# ROBUST RESPONSE SURFACE DESIGNS AGAINST MISSING OBSERVATIONS

by

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# ABSTRACT

Even though an experiment is carefully planned, some observations may be lost during the process of collecting data or may be suspicious in some way. Missing observations can be the result from many causes, for example, the loss of experimental units and miscoded data where their correct values are non-trackable. The risk of losing observations usually cannot be ignored in practice. When small response surface designs are used, the effects of missing points may be substantial. The ability to estimate all parameters could be completely lost, or the variances of predicted responses could be incredibly large in a certain part of an experimental region. With respect to design optimality, designs will usually no longer be optimal when missing values exist.

The robustness against a missing value of several standard response surface designs has been studied via newly proposed measures. The designs include central composite designs (CCDs), small composite designs (SCDs), hybrid designs, and exact alphabetic optimal designs. In addition, an R package has been developed to visualize the effect of missing data. The behaviors of $D$-, $A$-, $G$-, and $IV$-efficiencies for CCDs are studied, and the axial distance that makes a spherical CCD more robust to a missing point is found via a numerical search. Results show that the axial distance obtained from Min $D$ criterion is the largest and respectively followed by Min $G$, Min $IV$, and Min $A$.

The $D$-, $A$-, $G$-, and $IV$-optimality criteria, as well as the point-exchange algorithm, are modified for constructing optimal robust exact designs. The resulting robust exact designs are compared to existing optimal exact designs to observe how resulting designs are robust to a missing point. It is observed that $D$- and $IV$-optimal robust designs are slightly less optimal but their robustness properties are appreciably improved. The robustness of $G$-optimal robust designs is usually slightly improved but with considerable loss in design efficiency. The same robust optimality criteria are also applied to construct optimal robust exact mixture designs. Finally, the adaptive designs are introduced. This allows experimenters to change design points once a missing value occurs during experimentation.

# CHAPTER 1

# INTRODUCTION

## 1. Overview of Response Surface Methodology

Response Surface Methodology (RSM) is an efficient tool consisting of a series of experimental designs, analysis of data, and optimization. This tool plays an important role in the design, development, formulation of new products, and improvement of existing product designs. RSM was originated by Box and Wilson (1951), and then by Box (1952, 1954). Although published papers involving RSM have been largely found in the chemical and food industries, more recently RSM has been employed in other disciplines, e.g., Moberg et al. (2005) applied RSM to tandem mass spectrometric fragmentation data and Gandhi and Kumaran (2014) used RSM to optimize a biodiesel data study. A goal of response surface methodology (RSM) is to seek the factor settings, which can be varied over a continuous region, that maximize or minimize a single response or multiple responses. RSM is conventionally divided into three stages or phases. First, active factors or independent variables will be identified among a wider set of possible controllable factors by conducting a screening experiment usually requiring a small number of experimental runs or tests. Second, sequential experimentation is conducted to find a path to a new region where the process is improved using an optimization technique like the method of steepest ascent. Implementation of this method involves running an experiment and fitting a first-order model and a test for curvature. If the lack-of-fit test for curvature indicates no problem, then there is a “better” region of experimentation to be explored. The process variables are adjusted, and a new experiment is conducted. This stage is continually repeated until the aforementioned test of curvature indicates the first-order model is inadequate due to a significant lack-of-fit. Then, an experiment is run in the final stage in which the process variable region is expected to contain an optimum response and a second-order empirical model will be fitted to determine the optimum settings.

The process or system involves the single response $y$ and $k$ controllable independent variables $\varphi_1, \varphi_2, \ldots, \varphi_k$, and $N$ experimental runs are conducted. Assume there is a true relationship between the $\varphi$'s and $y$ of the form

$$y = g(\varphi_1, \varphi_2, \ldots, \varphi_k) + \epsilon,$$

where function $g$ is unknown and directly inaccessible to experimenters and $\epsilon$ is the error term, often assumed to be normally distributed with mean zero and some constant variance. The true relationship between the response and predictors, which is typically complex and not known, can be approximated by an empirical model within a constrained experimental region. The approximating function usually is a low-order polynomial function which is based on the Taylor series expansion of $g$ and is also a linear regression function whose parameters are estimated by the least squares criterion. Once the empirical model is fitted and model assumptions are satisfied, a researcher can characterize the process over a region of experimentation.

The second-order model is the most popular choice of a model to approximate the true relationship between the response and predictors because: (1) it is found to be successful in much of the published case study literature; (2) the fitted surface has a simple interpretation with respect to the maximum, minimum, and saddle points; and (3) the experimental region of interest is usually small enough to use the second-order model as an approximating function (Myers et al., 2009). This RSM situation in which second-order designs play a role is where our research begins. It is important to note that designs for second-order models, or simply, second-order designs, are not used to explore active factors but, rather, they are used in the last stage where all active factors are known or assumed to be important. Furthermore, we assume that the second-order model is sufficient in a small region in which the optimal point occurs, so that if necessary, saturated or near-saturated designs can be used despite having few to no degrees of freedom left to perform a lack-of-fit test. The analysis and optimization of second-order models are not of interest in the dissertation. The focus is on the problem of selecting the points in an experimental region to estimate all model parameters for a second-order model and simultaneously satisfy particular criteria, e.g., robustness to missing data, orthogonality, and minimizing the generalized variances.

