]	J_{PCA}
7	0.81	0.3749	17.8344
8	0.89	0.3961	8.0116
9	0.98	0.4268	5.5740
10	1.00	0.4000	4.5797
11	1.00	0.3636	4.1703
12	1.00	0.3333	4.0198
13	1.00	0.3077	4.0030

k=3

n	g	[ii]	J_{PCA}
11	0.69	0.3463	59.4860
12	0.74	0.3651	22.0349
13	0.80	0.3938	13.2580
14	0.86	0.4226	9.6966
15	0.91	0.4417	7.8179
16	0.97	0.4705	6.6650
17	1.00	0.4705	5.8971
18	1.00	0.4444	5.3961

k=4

n	g	[ii]	J_{PCA}
19	0.61	0.3133	155.3430
20	0.64	0.3277	52.8160
21	0.68	0.3523	29.4479
22	0.72	0.3770	20.2103
23	0.76	0.4000	15.4627
24	0.80	0.4267	12.6209
25	0.84	0.4516	10.7429
26	0.88	0.4766	9.4131
27	0.92	0.5016	8.4230

k=5

n	g	[ii]	J_{PCA}
36	0.57	0.2888	114.2230
37	0.59	0.3011	61.0787
38	0.62	0.3237	40.3896
39	0.64	0.3361	29.9206
40	0.67	0.3591	23.7440
41	0.70	0.3824	19.7233
42	0.72	0.3950	16.9118
43	0.75	0.4186	14.8456
44	0.78	0.4425	13.2658

k=5 (1/2 fraction)

n	g	[ii]	J_{PCA}
20	0.65	0.3380	66.7850
21	0.70	0.3730	36.1250
22	0.74	0.3983	24.1154
23	0.79	0.4342	18.0014
24	0.84	0.4704	14.3794
25	0.89	0.5069	12.0102
26	0.95	0.5554	10.3487
27	1.00	0.5926	9.1229
28	1.00	0.5714	8.2078

Table C.4
Factorial Designs - Minimum J_{PCMAX} For Designs With Given Sample Size and Power < 0.90 For $\alpha = 0.05$ Test
Design Region : Cuboidal Region of Interest : Cuboidal

k = 2

n	g	[ii]	J_{PCMAX}
7	1.00	0.5710	55.6974
8	1.00	0.5000	22.3424
9	1.00	0.4444	14.9730
10	1.00	0.4000	12.4026
11	1.00	0.3636	11.4089
12	1.00	0.3333	11.1056
13	1.00	0.3080	11.1612

k = 3

n	g	[ii]	J_{PCMAX}
11	0.91	0.6020	213.4180
12	0.95	0.6020	71.1770
13	1.00	0.6154	39.0306
14	1.00	0.5714	20.5520
15	1.00	0.5333	17.2044
16	1.00	0.5000	15.2055
17	1.00	0.4706	13.9674
18	1.00	0.4444	13.1961
19	1.00	0.4211	12.7300

k = 4

n	g	[ii]	J_{PCMAX}
19	0.84	0.5940	736.9390
20	0.87	0.6055	230.2840
21	0.89	0.6035	119.0520
22	0.91	0.6023	76.4968
23	0.94	0.6147	55.2868
24	0.96	0.6144	42.9645
25	0.98	0.6147	35.0564
26	1.00	0.6154	29.6127
27	1.00	0.5926	25.7379
28	1.00	0.5714	22.9060

k = 5

n	g	[ii]	J_{PCMAX}
36	0.82	0.5980	697.0200
37	0.83	0.5960	349.3640
38	0.85	0.6080	218.0470
39	0.86	0.6070	153.4230
40	0.87	0.6055	116.3290
41	0.88	0.6040	92.7825
42	0.89	0.6030	76.7415
43	0.90	0.6030	65.2266
44	0.92	0.6160	56.6030
45	0.93	0.6150	49.9575

k = 5 (1/2 fraction)

n	g	[ii]	J_{PCMAX}
20	0.87	0.6055	350.3980
21	0.89	0.6035	176.5420
22	0.91	0.6023	110.8970
23	0.94	0.6147	78.5911
24	0.96	0.6144	60.0335
25	0.98	0.6147	48.2527
26	1.00	0.6154	40.2252
27	1.00	0.5926	34.5485
28	1.00	0.5714	30.4258

Table C.5
Factorial Designs - Minimum J_{PCMAX} For Designs With Given Sample Size and Power < 0.90 For $\alpha = 0.05$ Test
Design Region : Spherical   Region of Interest : Spherical

k = 2

n	g	[ii]	J_{PCMAX}
7	0.70	0.2800	99.8820
8	0.70	0.2450	47.7030
9	0.70	0.2177	35.9010
10	0.70	0.1960	31.9720
11	0.70	0.1780	30.7140
12	0.70	0.1633	30.6510

k = 3

n	g	[ii]	J_{PCMAX}
11	0.57	0.2363	402.9780
12	0.57	0.2166	154.8850
13	0.57	0.1999	97.5998
14	0.57	0.1857	75.4705
15	0.57	0.1733	64.7847
16	0.57	0.1625	59.0463
17	0.57	0.1529	55.8451
18	0.57	0.1444	54.1025

k = 4

n	g	[ii]	J_{PCMAX}
19	0.50	0.2105	1368.9300
20	0.50	0.2000	461.9970
21	0.50	0.1905	258.0080
22	0.50	0.1818	178.9970
23	0.50	0.1739	139.5610
24	0.50	0.1666	116.8450
25	0.50	0.1600	102.5340
26	0.50	0.1538	92.9706

k = 5

n	g	[ii]	J_{PCMAX}
36	0.447	0.1777	241.7000
37	0.447	0.1730	198.7050
38	0.447	0.1684	170.5570
39	0.447	0.1641	150.8650
40	0.447	0.1600	136.4370
41	0.447	0.1560	125.5030
42	0.447	0.1240	117.0050
43	0.447	0.1488	110.2700
44	0.447	0.1455	104.8500

k = 5 (1/2 fraction)

n	g	[ii]	J_{PCMAX}
20	0.447	0.1600	824.9000
21	0.447	0.1524	452.1370
22	0.447	0.1455	308.4680
23	0.447	0.1391	236.9620
24	0.447	0.1333	195.7930
25	0.447	0.1280	169.8030
26	0.447	0.1231	152.3500
27	0.447	0.1185	140.1160
28	0.447	0.1143	131.2790

Table C.6
Factorial Designs - Minimum J_{PCMAX} For Designs With Given Sample Size and Power < 0.90 For $\alpha = 0.05$ Test
Design Region : Cuboidal Region of Interest : Spherical

k = 2

n	g	[ii]	J_{PCMAX}
7	0.94	0.5050	62.0300
8	1.00	0.5000	23.4380
9	1.00	0.4444	14.4840
10	1.00	0.4000	11.1170
11	1.00	0.3636	9.5760
12	1.00	0.3333	8.8330

k = 3

n	g	[ii]	J_{PCMAX}
11	0.77	0.4310	255.3040
12	0.81	0.4374	84.6180
13	0.84	0.4342	46.0408
14	0.88	0.4425	30.8998
15	0.91	0.4417	23.1806
16	0.95	0.4513	18.5991
17	0.98	0.4520	15.6032
18	1.00	0.4444	13.5155

k = 4

n	g	[ii]	J_{PCMAX}
19	0.67	0.3780	918.8200
20	0.69	0.3810	286.6270
21	0.70	0.3730	147.5850
22	0.72	0.3770	94.3720
23	0.74	0.3810	67.8630
24	0.76	0.3850	52.4670
25	0.78	0.3890	42.5860
26	0.79	0.3840	35.7822
27	0.81	0.3890	30.8474

k = 5

n	g	[ii]	J_{PCMAX}
36	0.62	0.3420	156.4590
37	0.62	0.3320	123.2690
38	0.63	0.3340	101.3590
39	0.64	0.3360	85.8710
40	0.65	0.3380	74.3760
41	0.66	0.3400	65.5290
42	0.67	0.3420	58.5240
43	0.68	0.3440	52.8510
44	0.69	0.3460	48.1700

k = 5 (1/2 fraction)

n	g	[ii]	J_{PCMAX}
20	0.65	0.3380	448.8200
21	0.66	0.3320	225.2920
22	0.68	0.3360	140.8680
23	0.70	0.3410	99.3360
24	0.71	0.3360	75.4920
25	0.73	0.3410	60.3430
26	0.75	0.3460	50.0250
27	0.76	0.3420	42.6170
28	0.78	0.3480	37.0750

Table C.7
Central Composite Designs - Minimum J_{PCA} and J_{PCMAX} For Designs With Given Sample Size and Power < 0.90 For $\alpha = 0.05$ Test
Design Region : Cuboidal Region of Interest : Cuboidal

$k = 2$ $(g = 1, \alpha = 1)$

n	n_0	[ii]	J_{PCA}	J_{PCMAX}	D_s-efficiency	D-efficiency
11	3	0.5455	38.7609	78.5108	0.9626	0.9026
12	4	0.5000	17.9518	34.3712	0.9266	0.8602
13	5	0.4615	13.0267	26.0754	0.8870	0.8195
14	6	0.4286	11.1827	22.8950	0.8473	0.7814
15	7	0.4000	10.3779	21.4922	0.8090	0.7462
16	8	0.3750	10.0347	20.8943	0.7728	0.7137
17	9	0.3529	9.9336	20.7240	0.7388	0.6839
18	10	0.3333	9.9742	20.8064	0.7071	0.6565

$k = 3$ $(g = 1, \alpha = 1)$

n	n_0	[ii]	J_{PCA}	J_{PCMAX}	D_s-efficiency	D-efficiency
17	3	0.5882	95.5630	203.3764	0.9054	0.8704
18	4	0.5556	41.7049	91.4993	0.8710	0.8360
19	5	0.5263	28.3689	63.1889	0.8376	0.8035
20	6	0.5000	22.9723	51.5682	0.8057	0.7730
21	7	0.4762	20.2653	45.6698	0.7754	0.7444
22	8	0.4545	18.7554	42.3396	0.7469	0.7178
23	9	0.4348	17.8733	40.3648	0.7200	0.6928
24	10	0.4167	17.3586	39.1870	0.6947	0.6696
25	11	0.4000	17.0764	38.5156	0.6710	0.6477
26	12	0.3846	16.9501	38.1850	0.6487	0.6273
27	13	0.3704	16.9335	38.0945	0.6277	0.6081
28	14	0.3571	16.9966	38.1791	0.6079	0.5901
29	15	0.3448	17.1196	38.3955	0.5893	0.5731
30	16	0.3333	17.2887	38.7132	0.5717	0.5571

Table C.7 (continued)
Central Composite Designs - Minimum J_{PCA} and J_{PCMAX}

***k* = 4** (g = 1, α = 1)

n	n_0	[ii]	J_{PCA}	J_{PCMAX}	D_s-efficiency	D-efficiency
28	4	0.6429	85.7819	224.7950	0.8411	0.8380
29	5	0.6207	55.5990	146.8462	0.8184	0.8153
30	6	0.6000	43.0616	114.2491	0.7965	0.7934
31	7	0.5806	36.5000	97.0988	0.7754	0.7726
32	8	0.5625	32.5978	86.8517	0.7551	0.7526
33	9	0.5455	30.0906	80.2372	0.7357	0.7336
34	10	0.5294	28.3998	75.7545	0.7171	0.7155
35	11	0.5143	27.2258	72.6239	0.6993	0.6982
36	12	0.5000	26.3986	70.4027	0.6822	0.6816
37	13	0.4865	25.8152	68.8213	0.6659	0.6658
38	14	0.4737	25.4091	67.7066	0.6503	0.6507
39	15	0.4615	25.1363	66.9425	0.6353	0.6363
40	16	0.4500	24.9658	66.4484	0.6210	0.6225
41	17	0.4390	24.8757	66.1665	0.6073	0.6092
42	18	0.4286	24.8499	66.0544	0.5941	0.5966

***k* = 4** - 1/2 fraction of factorial (g = 1, α = 1)

n	n_0	[ii]	J_{PCA}	J_{PCMAX}	D_s-efficiency	D-efficiency
20	4	0.5000	72.2474	162.0387	0.7507	0.7265
21	5	0.4762	48.2983	107.8572	0.7197	0.6972
22	6	0.4545	38.4351	85.3530	0.6909	0.6701
23	7	0.4348	33.3616	73.6621	0.6640	0.6450
24	8	0.4167	30.4259	66.8110	0.6391	0.6216
25	9	0.4000	28.6139	62.5097	0.6159	0.5999
26	10	0.3846	27.4607	59.7059	0.5942	0.5796
27	11	0.3704	26.7251	57.8528	0.5739	0.5607
28	12	0.3571	26.2701	56.6392	0.5549	0.5430
29	13	0.3448	26.0123	55.8758	0.5371	0.5263
30	14	0.3333	25.8984	55.4409	0.5204	0.5107
31	15	0.3226	25.8924	55.2529	0.5046	0.4960
32	16	0.3125	25.9695	55.2550	0.4898	0.4821
33	17	0.3030	26.1119	55.4067	0.4758	0.4690
34	18	0.2941	26.3064	55.6779	0.4625	0.4566
35	19	0.2857	26.5434	56.0463	0.4500	0.4449
36	20	0.2778	26.8151	56.4947	0.4381	0.4337

Table C.7 (continued)
Central Composite Designs - Minimum J_{PCA} and J_{PCMAX}

$k = 5$ (g = 1, α = 1)

n	n_0	[ii]	J_{PCA}	J_{PCMAX}	D_s-efficiency	D-efficiency
46	4	0.7391	171.7772	539.1523	0.8178	0.8405
47	5	0.7234	107.8351	340.4260	0.8042	0.8263
48	6	0.7083	81.0202	256.7879	0.7908	0.8123
49	7	0.6939	66.7628	212.2005	0.7777	0.7987
50	8	0.6800	58.0909	185.0238	0.7648	0.7854
51	9	0.6667	52.3484	166.9948	0.7522	0.7725
52	10	0.6538	48.3207	154.3290	0.7398	0.7599
53	11	0.6415	45.3789	145.0634	0.7278	0.7477
54	12	0.6296	43.1661	138.0836	0.7162	0.7358
55	13	0.6182	41.4658	132.7119	0.7048	0.7243
56	14	0.6071	40.1388	128.5132	0.6937	0.7131
57	15	0.5965	39.0923	125.1960	0.6829	0.7022
58	16	0.5862	38.2614	122.5576	0.6724	0.6916
59	17	0.5763	37.6000	120.4529	0.6622	0.6813
60	18	0.5667	37.0741	118.7753	0.6522	0.6712
61	19	0.5574	36.6582	117.4447	0.6426	0.6615
62	20	0.5484	36.3329	116.4000	0.6331	0.6520
63	21	0.5397	36.0830	115.5935	0.6240	0.6428
64	22	0.5313	35.8966	114.9875	0.6151	0.6339
65	23	0.5231	35.7641	114.5520	0.6064	0.6252
66	24	0.5152	35.6778	114.2626	0.5979	0.6167
67	25	0.5075	35.6313	114.0993	0.5897	0.6084
68	26	0.5000	35.6195	114.0457	0.5816	0.6004

$k = 5$ - 1/2 fraction of factorial (g = 1, α = 1)

n	n_0	[ii]	J_{PCA}	J_{PCMAX}	D_s-efficiency	D-efficiency
30	4	0.6000	125.4781	353.2761	0.7764	0.7706
31	5	0.5806	80.5325	226.2275	0.7543	0.7491
32	6	0.5625	61.7516	172.9196	0.7334	0.7286
33	7	0.5455	51.8421	144.6750	0.7134	0.7092
34	8	0.5294	45.8854	127.6176	0.6944	0.6907
35	9	0.5143	42.0044	116.4431	0.6763	0.6732
36	10	0.5000	39.3396	108.7195	0.6591	0.6564
37	11	0.4865	37.4456	103.1848	0.6427	0.6405
38	12	0.4737	36.0693	99.1220	0.6270	0.6253
39	13	0.4615	35.0571	96.0950	0.6120	0.6109
40	14	0.4500	34.3104	93.8238	0.5977	0.5970
41	15	0.4390	33.7630	92.1205	0.5841	0.5838
42	16	0.4286	33.3690	90.8545	0.5710	0.5711
43	17	0.4186	33.0957	89.9325	0.5585	0.5590
44	18	0.4091	32.9187	89.2857	0.5465	0.5474
45	19	0.4000	32.8200	88.8626	0.5350	0.5363
46	20	0.3913	32.7859	88.6237	0.5239	0.5256
47	21	0.3830	32.8054	88.5383	0.5133	0.5153
48	22	0.3750	32.8701	88.5821	0.5032	0.5055

Table C.8
Central Composite Designs - Minimum J_{PCA} and J_{PCMAX} For Designs With Given Sample Size and Power < 0.90 For $\alpha = 0.05$ Test
Design Region : Spherical   Region of Interest : Spherical

$k = 2$ $(g = 1/\sqrt{k}, \alpha = 1)$

n	n_0	[ii]	J_{PCA}	J_{PCMAX}	D-efficiency
11	3	0.3636	45.1601	93.5258	0.9689
12	4	0.3333	20.5213	32.5355	0.9318
13	5	0.3077	14.8267	24.7790	0.8927
14	6	0.2857	12.7381	21.8182	0.8545
15	7	0.2667	11.8507	20.5239	0.8183
16	8	0.2500	11.4921	19.9843	0.7844
17	9	0.2353	11.4087	19.8455	0.7529
18	10	0.2222	11.4855	19.9435	0.7237

$k = 3$ $(g = 1/\sqrt{k}, \alpha = 1)$

n	n_0	[ii]	J_{PCA}	J_{PCMAX}	D-efficiency
17	3	0.2745	116.9414	219.8223	0.9763
18	4	0.2593	49.6580	67.5760	0.9490
19	5	0.2456	33.5006	47.0447	0.9193
20	6	0.2333	27.1044	38.6966	0.8894
21	7	0.2222	23.9600	34.4871	0.8602
22	8	0.2121	22.2450	32.1349	0.8322
23	9	0.2029	21.2724	30.7629	0.8054
24	10	0.1944	20.7308	29.9674	0.7800
25	11	0.1867	20.4601	29.5381	0.7560
26	12	0.1795	20.3701	29.3553	0.7333
27	13	0.1728	20.4064	29.3460	0.7118
28	14	0.1667	20.5343	29.4635	0.6915
29	15	0.1609	20.7307	29.6762	0.6723
30	16	0.1556	20.9795	29.9623	0.6541

Table C.8 (continued)
Central Composite Designs - Minimum J_{PCA} and J_{PCMAX}

$k=4$ ($g=1/\sqrt{k}$, $\alpha=1$)

n	n_0	[ii]	J_{PCA}	J_{PCMAX}	D-efficiency
28	4	0.2143	93.1954	137.7375	0.9718
29	5	0.2069	60.0446	71.5807	0.9523
30	6	0.2000	46.5467	56.3772	0.9318
31	7	0.1935	39.6001	48.4144	0.9111
32	8	0.1875	35.5350	43.6874	0.8905
33	9	0.1818	32.9670	40.6633	0.8703
34	10	0.1765	31.2687	38.6384	0.8507
35	11	0.1714	30.1173	37.2473	0.8317
36	12	0.1667	29.3309	36.2825	0.8133
37	13	0.1622	28.7996	35.6176	0.7955
38	14	0.1579	28.4536	35.1715	0.7784
39	15	0.1538	28.2459	34.8897	0.7620
40	16	0.1500	28.1442	34.7345	0.7461
41	17	0.1463	28.1257	34.6788	0.7309
42	18	0.1429	28.1733	34.7026	0.7162