Suppose there are $N$ experimental design points, $k$ independent variables, and original-unit variables $\varphi_1, \varphi_2, \ldots, \varphi_k$, usually scaled into a unitless value in order to apply general principles of a design and also make an interpretation of experimental results easier. The most commonplace coding convention is an orthogonal coding which is defined as

$$x_{iu} = \frac{\varphi_{iu} - M_i}{R_i/2}, \;\; i = 1, 2, \ldots, k, \;\; \text{and } u = 1, 2, \ldots, N,$$

where

$$M_i = \frac{\min\limits_u(\varphi_{iu}) + \max\limits_u(\varphi_{iu})}{2},$$

and

$$R_i = \max_u(\varphi_{iu}) - \min_u(\varphi_{iu}).$$

This coding will map the highest, midpoint, and lowest values to $1, 0$, and $-1$, respectively (del Castillo, 2007). Another coding suggested by Box (1952) and Box and

Hunter (1957) is to standardize original variables as

$$x_{iu} = \frac{\varphi_{iu} - \bar{\varphi}_i}{S_i},$$

where

$$\bar{\varphi}_i = \frac{\sum_{u=1}^{N} \varphi_{iu}}{N}, \quad \text{and } S_i = \left\{ \sum_{u=1}^{N} \frac{(\varphi_{iu} - \bar{\varphi}_i)^2}{N} \right\}^{1/2},$$

$i = 1, 2, \ldots, k, \;\; u = 1, 2, \ldots, N$. This coding results in

$$\sum_{u=1}^{N} x_{iu} = 0 \quad \text{and} \quad \sum_{u=1}^{N} x_{iu}^2 = N.$$

This coding is less popular than the orthogonal coding because resulting scaled variables do not lie between $-1$ and $+1$ for which values of variables in most response surface designs are usually coded.

The second-order model is a polynomial having the form

$$y = \beta + \sum_{i=1}^{k} \beta_i x_i + \sum_{i=1}^{k} \beta_{ii} x_i^2 + \sum_{\substack{i=1 \\ j>i}}^{k} \sum_{j=1}^{k} \beta_{ij} x_i x_j + \epsilon, \tag{1.1}$$

where $k$ is the number of factors, $y$ is the response, $x_i$ is the level or value of factor $i$, $\beta_i$ is the $i$th parameter to be estimated, $i = 1, 2, \ldots, p$, and $\epsilon$ is an error term. This model has $p = (k+1)(k+2)/2$ coefficients and each controllable factor must have at least 3 levels. Also the number of distinct experimental design points must be at least $p$. The form of the second-order model in matrix notation is

$$y = \beta_0 + \mathbf{x}^{\mathrm{T}}\mathbf{b} + \mathbf{x}^{\mathrm{T}}\mathbf{B}\mathbf{x} + \epsilon,$$

where $\mathbf{x}^{\mathrm{T}} = [x_1, \ldots, x_k]$, $\mathbf{b}$ is the column vector containing the $k$ first-order parameters, i.e., $\mathbf{b}^{\mathrm{T}} = [\beta_1, \ldots, \beta_k]$, and the symmetric matrix $\mathbf{B}$ with dimension $k \times k$ contains pure quadratic and two-factor interaction parameters. The matrix $\mathbf{B}$ is defined as

$$\mathbf{B} = \begin{pmatrix} \beta_{11} & \beta_{12}/2 & \ldots & \beta_{1k}/2 \\ & \beta_{22} & \ldots & \beta_{2k}/2 \\ & & \ddots & \\ & & & \beta_{kk} \end{pmatrix}.$$

The matrix form is useful in the canonical analysis of the response surface; see Box and Draper (2007) for more details.

The general form of a linear model in which there are $p$ unknown parameters and $N$ design points can be written in a matrix notation as

$$\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon},$$

where $\boldsymbol{\beta}$ is a vector of unknown regression coefficients and matrix $\mathbf{X}$, called the *model matrix*, is the $N \times p$ expanded design matrix with each row having the vector form of

$$\mathbf{x}^{(m)} = [1, x_1, x_2, \ldots, x_k, x_1^2, x_2^2, \ldots, x_k^2, x_1x_2, x_1x_3, \ldots, x_{k-1}x_k].$$

That is to say, a design point $\mathbf{x} = [x_1, x_2, \ldots, x_k]$ is expanded to $\mathbf{x}^{(m)}$.

Given that $E(\mathbf{Y}) = \mathbf{X}\boldsymbol{\beta} = \boldsymbol{\mu}$ and the variance-covariance is $\sigma^2\mathbf{I}_N$, the vector $\hat{\boldsymbol{\beta}}$ of least squares estimates is

$$\hat{\boldsymbol{\beta}} = (\mathbf{X}^{\mathrm{T}}\mathbf{X})^{-1}\mathbf{X}^{\mathrm{T}}\mathbf{Y}\,,$$

and the variances and covariances of estimates are contained in the matrix

$$\text{var}(\hat{\boldsymbol{\beta}}) = \sigma^2(\mathbf{X}^{\mathrm{T}}\mathbf{X})^{-1}.$$

Suppose the model $\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}$ is inadequate, and in reality, an additional $p^*$ parameters are needed in the model. Then the estimate $\hat{\boldsymbol{\beta}} = (\mathbf{X}^{\mathrm{T}}\mathbf{X})^{-1}\mathbf{X}^{\mathrm{T}}\mathbf{Y}$ will be, in general, biased for estimating $\boldsymbol{\beta}$, and the expectation of the least squares estimates will be

$$E(\hat{\boldsymbol{\beta}}) = \boldsymbol{\beta} + \mathbf{A}\boldsymbol{\beta}_1,$$