$k=4$ - 1/2 fraction of factorial ($g=1/\sqrt{k}$, $\alpha=1$)

n	n_0	[ii]	J_{PCA}	J_{PCMAX}	D-efficiency
20	4	0.2000	103.9345	152.8071	0.9007
21	5	0.1905	68.7809	102.0537	0.8707
22	6	0.1818	54.4456	80.9976	0.8413
23	7	0.1739	47.1231	70.0790	0.8130
24	8	0.1667	42.9090	63.6978	0.7861
25	9	0.1600	40.3199	59.7070	0.7606
26	10	0.1538	38.6794	57.1201	0.7365
27	11	0.1481	37.6378	55.4245	0.7137
28	12	0.1429	36.9975	54.3284	0.6923
29	13	0.1379	36.6385	53.6544	0.6720
30	14	0.1333	36.4841	53.2883	0.6528
31	15	0.1290	36.4830	53.1538	0.6346
32	16	0.1250	36.5997	53.1974	0.6174
33	17	0.1212	36.8088	53.3812	0.6012
34	18	0.1176	37.0916	53.6772	0.5857
35	19	0.1143	37.4343	54.0642	0.5710
36	20	0.1111	37.8261	54.5263	0.5571

Table C.8 (continued)
Central Composite Designs - Minimum J_{PCA} and J_{PCMAX}

$k=5$ ($g=1/\sqrt{k}$, $\alpha=1$)

n	n_0	[ii]	J_{PCA}	J_{PCMAX}	D-efficiency
46	4	0.1826	154.3804	285.0650	0.9846
47	5	0.1787	96.3978	136.5835	0.9740
48	6	0.1750	72.5223	95.5941	0.9620
49	7	0.1714	60.0113	79.7376	0.9493
50	8	0.1680	52.4981	70.0991	0.9363
51	9	0.1647	47.5824	63.7277	0.9231
52	10	0.1615	44.1757	59.2718	0.9099
53	11	0.1585	41.7185	56.0302	0.8968
54	12	0.1556	39.8953	53.6049	0.8838
55	13	0.1527	38.5156	51.7539	0.8710
56	14	0.1500	37.4579	50.3219	0.8585
57	15	0.1474	36.6409	49.2048	0.8462
58	16	0.1448	36.0087	48.3300	0.8342
59	17	0.1424	35.5211	47.6458	0.8224
60	18	0.1400	35.1490	47.1142	0.8109
61	19	0.1377	34.8703	46.7065	0.7997
62	20	0.1355	34.6685	46.4010	0.7887
63	21	0.1333	34.5305	46.1804	0.7780
64	22	0.1312	34.4461	46.0316	0.7675
65	23	0.1292	34.4071	45.9435	0.7573
66	24	0.1273	34.4071	45.9077	0.7474
67	25	0.1254	34.4406	45.9169	0.7377
68	26	0.1235	34.5033	45.9653	0.7282

$k=5$ - 1/2 fraction of factorial ($g=1/\sqrt{k}$, $\alpha=1$)

n	n_0	[ii]	J_{PCA}	J_{PCMAX}	D-efficiency
30	4	0.1733	158.3653	200.1534	0.9463
31	5	0.1677	101.2030	129.3415	0.9256
32	6	0.1625	77.5775	99.6794	0.9045
33	7	0.1576	65.2221	84.0036	0.8836
34	8	0.1529	57.8549	74.5707	0.8630
35	9	0.1486	53.0931	68.4206	0.8431
36	10	0.1444	49.8512	64.1963	0.8238
37	11	0.1405	47.5689	61.1934	0.8052
38	12	0.1368	45.9293	59.0119	0.7872
39	13	0.1333	44.7403	57.4084	0.7700
40	14	0.1300	43.8792	56.2267	0.7534
41	15	0.1268	43.2638	55.3619	0.7374
42	16	0.1238	42.8372	54.7411	0.7221
43	17	0.1209	42.5586	54.3123	0.7073
44	18	0.1182	42.3983	54.0371	0.6931
45	19	0.1156	42.3340	53.8867	0.6795
46	20	0.1130	42.3485	53.8390	0.6663
47	21	0.1106	42.4288	53.8771	0.6537
48	22	0.1083	42.5641	53.9872	0.6415

Table C.9

Central Composite Designs - Minimum J_{PCA} and J_{PCMAX} For Designs With Given Sample Size and Power < 0.90 For $\alpha = 0.05$ Test

Design Region : Cuboidal   Region of Interest : Spherical

$k=2$ (g = 1, $\alpha = 1$)

n	n_0	[ii]	J_{PCA}	J_{PCMAX}	D_s-efficiency	D-efficiency
11	3	0.5455	35.7090	94.1444	0.9626	0.9026
12	4	0.5000	15.5160	32.0355	0.9266	0.8602
13	5	0.4615	10.7481	24.2373	0.8870	0.8195
14	6	0.4286	8.9207	21.2349	0.8473	0.7814
15	7	0.4000	8.0741	19.8989	0.8090	0.7462
16	8	0.3750	7.6602	19.3176	0.7728	0.7137
17	9	0.3529	7.4719	19.1371	0.7388	0.6839
18	10	0.3333	7.4153	19.1935	0.7071	0.6565

$k=3$ (g = 1, $\alpha \doteq 1$)

n	n_0	[ii]	J_{PCA}	J_{PCMAX}	D_s-efficiency	D-efficiency
17	3	0.5882	72.4166	258.8034	0.9054	0.8704
18	4	0.5556	29.7561	88.0640	0.8710	0.8360
19	5	0.5263	19.3305	47.6161	0.8376	0.8035
20	6	0.5000	15.1059	33.4224	0.8057	0.7730
21	7	0.4762	12.9569	29.6263	0.7754	0.7444
22	8	0.4545	11.7239	27.4812	0.7469	0.7178
23	9	0.4348	10.9682	26.2074	0.7200	0.6928
24	10	0.4167	10.4903	25.4459	0.6947	0.6696
25	11	0.4000	10.1876	25.0100	0.6710	0.6477
26	12	0.3846	10.0020	24.7932	0.6487	0.6273
27	13	0.3704	9.8984	24.7307	0.6277	0.6081
28	14	0.3571	9.8544	24.7809	0.6079	0.5901
29	15	0.3448	9.8550	24.9157	0.5893	0.5731
30	16	0.3333	9.8899	25.1157	0.5717	0.5571

Table C.9 (continued)
Central Composite Designs - Minimum J_{PCA} and J_{PCMAX}

$k=4$ (g= 1, α= 1)

n	n_0	[ii]	J_{PCA}	J_{PCMAX}	D_s-efficiency	D-efficiency
28	4	0.6429	50.6878	235.0764	0.8411	0.8380
29	5	0.6207	31.6193	129.2817	0.8184	0.8153
30	6	0.6000	23.7333	85.9291	0.7965	0.7934
31	7	0.5806	19.5991	63.1614	0.7754	0.7726
32	8	0.5625	17.1234	49.3736	0.7551	0.7526
33	9	0.5455	15.5130	40.2224	0.7357	0.7336
34	10	0.5294	14.4068	36.1199	0.7171	0.7155
35	11	0.5143	13.6186	34.6547	0.6993	0.6982
36	12	0.5000	13.0433	33.6159	0.6822	0.6816
37	13	0.4865	12.6170	32.8769	0.6659	0.6658
38	14	0.4737	12.2990	32.3567	0.6503	0.6507
39	15	0.4615	12.0621	32.0008	0.6353	0.6363
40	16	0.4500	11.8874	31.7715	0.6210	0.6225
41	17	0.4390	11.7616	31.6417	0.6073	0.6092
42	18	0.4286	11.6746	31.5915	0.5941	0.5966

$k=4$ - 1/2 fraction of factorial (g= 1, α= 1)

n	n_0	[ii]	J_{PCA}	J_{PCMAX}	D_s-efficiency	D-efficiency
20	4	0.5000	35.2539	118.9913	0.7507	0.7265
21	5	0.4762	22.8245	64.5805	0.7197	0.6972
22	6	0.4545	17.7267	42.4666	0.6909	0.6701
23	7	0.4348	15.0963	35.1562	0.6640	0.6450
24	8	0.4167	13.5588	31.9489	0.6391	0.6216
25	9	0.4000	12.5925	29.9368	0.6159	0.5999
26	10	0.3846	11.9595	28.6267	0.5942	0.5796
27	11	0.3704	11.5368	27.7622	0.5739	0.5607
28	12	0.3571	11.2551	27.1975	0.5549	0.5430
29	13	0.3448	11.0721	26.8439	0.5371	0.5263
30	14	0.3333	10.9608	26.6442	0.5204	0.5107
31	15	0.3226	10.9034	26.5602	0.5046	0.4960
32	16	0.3125	10.8873	26.5654	0.4898	0.4821
33	17	0.3030	10.9035	26.6406	0.4758	0.4690
34	18	0.2941	10.9455	26.7719	0.4625	0.4566
35	19	0.2857	11.0085	26.9488	0.4500	0.4449
36	20	0.2778	11.0887	27.1632	0.4381	0.4337

Table C.9 (continued)
Central Composite Designs - Minimum J_{PCA} and J_{PCMAX}

$k=5$ (g = 1, α = 1)

n	n_0	[ii]	J_{PCA}	J_{PCMAX}	D_s-efficiency	D-efficiency
46	4	0.7391	85.3845	594.6961	0.8178	0.8405
47	5	0.7234	51.9032	331.3274	0.8042	0.8263
48	6	0.7083	37.9392	222.4965	0.7908	0.8123
49	7	0.6939	30.5292	164.9392	0.7777	0.7987
50	8	0.6800	26.0193	129.8669	0.7648	0.7854
51	9	0.6667	23.0241	106.4554	0.7522	0.7725
52	10	0.6538	20.9126	89.8063	0.7398	0.7599
53	11	0.6415	19.3589	77.4045	0.7278	0.7477
54	12	0.6296	18.1789	67.8343	0.7162	0.7358
55	13	0.6182	17.2609	60.2409	0.7048	0.7243
56	14	0.6071	16.5334	54.0797	0.6937	0.7131
57	15	0.5965	15.9487	48.9875	0.6829	0.7022
58	16	0.5862	15.4736	44.7135	0.6724	0.6916
59	17	0.5763	15.0844	43.8683	0.6622	0.6813
60	18	0.5667	14.7639	43.2727	0.6522	0.6712
61	19	0.5574	14.4991	42.8010	0.6426	0.6615
62	20	0.5484	14.2799	42.4314	0.6331	0.6520
63	21	0.5397	14.0988	42.1468	0.6240	0.6428
64	22	0.5313	13.9496	41.9339	0.6151	0.6339
65	23	0.5231	13.8275	41.7819	0.6064	0.6252
66	24	0.5152	13.7286	41.6820	0.5979	0.6167
67	25	0.5075	13.6497	41.6272	0.5897	0.6084
68	26	0.5000	13.5882	41.6116	0.5816	0.6004