where $\mathbf{A} = (\mathbf{X}^{\mathrm{T}}\mathbf{X})^{-1}\mathbf{X}^{\mathrm{T}}\mathbf{X}_1$ and $\mathbf{X}_1$ is the $N \times p^*$ matrix corresponding to the $p^*$ additional model parameters. Box and Hunter (1957) called matrix $\mathbf{A}$ the alias matrix which contains the coefficients of biases. Note that $\mathbf{X}^{\mathrm{T}}\mathbf{X}$, called the information matrix, is important because the variance of $\hat{\beta}_j$ is proportional to the $j$th diagonal element in matrix $(\mathbf{X}^{\mathrm{T}}\mathbf{X})^{-1}$. To compare experimental designs, only the $(\mathbf{X}^{\mathrm{T}}\mathbf{X})^{-1}$ matrices are relevant because $\sigma^2$ is the same for all proposed experimental designs (Atkinson et al., 2007). The matrix $N^{-1}\mathbf{X}^{\mathrm{T}}\mathbf{X}$ is called the moment matrix and its inverse $N(\mathbf{X}^{\mathrm{T}}\mathbf{X})^{-1}$ is called the precision matrix. The prediction variance of a predicted value at an arbitrary point $\mathbf{x}$ is

$$\text{Var}[\hat{y}(\mathbf{x})] = \sigma^2\mathbf{x}^{(m)^{\mathrm{T}}}(\mathbf{X}^{\mathrm{T}}\mathbf{X})^{-1}\mathbf{x}^{(m)}.$$

The prediction variance tells how well the fitted model predicts a response. Scaling the prediction variance enables one to compare designs with different sample sizes. This is achieved by dividing and multiplying the $\text{Var}[\hat{y}(\mathbf{x})]$ by $\sigma^2$ and $N$, respectively, and the resulting quantity is scale-free and on a per observation basis. The scaled prediction variance (SPV) is defined as

$$\mathrm{SPV}(\mathbf{x}) = \frac{N\mathrm{Var}[\hat{y}(\mathbf{x})]}{\sigma^2} = N\mathbf{x}^{(m)^{\mathrm{T}}}(\mathbf{X}^{\mathrm{T}}\mathbf{X})^{-1}\mathbf{x}^{(m)} \tag{1.2}$$

For more details in RSM, see Box and Draper (1987), Khuri and Cornell (1996), Whitcomb and Anderson (2005), Atkinson et al. (2007), Box and Draper (2007), del Castillo (2007), Myers et al. (2009), and Goos and Jones (2011).

## 2. Desirable Properties of Second-Order Designs

A response surface design is a set of points in $k$-dimensional $x$-space carefully selected according to a predetermined single criterion or multiple criteria of goodness. Myers et al. (2009) listed desirable properties of "good" response surface designs as summarized in the following.

1. Give fitted values as close as possible to the true values.
2. Be able to perform a lack-of-fit test.
3. Allow a sequential increase to the order of the model.
4. Provide an estimate of "pure" experimental error.
5. Be robust to unusual observations.
6. Be insensitive to errors in a control of design levels.
7. Be cost-effective.
8. Allow experiments to be conducted in blocks.
9. Be able to check on the homogeneous variance assumption.
10. Generate a satisfactory distribution of SPVs throughout the region of interest.

Box (1968) also gave a list of 12 characteristics of a "good" experimental design, similar to those by Myers et al. (2009). An additional desirable property listed by Box (1968) is to require a minimum number of experimental points, but this conflicts with the robustness-to-outliers property because designs with fewer points will be less stable to outliers or missing values (Akhtar and Prescott, 1986). The desirable characteristics, however, are not equally important in every RSM application. For example, the second-order model is primarily used in response optimization. Thus, a model giving precise predictions will be more attractive, and in this case, the prediction variance is more important than other design properties (Anderson-Cook et al., 2009). Atkinson et al. (2007) added the orthogonality and rotatability properties for a favorable response surface design which will now be discussed.

## 2.1. Orthogonality

The orthogonality property is easily attainable for a first-order response surface design. If all design points are at $\pm 1$ extremes and the $\mathbf{X}^{\mathrm{T}}\mathbf{X}$ is orthogonal, the estimates contained in $\hat{\boldsymbol{\beta}}$ are uncorrelated (Box and Hunter, 1957), and the corresponding variances of estimates are minimized. Note that $\mathrm{Var}(\hat{\boldsymbol{\beta}}) = \sigma^2(\mathbf{X}^{\mathrm{T}}\mathbf{X})^{-1}$, thus minimizing the $i$th diagonal element of $(\mathbf{X}^{\mathrm{T}}\mathbf{X})^{-1}$ is equivalent to minimizing the $\mathrm{Var}(\beta_i)$. The formal proofs of the variance optimality for the first-order design are presented in Box (1952) and Plackett and Burman (1946). For the second-order model, the moment matrix is not diagonal because the sums of products between $x_i^2$ and 1 (an intercept) and between $x_i^2$ and $x_j^2$ will not be zeros unless all $x_{iu}$'s are zeros. So, it is impossible to have an (completely) orthogonal matrix in unscaled variables. Box and Hunter (1957) discussed how to construct the second-order orthogonal designs by making use of an orthogonal polynomial coding.

Box and Wilson (1951) derived a formula to find the axial distance that makes central composite designs (CCDs) "orthogonal" and also the $\alpha$ that gives the same variance of second-order effects. Unfortunately, these two properties cannot be satisfied by using the same $\alpha$. Note that the term "orthogonal" in Box and Wilson (1951) does not mean an orthogonal matrix but it means the covariances of estimates $\hat{\beta}_{ii}$ and $\hat{\beta}_{jj}$ are zeros and, therefore, estimates associated with quadratic terms are uncorrelated.