$k=5$ - 1/2 fraction of factorial (g = 1, α = 1)

n	n_0	[ii]	J_{PCA}	J_{PCMAX}	D_s-efficiency	D-efficiency
30	4	0.6000	53.5611	298.1942	0.7764	0.7706
31	5	0.5806	33.4073	164.9548	0.7543	0.7491
32	6	0.5625	25.0266	110.0539	0.7334	0.7286
33	7	0.5455	20.6072	81.0971	0.7134	0.7092
34	8	0.5294	17.9432	63.5012	0.6944	0.6907
35	9	0.5143	16.1968	51.7900	0.6763	0.6732
36	10	0.5000	14.9864	43.4878	0.6591	0.6564
37	11	0.4865	14.1144	37.7393	0.6427	0.6405
38	12	0.4737	13.4693	36.2949	0.6270	0.6253
39	13	0.4615	12.9833	35.2205	0.6120	0.6109
40	14	0.4500	12.6130	34.4159	0.5977	0.5970
41	15	0.4390	12.3294	33.8142	0.5841	0.5838
42	16	0.4286	12.1125	33.3687	0.5710	0.5711
43	17	0.4186	11.9479	33.0460	0.5585	0.5590
44	18	0.4091	11.8250	32.8216	0.5465	0.5474
45	19	0.4000	11.7359	32.6771	0.5350	0.5363
46	20	0.3913	11.6747	32.5984	0.5239	0.5256
47	21	0.3830	11.6366	32.5745	0.5133	0.5153
48	22	0.3750	11.6179	32.5968	0.5032	0.5055

Table C.10
Box-Behnken Designs - Minimum J_{PCA} and J_{PCMAX} For Designs With Given Sample Size and Power < 0.90 For $\alpha = 0.05$ Test
Design Region : Cuboidal Region of Interest : Cuboidal

$k=3$ (g=1)

n	n_0	[ii]	J_{PCA}	J_{PCMAX}	D_s-efficiency	D-efficiency
15	3	0.5333	99.0171	262.9427	0.7790	0.7723
16	4	0.5000	40.8820	79.3800	0.7580	0.7452
17	5	0.4706	27.1984	40.6271	0.7330	0.7172
18	6	0.4444	21.8615	30.5696	0.7069	0.6898
19	7	0.4211	19.2742	27.4472	0.6810	0.6636
20	8	0.4000	17.8855	25.7384	0.6558	0.6389
21	9	0.3810	17.1151	24.7761	0.6318	0.6157
22	10	0.3636	16.7018	24.2530	0.6091	0.5940
23	11	0.3478	16.5120	24.0090	0.5875	0.5736
24	12	0.3333	16.4706	23.9529	0.5672	0.5545
25	13	0.3200	16.5326	24.0292	0.5481	0.5366

$k=4$ (g=1)

n	n_0	[ii]	J_{PCA}	J_{PCMAX}	D_s-efficiency	D-efficiency
28	4	0.4286	102.4338	186.2390	0.4659	0.5073
29	5	0.4138	65.5830	94.0335	0.4583	0.4971
30	6	0.4000	50.5945	73.7251	0.4497	0.4864
31	7	0.3871	42.8804	63.0710	0.4405	0.4756
32	8	0.3750	38.3612	56.7314	0.4311	0.4649
33	9	0.3636	35.5001	52.6622	0.4217	0.4543
34	10	0.3529	33.6013	49.9252	0.4124	0.4441
35	11	0.3429	32.3072	48.0335	0.4033	0.4341
36	12	0.3333	31.4164	46.7100	0.3944	0.4245
37	13	0.3243	30.8073	45.7865	0.3857	0.4153
38	14	0.3158	30.4026	45.1546	0.3774	0.4063
39	15	0.3077	30.1506	44.7419	0.3693	0.3978
40	16	0.3000	30.0156	44.4979	0.3615	0.3895
41	17	0.2927	29.9721	44.3865	0.3539	0.3815
42	18	0.2857	30.0015	44.3812	0.3466	0.3739

Table C.10 (continued)
Box-Behnken Designs - Minimum J_{PCA} and J_{PCMAX}

$k=5$ (g=1)

n	n_0	[ii]	J_{PCA}	J_{PCMAX}	D_s-efficiency	D-efficiency
44	4	0.3636	235.9410	376.1972	0.2913	0.3396
45	5	0.3556	147.9900	207.4228	0.2886	0.3356
46	6	0.3478	111.5351	157.5886	0.2854	0.3312
47	7	0.3404	92.3385	131.0684	0.2818	0.3265
48	8	0.3333	80.7653	114.9437	0.2780	0.3217
49	9	0.3265	73.1679	104.2812	0.2741	0.3169
50	10	0.3200	67.8874	96.8213	0.2702	0.3122
51	11	0.3137	64.0681	91.3919	0.2662	0.3074
52	12	0.3077	61.2268	87.3276	0.2623	0.3028
53	13	0.3019	59.0709	84.2235	0.2584	0.2982
54	14	0.2963	57.4133	81.8201	0.2545	0.2937
55	15	0.2909	56.1289	79.9430	0.2507	0.2893
56	16	0.2857	55.1313	78.4714	0.2470	0.2850
57	17	0.2807	54.3585	77.3184	0.2434	0.2808
58	18	0.2759	53.7653	76.4206	0.2398	0.2767
59	19	0.2712	53.3177	75.7300	0.2363	0.2728
60	20	0.2667	52.9899	75.2102	0.2329	0.2689
61	21	0.2623	52.7616	74.8325	0.2296	0.2651
62	22	0.2581	52.6170	74.5747	0.2264	0.2614
63	23	0.2540	52.5434	74.4187	0.2232	0.2578
64	24	0.2500	52.5307	74.3499	0.2201	0.2543

Table C.11

Box-Behnken Designs - Minimum J_{PCA} and J_{PCMAX} For Designs With Given Sample Size and Power < 0.90 For $\alpha = 0.05$ Test

Design Region : Spherical   Region of Interest : Spherical

$k=3$ $(g = 1/\sqrt{2})$

n	n_0	[ii]	J_{PCA}	J_{PCMAX}	D-efficiency
15	3	0.2667	125.3791	230.9081	0.9382
16	4	0.2500	54.4813	104.7706	0.9053
17	5	0.2353	37.3223	72.9049	0.8712
18	6	0.2222	30.5318	59.9003	0.8380
19	7	0.2105	27.2195	53.3699	0.8062
20	8	0.2000	25.4442	49.7476	0.7762
21	9	0.1905	24.4702	47.6608	0.7480
22	10	0.1818	23.9629	46.4776	0.7215
23	11	0.1739	23.7498	45.8685	0.6968
24	12	0.1667	23.7334	45.6460	0.6736
25	13	0.1600	23.8548	45.6958	0.6518

$k=4$ $(g = 1/\sqrt{2})$

n	n_0	[ii]	J_{PCA}	J_{PCMAX}	D-efficiency
28	4	0.2143	93.1954	137.7375	0.9718
29	5	0.2069	60.0446	71.5807	0.9523
30	6	0.2000	46.5467	56.3772	0.9318
31	7	0.1935	39.6001	48.4144	0.9111
32	8	0.1875	35.5350	43.6874	0.8905
33	9	0.1818	32.9670	40.6633	0.8703
34	10	0.1765	31.2687	38.6384	0.8507
35	11	0.1714	30.1173	37.2473	0.8317
36	12	0.1667	29.3309	36.2825	0.8133
37	13	0.1622	28.7996	35.6176	0.7955
38	14	0.1579	28.4536	35.1715	0.7784
39	15	0.1538	28.2459	34.8897	0.7620
40	16	0.1500	28.1442	34.7345	0.7461
41	17	0.1463	28.1257	34.6788	0.7309
42	18	0.1429	28.1733	34.7026	0.7162

Table C.11 (continued)
Box-Behnken Designs - Minimum J_{PCA} and J_{PCMAX}

$k=5$ $(g=1/\sqrt{2})$

n	n_0	[ii]	J_{PCA}	J_{PCMAX}	D-efficiency
44	4	0.1818	156.8755	269.1327	0.9750
45	5	0.1778	98.2003	128.9410	0.9635
46	6	0.1739	74.0175	91.8483	0.9508
47	7	0.1702	61.3415	76.7236	0.9374
48	8	0.1667	53.7306	67.5392	0.9238
49	9	0.1633	48.7539	61.4762	0.9100
50	10	0.1600	45.3086	57.2431	0.8963
51	11	0.1569	42.8274	54.1704	0.8827
52	12	0.1538	40.9902	51.8777	0.8693
53	13	0.1509	39.6037	50.1337	0.8562
54	14	0.1481	38.5444	48.7900	0.8433
55	15	0.1455	37.7299	47.7472	0.8307
56	16	0.1429	37.1033	46.9360	0.8184
57	17	0.1404	36.6240	46.3070	0.8063
58	18	0.1379	36.2620	45.8237	0.7946
59	19	0.1356	35.9952	45.4588	0.7831
60	20	0.1333	35.8065	45.1915	0.7720
61	21	0.1311	35.6829	45.0055	0.7611
62	22	0.1290	35.6139	44.8879	0.7505
63	23	0.1270	35.5911	44.8285	0.7401
64	24	0.1250	35.6080	44.8190	0.7300