## 2.2. Rotatability

The rotatable property has been discussed in many textbooks and was formally introduced by Box and Hunter (1957). A rotatable design is a design whose SPVs, as in (1.2), are the same for all points $\mathbf{x}$ equidistant from the center point of the design (Tanco et al., 2013). The SPV function of a rotatable design can be written as a function of radius, $\rho$, which is the distance between the point $\mathbf{x}$ and the center point. Points on different spheres can, however, yield different SPVs, so the rotatable design does not necessarily possess a nice variance distribution over an experimental region. Myers et al. (2009) pointed out that the rotatability or near-rotatability is not difficult to achieve without loss of other desirable properties. Whether or not the design is rotatable is determined by the structure of the moment matrix, $N^{-1}\mathbf{X}^{\mathrm{T}}\mathbf{X}$ (Khuri and Cornell, 1996).

The moment matrix simply contains the moments. In general, for fitting a response surface of order $d$ with $k$ coded independent variables, a moment of order $q$ is defined as

$$\frac{1}{N}\sum_{u=1}^{N} x_{1u}^{q_1} x_{2u}^{q_2} \cdots x_{ku}^{q_k} = [1^{q_1} 2^{q_2} \ldots k^{q_k}],$$

where $q_1, q_2, \ldots, q_k$ are nonnegative integers, $x_{iu}$ is the level of the $i$th factor used in the $u$th experimental run ($i = 1, 2, \ldots, k$; $u = 1, 2, \ldots, N$), and $q = \sum_{i=1}^{k} q_i$. The $q$

is called *the order of the design moment.* For instance, $[1^0 2^2 3^1]$ is the design moment of order $q = 0 + 2 + 1 = 3$ and is equal to $\sum_{u=1}^{N} x_{2u}^2 x_{3u}/N$. The moment matrix of a second-order model for $k = 2$ is

$$\frac{\mathbf{X}^{\mathrm{T}}\mathbf{X}}{N} = \begin{array}{c} \begin{matrix} 1 & x_1 & x_2 & x_1^2 & x_2^2 & x_1x_2 \end{matrix} \\ \begin{pmatrix} 1 & [1] & [2] & [11] & [22] & [12] \\ [1] & [11] & [12] & [111] & [122] & [112] \\ [2] & [12] & [22] & [112] & [222] & [122] \\ [11] & [111] & [112] & [1111] & [1122] & [1112] \\ [22] & [122] & [222] & [1122] & [2222] & [1222] \\ [12] & [112] & [122] & [1112] & [1222] & [1122] \end{pmatrix} \begin{matrix} 1 \\ x_1 \\ x_2 \\ x_1^2 \\ x_2^2 \\ x_1x_2 \end{matrix} \end{array} .$$

Box and Hunter (1957) showed that if the moment of a design is the same as the moment of a spherical normal distribution for all orders up to order $2d$, then the design is rotatable for a polynomial model of order $d$. Given that independent variables are coded by Box's convention (Box, 1952), the moment of a rotatable design of order $q$ will be

$$[1^{q_1} 2^{q_2} \ldots k^{q_k}] = \begin{cases} 0 & \text{if at least one of the } q_i \text{ is odd;} \\ \frac{\lambda_q \prod_{i=1}^{k} q_i!}{2^{q/2} \prod_{i=1}^{k} \left(\frac{q_i}{2}\right)!} & \text{if all of the } q_i \text{ are even.} \end{cases}$$

The quantity $\lambda_q$ depends only on $q$ and is a parameter that can be freely chosen by the experimenter. If design moments deviate from the aforementioned form, the rotatability property is weakened or destroyed.

For rotatable designs of order two, the fourth-order moments $[iiii]$ and $[iijj]$ are $3\lambda_4$ and $\lambda_4$, respectively. Accordingly, one might consider $[iiii] = 3[iijj]$ as a sufficient condition to check whether the design is rotatable. Also, if it is a rotatable design, all odd moments, i.e., [1], [2], [12], [111], [112], [122], [1112], and [1222], will be zero. The corresponding moment matrix $N^{-1}\mathbf{X}^{\mathrm{T}}\mathbf{X}$, and its inverse are presented on page 212 in Box and Hunter (1957).

Box and Hunter (1957) showed that the variance function for any second-order rotatable designs can be written as

$$\mathrm{Var}(\rho) = A\{2(k+2)q_4^2 + 2q_4(q_4-1)(k+2)\rho^2 + [(k+1)q_4 - (k-1)]\rho^4\},$$

where $A = [2q_4\{(k+2)q_4 - k\}]^{-1}$ and $\rho = \sqrt{\mathbf{x}^{\mathrm{T}}\mathbf{x}}$. Also, the variances and covariances of the estimated coefficients in a second-order rotatable design are given by

$$\begin{aligned}
\mathrm{Var}(\hat{\beta}_0) &= 2q_4^2(k+2)A\sigma^2/N; \qquad \mathrm{Var}(\hat{\beta}_i) = \sigma^2/N;\\
\mathrm{Var}(\hat{\beta}_{ii}) &= [(k+1)q_4 - (k-1)]A\sigma^2/N; \qquad \mathrm{Var}(\hat{\beta}_{ij}) = \sigma^2/(Nq_4);\\
\mathrm{Cov}(\hat{\beta}_0, \hat{\beta}_{ii}) &= -2q_4A\sigma^2/N; \qquad \mathrm{Cov}(\hat{\beta}_{ii}, \hat{\beta}_{jj}) = (1-q_4)A\sigma^2/N,
\end{aligned}$$

and all remaining covariances are zero. The parameter $q_4$ is freely selected by experimenters, but it should be chosen based on particular criteria. For example, $q_4 = 1$ nullifies correlations between the quadratic coefficients and such a design is called an *orthogonal rotatable design*. Note that the term orthogonal here does not mean completely orthogonal because the intercept and quadratic terms are still correlated (Box and Hunter, 1957).