Table C.12
Box-Behnken Designs - Minimum J_{PCA} and J_{PCMAX} For Designs With Given Sample Size and Power < 0.90 For $\alpha = 0.05$ Test
Design Region : Cuboidal   Region of Interest : Spherical

$k=3$ (g= 1)

n	n_0	[ii]	J_{PCA}	J_{PCMAX}	D_s-efficiency	D-efficiency
15	3	0.5333	82.4575	445.5840	0.7790	0.7723
16	4	0.5000	29.5226	132.0811	0.7580	0.7452
17	5	0.4706	17.6791	64.8219	0.7330	0.7172
18	6	0.4444	13.1559	39.6218	0.7069	0.6898
19	7	0.4211	10.9551	27.3362	0.6810	0.6636
20	8	0.4000	9.7374	20.3701	0.6558	0.6389
21	9	0.3810	9.0148	16.0211	0.6318	0.6157
22	10	0.3636	8.5722	13.1944	0.6091	0.5940
23	11	0.3478	8.3020	13.0796	0.5875	0.5736
24	12	0.3333	8.1445	13.0615	0.5672	0.5545
25	13	0.3200	8.0646	13.1115	0.5481	0.5366

$k=4$ (g= 1)

n	n_0	[ii]	J_{PCA}	J_{PCMAX}	D_s-efficiency	D-efficiency
28	4	0.4286	56.9960	421.9941	0.4659	0.5073
29	5	0.4138	32.0514	204.3381	0.4583	0.4971
30	6	0.4000	22.4722	123.2349	0.4497	0.4864
31	7	0.3871	17.7250	83.8234	0.4405	0.4756
32	8	0.3750	15.0065	61.4756	0.4311	0.4649
33	9	0.3636	13.3020	47.4655	0.4217	0.4543
34	10	0.3529	12.1674	38.0442	0.4124	0.4441
35	11	0.3429	11.3808	31.3737	0.4033	0.4341
36	12	0.3333	10.8206	26.4619	0.3944	0.4245
37	13	0.3243	10.4153	22.7326	0.3857	0.4153
38	14	0.3158	10.1199	19.8309	0.3774	0.4063
39	15	0.3077	9.9053	17.5280	0.3693	0.3978
40	16	0.3000	9.7515	15.6705	0.3615	0.3895
41	17	0.2927	9.6446	14.1520	0.3539	0.3815
42	18	0.2857	9.5745	12.8967	0.3466	0.3739

Table C.12 (continued)
Box-Behnken Designs - Minimum J_{PCA} and J_{PCMAX}

$k=5$ (g= 1)

n	n_0	[ii]	J_{PCA}	J_{PCMAX}	D_s-efficiency	D-efficiency
44	4	0.3636	96.0190	1005.1715	0.2913	0.3396
45	5	0.3556	52.7505	483.5712	0.2886	0.3356
46	6	0.3478	36.0876	289.9514	0.2854	0.3312
47	7	0.3404	27.7811	196.2040	0.2818	0.3265
48	8	0.3333	22.9785	143.2133	0.2780	0.3217
49	9	0.3265	19.9252	110.0747	0.2741	0.3169
50	10	0.3200	17.8533	87.8258	0.2702	0.3122
51	11	0.3137	16.3803	72.0829	0.2662	0.3074
52	12	0.3077	15.2964	60.4851	0.2623	0.3028
53	13	0.3019	14.4780	51.6644	0.2584	0.2982
54	14	0.2963	13.8482	44.7808	0.2545	0.2937
55	15	0.2909	13.3566	39.2937	0.2507	0.2893
56	16	0.2857	12.9690	34.8416	0.2470	0.2850
57	17	0.2807	12.6615	31.1748	0.2434	0.2808
58	18	0.2759	12.4169	28.1159	0.2398	0.2767
59	19	0.2712	12.2225	25.5357	0.2363	0.2728
60	20	0.2667	12.0689	23.3385	0.2329	0.2689
61	21	0.2623	11.9486	21.4516	0.2296	0.2651
62	22	0.2581	11.8561	19.8194	0.2264	0.2614
63	23	0.2540	11.7868	18.3984	0.2232	0.2578
64	24	0.2500	11.7372	17.1541	0.2201	0.2543

Table C.13
Small Composite Designs - Minimum J_{PCA} and J_{PCMAX} For Designs With Given Sample Size and Power $<$ 0.90 For $\alpha = 0.05$ Test
Design Region : Cuboidal Region of Interest : Cuboidal

$k=3$ ($g=1$, $\alpha=1$)

n	n_0	[ii]	J_{PCA}	J_{PCMAX}	D_s-efficiency	D-efficiency
13	3	0.4615	303.7775	674.5472	0.4534	0.5345
14	4	0.4286	137.3482	305.1574	0.4280	0.5050
15	5	0.4000	95.4995	211.7348	0.4048	0.4783
16	6	0.3750	78.5444	173.6554	0.3836	0.4542
17	7	0.3529	70.1278	154.6012	0.3642	0.4324
18	8	0.3333	65.5448	144.1019	0.3466	0.4126
19	9	0.3158	62.9853	138.1237	0.3305	0.3945
20	10	0.3000	61.6160	134.8069	0.3157	0.3780
21	11	0.2857	61.0029	133.1823	0.3022	0.3628
22	12	0.2727	60.8989	132.6978	0.2897	0.3488
23	13	0.2609	61.1535	133.0165	0.2782	0.3359
24	14	0.2500	61.6699	133.9218	0.2675	0.3240
25	15	0.2400	62.3829	135.2682	0.2576	0.3129

$k=4$ ($g=1$, $\alpha=1$)

n	n_0	[ii]	J_{PCA}	J_{PCMAX}	D_s-efficiency	D-efficiency
20	4	0.5000	106.6664	190.8337	0.6275	0.6447
21	5	0.4762	70.9130	126.7767	0.6015	0.6187
22	6	0.4545	56.1301	100.1566	0.5774	0.5946
23	7	0.4348	48.4868	86.3158	0.5550	0.5723
24	8	0.4167	44.0331	78.1948	0.5342	0.5516
25	9	0.4000	41.2573	73.0872	0.5147	0.5323
26	10	0.3846	39.4658	69.7494	0.4966	0.5143
27	11	0.3704	38.2985	67.5351	0.4797	0.4975
28	12	0.3571	37.5508	66.0766	0.4638	0.4818
29	13	0.3448	37.0981	65.1502	0.4489	0.4670
30	14	0.3333	36.8607	64.6120	0.4349	0.4532
31	15	0.3226	36.7849	64.3655	0.4218	0.4401
32	16	0.3125	36.8335	64.3438	0.4094	0.4278
33	17	0.3030	36.9798	64.4988	0.3976	0.4162
34	18	0.2941	37.2043	64.7951	0.3866	0.4052
35	19	0.2857	37.4923	65.2062	0.3761	0.3948
36	20	0.2778	37.8326	65.7120	0.3662	0.3849

Table C.14
Small Composite Designs - Minimum J_{PCA} and J_{PCMAX} For Designs With Given Sample Size and Power $<$ 0.90 For $\alpha = 0.05$ Test
Design Region : Spherical   Region of Interest : Spherical

$k=3$ $(g = 1/\sqrt{k}, \alpha = 1)$

n	n_0	[ii]	J_{PCA}	J_{PCMAX}	D-efficiency
13	3	0.2564	236.7053	511.3970	0.7776
14	4	0.2381	105.8014	231.9207	0.7432
15	5	0.2222	73.3737	161.2785	0.7093
16	6	0.2083	60.3796	132.5163	0.6772
17	7	0.1961	54.0000	118.1513	0.6472
18	8	0.1852	50.5737	110.2600	0.6195
19	9	0.1754	48.6999	105.7899	0.5939
20	10	0.1667	47.7361	103.3339	0.5701
21	11	0.1587	47.3490	102.1584	0.5482
22	12	0.1515	47.3492	101.8456	0.5278
23	13	0.1449	47.6217	102.1407	0.5089
24	14	0.1389	48.0925	102.8796	0.4914
25	15	0.1333	48.7123	103.9523	0.4750

$k=4$ $(g = 1/\sqrt{k}, \alpha = 1)$

n	n_0	[ii]	J_{PCA}	J_{PCMAX}	D-efficiency
20	4	0.2000	132.9837	269.0040	0.8431
21	5	0.1905	87.8675	178.4000	0.8150
22	6	0.1818	69.3800	140.7349	0.7875
23	7	0.1739	59.8886	121.1409	0.7610
24	8	0.1667	54.3934	109.6353	0.7358
25	9	0.1600	50.9909	102.3908	0.7120
26	10	0.1538	48.8116	97.6489	0.6894
27	11	0.1481	47.4057	94.4958	0.6681
28	12	0.1429	46.5183	92.4115	0.6480
29	13	0.1379	45.9948	91.0795	0.6290
30	14	0.1333	45.7362	90.2966	0.6111
31	15	0.1290	45.6762	89.9263	0.5941
32	16	0.1250	45.7688	89.8737	0.5780
33	17	0.1212	45.9812	90.0709	0.5627
34	18	0.1176	46.2894	90.4680	0.5483
35	19	0.1143	46.6751	91.0276	0.5345
36	20	0.1111	47.1247	91.7208	0.5215

Table C.15
Small Composite Designs - Minimum J_{PCA} and J_{PCMAX} For Designs With Given Sample Size and Power < 0.90 For $\alpha = 0.05$ Test
Design Region : Cuboidal Region of Interest : Spherical

$k=3$ ($g=1$, $\alpha=1$)

n	n_0	[ii]	J_{PCA}	J_{PCMAX}	D_s-efficiency	D-efficiency
13	3	0.4615	158.3214	306.4765	0.4534	0.5345
14	4	0.4286	70.3104	139.1448	0.4280	0.5050
15	5	0.4000	48.3404	96.8431	0.4048	0.4783
16	6	0.3750	39.4546	79.6153	0.3836	0.4542
17	7	0.3529	35.0327	71.0071	0.3642	0.4324
18	8	0.3333	32.6074	66.2747	0.3466	0.4126
19	9	0.3158	31.2331	63.5907	0.3305	0.3945
20	10	0.3000	30.4756	62.1125	0.3157	0.3780
21	11	0.2857	30.1093	61.4010	0.3022	0.3628
22	12	0.2727	30.0060	61.2059	0.2897	0.3488
23	13	0.2609	30.0877	61.3748	0.2782	0.3359
24	14	0.2500	30.3043	61.8095	0.2675	0.3240
25	15	0.2400	30.6222	62.4439	0.2576	0.3129