Box and Hunter (1957) used an inverse of the prediction variance denoted by $W(\rho) = 1/\mathrm{Var}(\rho)$ to describe a precision of the estimate $\hat{y}(\mathbf{x})$ at a distance $\rho$ from the center run(s). They graphed the standardized weight function with different values of $q_4$. The precision falls rapidly after $\rho = 1$ regardless of $q_4$ values. When $q_4$ exceeds 1, the precision is high especially at the center of the design, but if the true model is a third-order polynomial, the biases of $\hat{\beta}_{ii}$ are also large. Box and Hunter (1957) suggested choosing the value of $q_4$ which gives the same variance for all design points having $0 \leq \rho \leq 1$, and this is a concept referred to as *uniform precision.* del Castillo (2007) showed that $q_4 = (k + 3 + \sqrt{9k^2 + 14k - 7})/[4(k + 2)]$ makes a design to be uniform precision rotatable, and thus, for $k = 2$ to 8, the corresponding $q_4$'s are .7844, .8385, .8704, .8918, .9070, .9184, and .9274, respectively (Box and Hunter, 1957).

Khuri (1988) proposed a measure that quantifies the amount of rotatability as a percentage, and a design is said to be rotatable if and only if the percentage is exactly 100. Khuri's measure is a function of design moments of the second or higher order as shown in equation (2.15) in Khuri (1988).

Park et al. (1993) proposed a new measure of rotatability symbolized as $P_k(D)$ for $3^k$ factorial designs and CCDs as in equation (3.5) in their paper. The value of $P_k(D)$ is between zero and one and equals one for rotatable designs. Other rotatability measures can be found in Draper and Guttman (1988) and Draper and Pukelsheim (1990).

## 3. Relevant Response Surface Designs

In this section, the second-order response surface designs used later in Chapter 2 will now be summarized. Most of these designs are widely used in practice and some can be generated by statistical software, e.g., SAS, R, Matlab, and Minitab. With SAS® 9.2 ADX Interface (SAS Institute Inc., 2008), central composite designs with specific values of $\alpha$, Plackett-Burman designs, hybrid designs, optimal designs, etc., can be generated. R packages such as `DoE.base`, `FrF2`, `DoE.wrapper`, `BsMD`, `lhs`, `AlgDesign`, `rsm`, and `VdgRsm` are able to generate many response surface designs. More recently, package `RcmdrPlugin.DoE` provides a Graphical User Interface

(GUI) to generate several designs, e.g., D-optimal designs, Taguchi parameter designs, latin hypercube designs. For more information about package `RcmdrPlugin.DoE`, see Grömping (2011). In the dissertation, standard designs being used are available in the VdgRsm package (Srisuradetchai and Borkowski, 2014).

## 3.1. Central Composite Designs

The central composite design (CCD), introduced by Box and Wilson (1951), is the most popular design for collecting data to fit a second-order model when the process is near optimum because it satisfies many desirable criteria previously listed in Section 2. Thus, it has become a keystone of RSM. The CCD typically described in the coded $x$-space is composed of three sets of points:

(a) the $2^k$ vertices $(\pm 1, \pm 1, \ldots, \pm 1)$ of a $k$-dimensional "cube" $(k \leq 4)$, or a fraction of it $(k \geq 5)$;

(b) the $2k$ $k$-dimensional points $(\pm\alpha, 0, \ldots, 0)$, $(0, \pm\alpha, \ldots, 0)$, ..., $(0, 0, \ldots, \pm\alpha)$, referred to as "axial" or "star" points;

(c) a set of $n_0$, "center points", $(0, 0, \ldots, 0)$.

Set (a) is a full $2^k$ factorial for $k \leq 4$ and a $2^{k-p}$ fractional factorial for $k \geq 5$. Although the full factorial design could be used for $k \geq 5$, the number of experimental units swiftly increases as $k$ increases. Factorial points contribute to the estimation of linear and two-factor interaction terms. Set (b), consisting of pairs of points on the coordinate axes with the same distance $\alpha$ from the center point, primarily contributes to the estimation of pure quadratic terms, and set (c) represents the center points allowing us to estimate the pure error. Set (c) also contributes to the estimation of pure quadratic terms (Draper and Lin, 1996, Myers et al., 2009). Figure 1.1

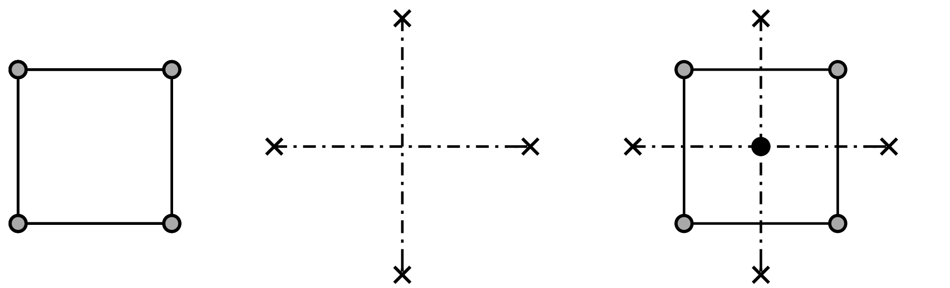



Figure 1.1: Central composite design for $k = 2$.

presents sets (a), (b) and a complete CCD with a single center point (solid black) for $k = 2$. In general, the total number of runs, $N$, is $n_f + n_a + n_c$ where $n_f, n_a$, and $n_c$ are respectively the number of factorial, axial (star), and center points. If a fractional factorial is used in the CCD, the required resolution is at least V. This means the smallest fractional factorial design for fitting a second-order model is a $2^{k-1}$ for $k = 5, 6, 7$, a $2^{k-2}$ for $k = 8, 9$, $2^{k-3}$ for $k = 10$, and a $2^{k-4}$ for $k = 11$ (Box et al., 2005, Draper and Lin, 1996). For more details on the construction of fractional factorial designs, refer to Box et al. (2005).

Choices of the $\alpha$ and $n_c$ are very important. By choosing a particular value of $\alpha$, the CCD can be spherical, rotatable, orthogonal, cuboidal, or minimum variance (Akram, 1993). If the experimentation consists of three levels in each factor and $\alpha$ equals one, such a design is called the *face-centered central composite design* (FCD). The fourth-order moments of CCDs are

$$[iiii] = \frac{1}{N}(n_f + 2\alpha^2) \quad \text{and} \quad [iijj] = \frac{n_f}{n_c}.$$

Solving the equation $[iiii] = 3[iijj]$ results in $\alpha$ of $n_f^{1/4}$. Thus, rotatability can be achieved regardless of the number of center runs. The importance of center runs is related to the uniform precision and orthogonality properties. Based on Box and Hunter (1957) coding convention, the uniform precision rotatable CCD can be attained by using $n_c$ satisfying the following equation (del Castillo, 2007):

$$\frac{n_f + 2k + n_c}{n_f + 4\sqrt{n_f} + 4} = \frac{k + 3 + \sqrt{9k^2 + 14k - 4}}{4(k+2)}.$$

The closest integer to the exact $n_c$ solution value will be used, and with this $n_c$ the design will be a near-uniform precision and rotatable design. Box and Draper (1963) applied the variance-plus-bias criterion to determine the number of center runs. They commented that choices of $n_c$ may be based on one's belief in the relative sizes of the integrated variance error and integrated bias error. Table 1.1, adapted from Draper and Lin (1996), shows the number of parameters to be estimated, the number of factorial, axial, and center runs recommended by Box and Hunter (1957) and Box and Draper (1963).

Table 1.1: Features of certain central composite designs.

| No. of variables | 2 | 3 | 4 | 5 | 6 | 7 | 8 |
|---|---|---|---|---|---|---|---|
| No. of parameters | 6 | 10 | 15 | 21 | 28 | 36 | 45 |
| Cube+Star | 8 | 14 | 24 | – | – | – | – |
| $\frac{1}{2}$Cube+star | – | – | – | 26 | 44 | 78 | – |
| $\frac{1}{4}$Cube+star | – | – | – | – | – | – | 80 |
| $\alpha$ (rotatable) | 1.414 | 1.682 | 2.000 | 2.000 | 2.378 | 2.828 | 2.828 |
| No. of center runs | | | | | | | |
| Box and Hunter (1957) | 5 | 6 | 7 | 6 | 9 | 14 | 13 |
| Box and Draper (1963) | 3 | 3 | 4 | 2 | 3 | 3 | 4 |

## 3.2. Hartley's Small Composite Designs

Experimentation can be expensive and time-consuming. In CCDs, the total number of experimental runs increases rapidly as $k$ increases because of the factorial portion. Hartley (1959) pointed out that when center and axial runs are included, it is not necessary for the factorial portion to be resolution V. It could be of resolution as low as III* which means a design is resolution III but no words of length four in the defining relations. Consequently, two-factor interactions are not aliased with other two-factor interactions. For example, for $k = 4$, the usual defining equation for a $2^{4-1}$ design is $x_1x_2x_3x_4 = \pm 1$ with each $x_i = \pm 1$. With this design, all main effects are clear of two-factor interactions, but because of three aliases: $x_1x_2 = x_3x_4$, $x_1x_3 = x_2x_4$, and $x_1x_4 = x_2x_3$, only three $\hat{\beta}_{ij}$ can be estimated. Hartley (1959) used the defining relation $x_3 = x_1x_2$ for $2^{4-1}$ fractional portion yielding the corresponding 7 alias-sets of effects: $x_1 = x_2x_3$, $x_2 = x_1x_3$, $x_3 = x_1x_2$, $x_4 = x_1x_2x_3x_4$, $x_1x_4 = x_2x_3x_4$, $x_2x_4 = x_1x_3x_4$, and $x_3x_4 = x_1x_2x_4$. It can be seen that all two-factor interactions appear in different alias sets, so all $\hat{\beta}_{ij}$'s can be estimated. The three main-effect estimates, however, are aliased with two-factor interactions. Hartley's Small Composite Designs (HSCDs) are saturated or near-saturated for $k = 2, 3, 4$, and 6. For more details, see Hartley (1959). The HSCDs can be generated by using the SAS ADX (SAS Institute Inc., 2008) and R package VdgRsm (Srisuradetchai and Borkowski, 2014).