$k=4$ ($g=1$, $\alpha=1$)

n	n_0	[ii]	J_{PCA}	J_{PCMAX}	D_s-efficiency	D-efficiency
20	4	0.5000	49.2998	118.9913	0.6275	0.6447
21	5	0.4762	32.0533	64.5805	0.6015	0.6187
22	6	0.4545	24.9478	42.4666	0.5774	0.5946
23	7	0.4348	21.2687	35.1562	0.5550	0.5723
24	8	0.4167	19.1118	31.9489	0.5342	0.5516
25	9	0.4000	17.7521	29.9368	0.5147	0.5323
26	10	0.3846	16.8586	28.6267	0.4966	0.5143
27	11	0.3704	16.2598	27.7622	0.4797	0.4975
28	12	0.3571	15.8586	27.1975	0.4638	0.4818
29	13	0.3448	15.5960	26.8439	0.4489	0.4670
30	14	0.3333	15.4344	26.6442	0.4349	0.4532
31	15	0.3226	15.3485	26.5602	0.4218	0.4401
32	16	0.3125	15.3207	26.5654	0.4094	0.4278
33	17	0.3030	15.3385	26.6406	0.3976	0.4162
34	18	0.2941	15.3928	26.7719	0.3866	0.4052
35	19	0.2857	15.4767	26.9488	0.3761	0.3948
36	20	0.2778	15.5848	27.1632	0.3662	0.3849

Table C.16
Notz Type Designs - Minimum J_{PCA} and J_{PCMAX} For Designs With Given Sample Size and Power < 0.90 For $\alpha = 0.05$ Test
Design Region : Cuboidal Region of Interest : Cuboidal

$k=3$ ($g=1$, $\alpha=1$)

n	n_0	[ii]	J_{PCA}	J_{PCMAX}	D_s-efficiency	D-efficiency
14	3	0.6429	143.5098	391.6120	0.8249	0.8433
15	4	0.6000	62.3651	176.6775	0.7888	0.8043
16	5	0.5625	42.3760	122.2979	0.7534	0.7675
17	6	0.5294	34.3460	100.0759	0.7197	0.7334
18	7	0.5000	30.3610	88.8997	0.6880	0.7017
19	8	0.4737	28.1734	82.6875	0.6584	0.6726
20	9	0.4500	26.9272	79.0976	0.6309	0.6456
21	10	0.4286	26.2310	77.0509	0.6053	0.6207
22	11	0.4091	25.8824	75.9851	0.5815	0.5976
23	12	0.3913	25.7668	75.5800	0.5594	0.5761
24	13	0.3750	25.8147	75.6403	0.5388	0.5562
25	14	0.3600	25.9814	76.0405	0.5196	0.5376

$k=4$ ($g=1$, $\alpha=1$)

n	n_0	[ii]	J_{PCA}	J_{PCMAX}	D_s-efficiency	D-efficiency
19	4	0.6316	140.0998	365.7610	0.6328	0.6833
20	5	0.6000	92.0232	242.1681	0.6072	0.6560
21	6	0.5714	72.2116	190.7666	0.5831	0.6304
22	7	0.5455	61.9830	164.0256	0.5604	0.6066
23	8	0.5217	56.0214	148.3085	0.5392	0.5843
24	9	0.5000	52.2979	138.4157	0.5193	0.5636
25	10	0.4800	49.8843	131.9387	0.5008	0.5442
26	11	0.4615	48.2994	127.6325	0.4834	0.5261
27	12	0.4444	47.2706	124.7876	0.4671	0.5092
28	13	0.4286	46.6323	122.9614	0.4518	0.4933
29	14	0.4138	46.2783	121.8909	0.4374	0.4783
30	15	0.4000	46.1374	121.3889	0.4239	0.4643
31	16	0.3871	46.1604	121.3146	0.4111	0.4510
32	17	0.3750	46.3121	121.5831	0.3991	0.4385
33	18	0.3636	46.5666	122.1242	0.3877	0.4267

Table C.17
Notz Type Designs - Minimum J_{PCA} and J_{PCMAX} For Designs With Given Sample Size and Power < 0.90 For $\alpha = 0.05$ Test
Design Region : Spherical   Region of Interest : Spherical

$k=3$ ($g=1/\sqrt{k}$, $\alpha=1$)

n	n_0	[ii]	J_{PCA}	J_{PCMAX}	D-efficiency
14	3	0.2619	160.4562	371.6201	0.8725
15	4	0.2444	71.0067	168.2507	0.8381
16	5	0.2292	49.1065	116.8381	0.8035
17	6	0.2157	40.3948	95.8612	0.7701
18	7	0.2037	36.1415	85.3390	0.7387
19	8	0.1930	33.8692	79.5152	0.7092
20	9	0.1833	32.6343	76.1736	0.6817
21	10	0.1746	32.0056	74.2928	0.6561
22	11	0.1667	31.7602	73.3406	0.6323
23	12	0.1594	31.7717	73.0138	0.6101
24	13	0.1528	31.9633	73.1277	0.5894
25	14	0.1467	32.2862	73.5634	0.5700

$k=4$ ($g=1/\sqrt{k}$, $\alpha=1$)

n	n_0	[ii]	J_{PCA}	J_{PCMAX}	D-efficiency
19	4	0.1974	180.1491	427.9495	0.7585
20	5	0.1875	119.7223	283.7078	0.7313
21	6	0.1786	94.8802	223.7354	0.7050
22	7	0.1705	82.1090	192.5400	0.6799
23	8	0.1630	74.7158	174.2485	0.6562
24	9	0.1563	70.1455	162.7422	0.6338
25	10	0.1500	67.2283	155.2245	0.6127
26	11	0.1442	65.3580	150.2343	0.5929
27	12	0.1389	64.1905	146.9564	0.5743
28	13	0.1339	63.5169	144.8804	0.5567
29	14	0.1293	63.2030	143.6675	0.5402
30	15	0.1250	63.1592	143.1251	0.5246
31	16	0.1210	63.3231	143.0858	0.5099
32	17	0.1172	63.6501	143.4450	0.4959
33	18	0.1136	64.1075	144.1243	0.4827

Table C.18
Notz Type Designs - Minimum J_{PCA} and J_{PCMAX} For Designs With Given Sample Size and Power < 0.90 For $\alpha = 0.05$ Test
Design Region : Cuboidal   Region of Interest : Spherical

$k=3$ (g= 1, α= 1)

n	n_0	[ii]	J_{PCA}	J_{PCMAX}	D_s-efficiency	D-efficiency
14	3	0.6429	108.3271	314.2793	0.8249	0.8433
15	4	0.6000	44.5081	113.5644	0.7888	0.8043
16	5	0.5625	29.0539	78.7033	0.7534	0.7675
17	6	0.5294	22.8650	64.4539	0.7197	0.7334
18	7	0.5000	19.7670	57.2847	0.6880	0.7017
19	8	0.4737	18.0285	53.2974	0.6584	0.6726
20	9	0.4500	16.9961	50.9910	0.6309	0.6456
21	10	0.4286	16.3737	49.6737	0.6053	0.6207
22	11	0.4091	16.0089	48.9853	0.5815	0.5976
23	12	0.3913	15.8159	48.7204	0.5594	0.5761
24	13	0.3750	15.7430	48.7539	0.5388	0.5562
25	14	0.3600	15.7572	49.0053	0.5196	0.5376

$k=4$ (g= 1, α= 1)

n	n_0	[ii]	J_{PCA}	J_{PCMAX}	D_s-efficiency	D-efficiency
19	4	0.6316	72.7943	211.2199	0.6328	0.6833
20	5	0.6000	46.1898	113.3264	0.6072	0.6560
21	6	0.5714	35.3336	89.4222	0.5831	0.6304
22	7	0.5455	29.7463	76.9807	0.5604	0.6066
23	8	0.5217	26.4811	69.6721	0.5392	0.5843
24	9	0.5000	24.4236	65.0673	0.5193	0.5636
25	10	0.4800	23.0679	62.0589	0.5008	0.5442
26	11	0.4615	22.1535	60.0591	0.4834	0.5261
27	12	0.4444	21.5335	58.7363	0.4671	0.5092
28	13	0.4286	21.1192	57.8875	0.4518	0.4933
29	14	0.4138	20.8540	57.3973	0.4374	0.4783
30	15	0.4000	20.7003	57.1623	0.4239	0.4643
31	16	0.3871	20.6318	57.1302	0.4111	0.4510
32	17	0.3750	20.6301	57.2597	0.3991	0.4385
33	18	0.3636	20.6815	57.5142	0.3877	0.4267

Table C.19
Hybrid Designs - Minimum J_{PCA} and J_{PCMAX} For Designs With Given Sample Size and Power < 0.90 For $\alpha = 0.05$ Test
Design Region : Cuboidal Region of Interest : Cuboidal

Hybrid 310

n	n_0	[ii]	J_{PCA}	J_{PCMAX}	D_s-efficiency	D-efficiency
13	3	0.3119	193.6866	324.7064	0.3232	0.3879
14	4	0.2897	88.5364	146.1705	0.3078	0.3683
15	5	0.2704	62.3537	101.6547	0.2927	0.3501
16	6	0.2535	51.8873	83.7056	0.2786	0.3334
17	7	0.2385	46.7977	74.8289	0.2654	0.3180
18	8	0.2253	44.1173	70.0141	0.2532	0.3039
19	9	0.2134	42.7067	67.3395	0.2420	0.2909
20	10	0.2028	42.0420	65.9221	0.2316	0.2790
21	11	0.1931	41.8507	65.3030	0.2220	0.2681
22	12	0.1843	41.9779	65.2210	0.2131	0.2580
23	13	0.1763	42.3291	65.5172	0.2048	0.2486
24	14	0.1690	42.8438	66.0897	0.1972	0.2399