## 3.3. Plackett-Burman Composite Designs

Draper (1985) used columns of a Plackett-Burman design (PBD) to create a small composite design. Note that the PBD proposed by Plackett and Burman (1946) is a screening design used to fit a first-order model. The $k$-factor Plackett-Burman

Table 1.2: Columns that provided the highest $D$-optimality criterion.

| $k$ | $p$ | $n_{PBD}$ | Columns chosen from PBDs | Sample size (without center points) Factorial and axial points Draper and Lin (1990) | Hartley (1959) |
|---|---|---|---|---|---|
| 3 | 10 | 4 | $(1, 2, 3)$ | $4 + 6 = 10$ | $4 + 6 = 10$ |
| 4 | 15 | 8 | $(1, 2, 3, 6)$ | $8 + 8 = 16$ | $8 + 8 = 16$ |
| 5 | 21 | 12 | $(1, 2, 3, 4, 5)$ | $12 + 10 = 22$ | $16 + 10 = 26$ |
| 6 | 28 | 16 | $(1, 2, 3, 4, 5, 14)$ | $16 + 12 = 28$ | $16 + 12 = 28$ |
| 7 | 36 | 24 | $(1, 2, 3, 5, 6, 7, 9)$ | $24 + 14 = 38$ | $32 + 14 = 46$ |

Composite Design (PBCD) is constructed by choosing $k$ columns from the PBD, $3 \leq k \leq 10$, and adding axial and center points. Draper and Lin (1990) suggested selecting columns from the PBD so that the $D$-criterion is maximized. Table 1.2 shows columns in PBDs resulting in the highest of the $D$-criterion if they are used as a factorial portion. For $k = 5$, all possible column choices taken from the 12-point PBD will have either repeated runs or a mirror-image pair (two points that have opposite signs), so one of each set of duplicates can be removed. The HSCDs can be considered as special cases of PBCDs if appropriate columns are chosen; however, for $k = 5$ and 7, the PBCD has a smaller sample size than the HSCD as presented in Table 1.2. The PBCDs can be generated by using the SAS ADX (SAS Institute Inc., 2008) and R package VdgRsm (Srisuradetchai and Borkowski, 2014).

### 3.4. Hybrid Designs

Roquemore (1976) proposed a new design for fitting a second-order model with the following goals: (1) to achieve the orthogonality in a sense that first- and third-order moments are zero; (2) to yield constant moments $[ii]$ and $[iijj]$; (3) to be near-rotatable if possible; and (4) to minimize the number of experimental runs (del Castillo, 2007). The $k$-factor design, $k = 3, 4$, and 6, can be viewed as a composite design for $k-1$ factors with an augmented column for the $k$th factor. Two criteria - orthogonality and rotatability - were used to construct the hybrid designs, and for each $k$ there is more than one choice of designs depending on the criteria being used. Hybrid designs are saturated or near-saturated second-order designs, so they are very competitive to CCDs if design size is of concern. Myers et al. (2009) mentioned that hybrid designs are not used as much in industry as they should be because their values of levels are not as "normal" in scale as those in CCDs.

For $k = 3$, three choices of hybrid designs denoted as 310, 311A, and 311B are available. The first number represents the number of factors, and the next two digits represent the number of distinct design points. For $k = 4$, there are three hybrid designs, 416A, 416B, and 416C, and for $k = 6$, two designs are provided. The hybrid designs can be generated by using the SAS ADX (SAS Institute Inc., 2008) and R package VdgRsm (Srisuradetchai and Borkowski, 2014).

### 3.5. Box-Behnken Designs

The Box-Behnken designs (BBDs), proposed by Box and Behnken (1960), are used for fitting second-order models. BBDs are naturally spherical designs because they have only edge points and all factorial points are excluded. That is, all points (except for center points) lie on the surface of a sphere. Only three levels of independent variables $x_1, x_2, \ldots, x_k$ which are coded to $-1, 0, 1$ can be used. This design is an alternative to a CCD when the optimum response is not located at the extremes of the experimental region or one is not interested in predicting a response at the extremes (Myers et al., 2009). The BBD for $k = 3$ with a center point is illustrated in Figure 1.2.

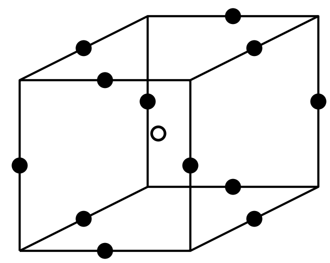


Figure 1.2: Box-Behnken design for $k = 3$ with center points (open circle).

BBDs are generated from balanced incomplete block designs (BIBDs) or partially balanced incomplete block designs (PBIBDs), and are available for $k = 3$ , 4, 5, 6, 7, 9, 10, 11, 12, and 16. A new set of BBDs were created for $k = 3$ to 12 and 16 (Nguyen and Borkowski, 2008). The BBDs possess desirable properties: (1) the designs are either rotatable (for $k = 4$ and 7) or near-rotatable; (2) they can be orthogonally blocked by adding additional center runs; and (3) few factors are changed at a time (del Castillo, 2007). Both SAS ADX (SAS Institute Inc., 2008) and R package VdgRsm (Srisuradetchai and Borkowski, 2014) can generate BBDs for $k = 3$ to 7.

### 3.6. Alphabetic Optimal Designs

The invention of optimal designs has been credited to Smith (1918), a Danish statistician. She wrote a dissertation introducing optimal designs where she determined $G$-optimal designs for single variable polynomial regression of order up to six (Guttorp and Lindgren, 2009). Later on, a general framework of the optimal design theory was created by Kiefer (1959, 1961) and Kiefer and Wolfowitz (1959). These original works used measure theoretic approaches, such that experimental designs are considered to be design measures and are called approximate designs. Let $\xi$ be an optimal design on design space $\mathcal{X}$. Because $\xi$ is a probability measure,

$$\xi(\mathbf{x}) \geq 0, \quad \mathbf{x} \in \mathcal{X}, \text{ and } \int_{\mathcal{X}} \xi(\mathbf{x})\, d\mathbf{x} = 1\,.$$

Continuous designs are represented by the measures $\xi$ over $\mathcal{X}$. If the *continuous* design has $n$ distinct points in a design region $\mathcal{X}$, it can be written as

$$\xi = \left\{ \begin{array}{cccc} \mathbf{x}_1 & \mathbf{x}_2 & \ldots & \mathbf{x}_n \\ w_1 & w_2 & \ldots & w_n \end{array} \right\},$$

where $\mathbf{x}_i \in \mathcal{X}$ is the $i$th design point, $\xi(\mathbf{x}_i) = w_i$ is the corresponding weight, and $\sum_{i=1}^{n} w_i = 1$, $i = 1, 2, \ldots, n$.