Hybrid 311A

n	n_0	[ii]	J_{PCA}	J_{PCMAX}	D_s-efficiency	D-efficiency
13	3	0.3077	226.4177	387.9108	0.2900	0.3619
14	4	0.2857	101.9399	176.9775	0.2790	0.3459
15	5	0.2667	71.1631	123.7459	0.2672	0.3301
16	6	0.2500	58.8812	102.1402	0.2555	0.3152
17	7	0.2353	52.8952	91.4064	0.2442	0.3012
18	8	0.2222	49.7204	85.5613	0.2336	0.2883
19	9	0.2105	48.0235	82.2998	0.2237	0.2764
20	10	0.2000	47.1931	80.5592	0.2144	0.2653
21	11	0.1905	46.9116	79.7856	0.2058	0.2551
22	12	0.1818	46.9989	79.6635	0.1978	0.2457
23	13	0.1739	47.3454	80.0004	0.1903	0.2369
24	14	0.1667	47.8807	80.6725	0.1833	0.2287

Hybrid 311B

n	n_0	[ii]	J_{PCA}	J_{PCMAX}	D_s-efficiency	D-efficiency
13	3	0.2564	369.7226	695.4559	0.1973	0.2720
14	4	0.2381	165.9630	315.6444	0.1898	0.2599
15	5	0.2222	115.2664	219.6822	0.1818	0.2481
16	6	0.2083	94.8898	180.6437	0.1738	0.2368
17	7	0.1961	84.8573	161.1739	0.1662	0.2264
18	8	0.1852	79.4511	150.5033	0.1589	0.2167
19	9	0.1754	76.4799	144.4829	0.1522	0.2077
20	10	0.1667	74.9375	141.1999	0.1459	0.1994
21	11	0.1587	74.3013	139.6576	0.1400	0.1917
22	12	0.1515	74.2741	139.2878	0.1346	0.1846
23	13	0.1449	74.6753	139.7442	0.1295	0.1780
24	14	0.1389	75.3887	140.8039	0.1247	0.1719

Table C.19 (continued)
Hybrid Designs - Minimum J_{PCA} and J_{PCMAX}

Hybrid 416A

n	n_0	[ii]	J_{PCA}	J_{PCMAX}	D_s-efficiency	D-efficiency
20	4	0.2148	366.5304	508.9650	0.1276	0.1758
21	5	0.2046	241.8834	337.1925	0.1232	0.1695
22	6	0.1953	190.3165	265.7815	0.1188	0.1634
23	7	0.1868	163.6005	228.6362	0.1147	0.1577
24	8	0.1790	147.9754	206.8172	0.1107	0.1524
25	9	0.1719	138.1795	193.0767	0.1070	0.1473
26	10	0.1653	131.8006	184.0809	0.1034	0.1425
27	11	0.1591	127.5871	178.0969	0.1001	0.1381
28	12	0.1534	124.8283	174.1394	0.0970	0.1338
29	13	0.1482	123.0924	171.6083	0.0940	0.1299
30	14	0.1432	122.1018	170.1180	0.0912	0.1261
31	15	0.1386	121.6710	169.4099	0.0885	0.1226
32	16	0.1343	121.6708	169.3042	0.0860	0.1192
33	17	0.1302	122.0088	169.6756	0.0836	0.1160
34	18	0.1264	122.6173	170.4224	0.0813	0.1130
35	19	0.1228	123.4454	171.4772	0.0792	0.1102
36	20	0.1193	124.4542	172.7854	0.0771	0.1075

Hybrid 416B

n	n_0	[ii]	J_{PCA}	J_{PCMAX}	D_s-efficiency	D-efficiency
20	4	0.2102	337.3317	466.9464	0.1326	0.1815
21	5	0.2002	222.8125	300.0872	0.1280	0.1750
22	6	0.1911	175.4670	236.7872	0.1235	0.1688
23	7	0.1828	150.9585	203.8751	0.1192	0.1629
24	8	0.1752	136.6401	184.5644	0.1151	0.1573
25	9	0.1682	127.6768	172.4192	0.1112	0.1521
26	10	0.1617	121.8522	164.4823	0.1075	0.1472
27	11	0.1557	118.0164	159.2169	0.1041	0.1426
28	12	0.1501	115.5167	155.7489	0.1008	0.1382
29	13	0.1450	113.9562	153.5460	0.0977	0.1341
30	14	0.1401	113.0802	152.2663	0.0948	0.1302
31	15	0.1356	112.7181	151.6805	0.0920	0.1266
32	16	0.1314	112.7514	151.6290	0.0894	0.1231
33	17	0.1274	113.0953	151.9975	0.0869	0.1198
34	18	0.1236	113.6874	152.7022	0.0846	0.1167
35	19	0.1201	114.4812	153.6800	0.0823	0.1138
36	20	0.1168	115.4409	154.8826	0.0802	0.1110

Table C.19 (continued)
Hybrid Designs - Minimum J_{PCA} and J_{PCMAX}

Hybrid 416C

n	n_0	[ii]	J_{PCA}	J_{PCMAX}	D_s-efficiency	D-efficiency
20	4	0.1976	384.0369	564.3146	0.1174	0.1646
21	5	0.1882	253.2477	351.9961	0.1133	0.1587
22	6	0.1797	199.1609	277.5164	0.1093	0.1531
23	7	0.1719	171.1457	238.7744	0.1055	0.1477
24	8	0.1647	154.7623	216.0285	0.1019	0.1427
25	9	0.1581	144.4907	201.7094	0.0984	0.1379
26	10	0.1520	137.8011	192.3350	0.0952	0.1335
27	11	0.1464	133.3811	186.1074	0.0921	0.1293
28	12	0.1412	130.4855	181.9936	0.0892	0.1253
29	13	0.1363	128.6616	179.3676	0.0865	0.1216
30	14	0.1318	127.6186	177.8273	0.0839	0.1181
31	15	0.1275	127.1620	177.1030	0.0814	0.1148
32	16	0.1235	127.1563	177.0070	0.0791	0.1116
33	17	0.1198	127.5050	177.4051	0.0769	0.1087
34	18	0.1163	128.1369	178.1985	0.0748	0.1059
35	19	0.1129	128.9987	179.3130	0.0729	0.1032
36	20	0.1098	130.0498	180.6888	0.0710	0.1006

Table C.20
Hybrid Designs - Minimum J_{PCA} and J_{PCMAX} For Designs With Given Sample Size and Power < 0.90 For $\alpha = 0.05$ Test
Design Region : Spherical Region of Interest : Spherical

Hybrid 310

n	n_0	[ii]	J_{PCA}	J_{PCMAX}	D-efficiency
13	3	0.2158	159.3617	420.5179	0.7668
14	4	0.2004	72.8835	189.9352	0.7282
15	5	0.1870	51.4004	131.9391	0.6922
16	6	0.1753	42.8349	108.4036	0.6590
17	7	0.1650	38.6849	96.6834	0.6286
18	8	0.1559	36.5121	90.2663	0.6008
19	9	0.1476	35.3810	86.6480	0.5752
20	10	0.1403	34.8614	84.6757	0.5517
21	11	0.1336	34.7299	83.7489	0.5300
22	12	0.1275	34.8594	83.5262	0.5100
23	13	0.1220	35.1724	83.7991	0.4914
24	14	0.1169	35.6192	84.4339	0.4742

Hybrid 311A

n	n_0	[ii]	J_{PCA}	J_{PCMAX}	D-efficiency
13	3	0.2462	122.1341	206.9597	0.8898
14	4	0.2286	54.5151	90.9279	0.8504
15	5	0.2133	38.0960	63.2156	0.8116
16	6	0.2000	31.6452	52.1889	0.7748
17	7	0.1882	28.5584	46.7791	0.7406
18	8	0.1778	26.9643	43.8685	0.7089
19	9	0.1684	26.1512	42.2703	0.6795
20	10	0.1600	25.7942	41.4414	0.6524
21	11	0.1524	25.7252	41.1003	0.6273
22	12	0.1455	25.8493	41.0871	0.6040
23	13	0.1391	26.1087	41.3047	0.5824
24	14	0.1333	26.4666	41.6906	0.5622

Hybrid 311B

n	n_0	[ii]	J_{PCA}	J_{PCMAX}	D-efficiency
13	3	0.2564	117.7045	180.9115	0.9345
14	4	0.2381	52.3036	83.3485	0.8931
15	5	0.2222	36.4644	58.7754	0.8523
16	6	0.2083	30.2493	48.8398	0.8138
17	7	0.1961	27.2766	43.9361	0.7778
18	8	0.1852	25.7408	41.2951	0.7445
19	9	0.1754	24.9562	39.8499	0.7136
20	10	0.1667	24.6099	39.1085	0.6851
21	11	0.1587	24.5402	38.8148	0.6588
22	12	0.1515	24.6559	38.8226	0.6343
23	13	0.1449	24.9014	39.0428	0.6116
24	14	0.1389	25.2413	39.4181	0.5905

Table C.20 (continued)
Hybrid Designs - Minimum J_{PCA} and J_{PCMAX}

Hybrid 416A

n	n_0	[ii]	J_{PCA}	J_{PCMAX}	D-efficiency
20	4	0.1867	113.6314	244.9257	0.8156
21	5	0.1778	75.8849	165.1309	0.7863
22	6	0.1697	60.3686	131.6032	0.7583
23	7	0.1623	52.4020	114.0835	0.7318
24	8	0.1556	47.8014	103.7924	0.7068
25	9	0.1494	44.9684	97.3285	0.6833
26	10	0.1436	43.1708	93.1299	0.6612
27	11	0.1383	42.0288	90.3685	0.6405
28	12	0.1334	41.3272	88.5786	0.6209
29	13	0.1288	40.9349	87.4775	0.6024
30	14	0.1245	40.7681	86.8727	0.5850
31	15	0.1205	40.7703	86.6540	0.5686
32	16	0.1167	40.9026	86.7214	0.5531
33	17	0.1132	41.1371	87.0176	0.5384
34	18	0.1098	41.4532	87.4997	0.5244
35	19	0.1067	41.8356	88.1296	0.5112
36	20	0.1037	42.2726	88.8872	0.4986

Hybrid 416B

n	n_0	[ii]	J_{PCA}	J_{PCMAX}	D-efficiency
20	4	0.1851	105.3513	183.5062	0.8599
21	5	0.1763	70.3730	122.2228	0.8290
22	6	0.1683	56.0176	96.8039	0.7996
23	7	0.1610	48.6590	83.6211	0.7717
24	8	0.1542	44.4177	75.9103	0.7454
25	9	0.1481	41.8123	71.0810	0.7206
26	10	0.1424	40.1648	67.9416	0.6973
27	11	0.1371	39.1236	65.8754	0.6754
28	12	0.1322	38.4893	64.5387	0.6548
29	13	0.1277	38.1410	63.7028	0.6354
30	14	0.1234	38.0008	63.2384	0.6170
31	15	0.1194	38.0168	63.0547	0.5997
32	16	0.1157	38.1530	63.0836	0.5833
33	17	0.1122	38.3835	63.2822	0.5678
34	18	0.1089	38.6893	63.6172	0.5531
35	19	0.1058	39.0563	64.0610	0.5392
36	20	0.1028	39.4736	64.5937	0.5259

Table C.20 (continued)
Hybrid Designs - Minimum J_{PCA} and J_{PCMAX}

Hybrid 416C

n	n_0	[ii]	J_{PCA}	J_{PCMAX}	D-efficiency
20	4	0.1854	105.0602	180.1981	0.8632
21	5	0.1766	70.1882	120.1443	0.8321
22	6	0.1686	55.8748	95.2279	0.8025
23	7	0.1612	48.5373	82.2991	0.7745
24	8	0.1545	44.3079	74.7301	0.7481
25	9	0.1483	41.7099	70.0000	0.7232
26	10	0.1426	40.0669	66.9193	0.6998
27	11	0.1374	39.0287	64.8974	0.6778
28	12	0.1324	38.3963	63.5848	0.6571
29	13	0.1279	38.0490	62.7710	0.6376
30	14	0.1236	37.9093	62.3216	0.6192
31	15	0.1196	37.9255	62.1458	0.6018
32	16	0.1159	38.0614	62.1772	0.5854
33	17	0.1124	38.2915	62.3781	0.5698
34	18	0.1091	38.5966	62.7114	0.5550
35	19	0.1060	38.9628	63.1526	0.5410
36	20	0.1030	39.3792	63.6791	0.5277

Table C.21
Hybrid Designs - Minimum J_{PCA} and J_{PCMAX} For Designs With Given Sample Size and Power < 0.90 For $\alpha = 0.05$ Test
Design Region : Cuboidal   Region of Interest : Spherical

Hybrid 310

n	n_0	[ii]	J_{PCA}	J_{PCMAX}	D_s-efficiency	D-efficiency
13	3	0.3119	86.8697	209.7824	0.3232	0.3879
14	4	0.2897	38.4424	93.1488	0.3078	0.3683
15	5	0.2704	26.6832	64.6421	0.2927	0.3501
16	6	0.2535	22.0585	53.2139	0.2786	0.3334
17	7	0.2385	19.8389	47.5715	0.2654	0.3180
18	8	0.2253	18.6854	44.5094	0.2532	0.3039
19	9	0.2134	18.0892	42.8038	0.2420	0.2909
20	10	0.2028	17.8180	41.8938	0.2316	0.2790
21	11	0.1931	17.7520	41.4883	0.2220	0.2681
22	12	0.1843	17.8234	41.4221	0.2131	0.2580
23	13	0.1763	17.9910	41.5944	0.2048	0.2486
24	14	0.1690	18.2285	41.9407	0.1972	0.2399

Hybrid 311A

n	n_0	[ii]	J_{PCA}	J_{PCMAX}	D_s-efficiency	D-efficiency
13	3	0.3077	89.9824	192.1668	0.2900	0.3619
14	4	0.2857	38.4415	64.0807	0.2790	0.3459
15	5	0.2667	26.2623	42.0073	0.2672	0.3301
16	6	0.2500	21.5482	34.4312	0.2555	0.3152
17	7	0.2353	19.3102	30.8600	0.2442	0.3012
18	8	0.2222	18.1571	28.9759	0.2336	0.2883
19	9	0.2105	17.5660	27.9590	0.2237	0.2764
20	10	0.2000	17.3005	27.4453	0.2144	0.2653
21	11	0.1905	17.2393	27.2487	0.2058	0.2551
22	12	0.1818	17.3141	27.2644	0.1978	0.2457
23	13	0.1739	17.4840	27.4292	0.1903	0.2369
24	14	0.1667	17.7226	27.7024	0.1833	0.2287

Hybrid 311B

n	n_0	[ii]	J_{PCA}	J_{PCMAX}	D_s-efficiency	D-efficiency
13	3	0.2564	117.7060	180.9145	0.1973	0.2720
14	4	0.2381	52.3044	83.3499	0.1898	0.2599
15	5	0.2222	36.4649	58.7763	0.1818	0.2481
16	6	0.2083	30.2498	48.8406	0.1738	0.2368
17	7	0.1961	27.2770	43.9368	0.1662	0.2264
18	8	0.1852	25.7412	41.2958	0.1589	0.2167
19	9	0.1754	24.9566	39.8505	0.1522	0.2077
20	10	0.1667	24.6103	39.1091	0.1459	0.1994
21	11	0.1587	24.5406	38.8154	0.1400	0.1917
22	12	0.1515	24.6563	38.8232	0.1346	0.1846
23	13	0.1449	24.9018	39.0434	0.1295	0.1780
24	14	0.1389	25.2417	39.4187	0.1247	0.1718

Table C.21 (continued)
Hybrid Designs - Minimum J_{PCA} and J_{PCMAX}

Hybrid 416A

n	n_0	[ii]	J_{PCA}	J_{PCMAX}	D_s-efficiency	D-efficiency
20	4	0.2148	88.0980	181.5988	0.1276	0.1758
21	5	0.2046	58.6073	124.3814	0.1232	0.1695
22	6	0.1953	46.5420	99.8379	0.1188	0.1634
23	7	0.1868	40.3715	86.8975	0.1147	0.1577
24	8	0.1790	36.8213	79.2737	0.1107	0.1524
25	9	0.1719	34.6436	74.4908	0.1070	0.1473
26	10	0.1653	33.2683	71.3757	0.1034	0.1425
27	11	0.1591	32.4002	69.3394	0.1001	0.1381
28	12	0.1534	31.8723	68.0263	0.0970	0.1338
29	13	0.1482	31.5829	67.2331	0.0940	0.1299
30	14	0.1432	31.4672	66.8144	0.0912	0.1261
31	15	0.1386	31.4817	66.6779	0.0885	0.1226
32	16	0.1343	31.5961	66.7594	0.0860	0.1192
33	17	0.1302	31.7891	67.0142	0.0836	0.1160
34	18	0.1264	32.0447	67.4102	0.0813	0.1130
35	19	0.1228	32.3511	67.9165	0.0792	0.1102
36	20	0.1193	32.6993	68.5150	0.0771	0.1075

Hybrid 416B

n	n_0	[ii]	J_{PCA}	J_{PCMAX}	D_s-efficiency	D-efficiency
20	4	0.2102	83.8791	143.0494	0.1326	0.1815
21	5	0.2002	55.7937	95.4301	0.1280	0.1750
22	6	0.1911	44.3217	75.7191	0.1235	0.1688
23	7	0.1828	38.4637	65.5062	0.1192	0.1629
24	8	0.1752	35.0990	59.5397	0.1151	0.1573
25	9	0.1682	33.0397	55.8105	0.1112	0.1521
26	10	0.1617	31.7430	53.3945	0.1075	0.1472
27	11	0.1557	30.9281	51.8138	0.1041	0.1426
28	12	0.1501	30.4363	50.7917	0.1008	0.1382
29	13	0.1450	30.1709	50.1640	0.0977	0.1341
30	14	0.1401	30.0703	49.8233	0.0948	0.1302
31	15	0.1356	30.0933	49.6971	0.0920	0.1266
32	16	0.1314	30.2111	49.7417	0.0894	0.1231
33	17	0.1274	30.4033	49.9145	0.0869	0.1198
34	18	0.1236	30.6549	50.1933	0.0846	0.1167
35	19	0.1201	30.9547	50.5580	0.0823	0.1138
36	20	0.1168	31.2942	50.9864	0.0802	0.1110

Table C.21 (continued)
Hybrid Designs - Minimum J_{PCA} and J_{PCMAX}

Hybrid 416C

n	n_0	[ii]	J_{PCA}	J_{PCMAX}	D_s-efficiency	D-efficiency
20	4	0.1976	93.4907	158.9163	0.1174	0.1646
21	5	0.1882	62.3556	106.0865	0.1133	0.1587
22	6	0.1797	49.6040	84.1666	0.1093	0.1531
23	7	0.1719	43.0791	72.7979	0.1055	0.1477
24	8	0.1647	39.3247	66.1459	0.1019	0.1427
25	9	0.1581	37.0229	61.9887	0.0984	0.1379
26	10	0.1520	35.5706	59.2877	0.0952	0.1335
27	11	0.1464	34.6559	57.5192	0.0921	0.1293
28	12	0.1412	34.1016	56.3747	0.0892	0.1253
29	13	0.1363	33.8004	55.6694	0.0865	0.1216
30	14	0.1318	33.6834	55.2846	0.0839	0.1181
31	15	0.1275	33.7046	55.1407	0.0814	0.1148
32	16	0.1235	33.8320	55.1786	0.0791	0.1116
33	17	0.1198	34.0427	55.3661	0.0769	0.1087
34	18	0.1163	34.3200	55.6702	0.0748	0.1059
35	19	0.1129	34.6513	56.0659	0.0729	0.1032
36	20	0.1098	35.0270	56.5429	0.0710	0.1006

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