In practice, a weight $\xi(\mathbf{x}_i)$ needs to be a rational number $n_i/N$ so that $n_i$ observations will be taken at design point $\mathbf{x}_i \in \mathcal{X}$, and such a design is called an *exact* design. Since the computer age arrived, algorithms have been employed to generate the "best" exact designs with respect to optimality criteria. A resulting design could be custom-tailored as experimenters can choose the number of experimental runs, model to fit, ranges on factors, and other constraints to meet their requirements (Myers et al., 2009).

For exact designs, the information matrix per observation, also called the moment matrix, is

$$\mathbf{M}(\xi_N) = \sum_{i=1}^{N} \mathbf{x}_i^{(m)} \mathbf{x}_i^{(m)^{\mathrm{T}}} w_i = \frac{1}{N} \mathbf{X}^{\mathrm{T}} \mathbf{X} = \frac{\sigma^2}{N} [\mathrm{var}(\hat{\boldsymbol{\beta}})]^{-1}\,.$$

The variance-covariance matrix $\mathrm{var}(\hat{\boldsymbol{\beta}})$ can be considered as a measure of the expected loss or risk in estimating $\boldsymbol{\beta}$ by the estimate $\hat{\boldsymbol{\beta}}$ if the loss function is a quadratic function (Hackl, 1995).

Suppose $\xi$ is a design which has $n_i$ observations at $\mathbf{x}_i$, $i = 1, 2, \ldots, n$, and

$\sum_{i=1}^{n} n_i = N$. If there are no missing observations or failed trials, the Fisher information matrix is proportional to

$$I(\xi, \beta) = \sum_{i=1}^{n} \frac{n_i}{N} \frac{\partial f(x_i, \beta)}{\partial \beta} \frac{\partial f(x_i, \beta)^{\mathrm{T}}}{\partial \beta} = \mathbf{M}(\xi_N) \,. \tag{1.3}$$

Without missing observations, the covariance matrix of the maximum likelihood estimator of $\boldsymbol{\beta}$ is proportional to $[I(\xi, \beta)]^{-1}$. Also an optimal design for estimating $\boldsymbol{\beta}$ can be found by maximizing the appropriate function of $I(\xi, \boldsymbol{\beta})$ (Imhof et al., 2002).

The $D$-, $A$-, $G$-, and $IV$-optimality criteria are of interest in the dissertation. The first two criteria are related to the variance of estimates while the last two criteria are concerned with the prediction variance. Because design criteria are described by letters of the alphabet, they are often called alphabetic optimality criteria which we will now summarize.

1. **D-Optimality**

   This criterion, introduced by Wald (1943), minimizes $\Psi[\mathbf{M}(\xi)] = \log|\mathbf{M}(\xi)|^{-1} = -\log|\mathbf{M}(\xi)|$, and is equivalent to minimizing the determinant $|(\mathbf{X}^{\mathrm{T}}\mathbf{X})^{-1}|$ (known as the generalized variance). Minimizing the aforementioned quantities is also the same as maximizing $|\mathbf{X}^{\mathrm{T}}\mathbf{X}|$ and maximizing $|I(\xi, \boldsymbol{\beta})|$, the Fisher information. The $D$ in the name stands for "determinant". For this criterion, we seek a design $\xi^*$ satisfying

$$\begin{aligned} \xi^* &= \arg\min_{\xi \in \Xi} |\mathbf{M}^{-1}(\xi)|, \\ &= \arg\min_{\xi \in \Xi} |N(\mathbf{X}^{\mathrm{T}}\mathbf{X})^{-1}|, \end{aligned}$$

   where $\Xi$ is the set of all continuous designs on $\mathcal{X}$. Under the assumptions of independent normal errors and constant variances, $|\mathbf{X}^{\mathrm{T}}\mathbf{X}|$ is inversely proportional to the square of the volume of the confidence region of the regression coefficients. The smaller the volume of the confidence region, then the better coefficients are estimated. Thus, the goal of $D$-optimality is to estimate the parameters as precisely as possible. Because $D$-optimal designs minimize the generalized variance of the parameter estimates, the variances for estimated parameters will tend to be small as well as the correlations between estimated parameters. To compare designs with different sample sizes, we use the $D^*$-efficiency defined as

$$D^*\text{-efficiency} = \left(\frac{|\mathbf{M}(\xi)|}{|\mathbf{M}(\xi^*)|}\right)^{1/p} \times 100,$$

where $p$ is the number of model parameters. The ratio $\left(|\mathbf{M}(\xi)|/|\mathbf{M}(\xi^*)|\right)^{1/p}$ is equivalent to the number of times the experiment needs to be replicated in order to have the same value of the $D$-criterion as that of the $D$-optimal design $\xi^*$. Thus, to calculate the $D$-efficiency of an exact design $\xi$, the $D$-optimal design $\xi^*$ is needed beforehand. This is, unfortunately, not usually the case. The best exact $D$-optimal design, generated from a computer algorithm, could replace the $D$-optimal design $\xi^*$, but the efficiency ratio will be overestimated. It would, however, provide an upper bound on $D^*$-efficiency. Some statistical software, e.g., SAS, assumes a hypothetical orthogonal design for the first-order model to calculate the denominator. The hypothetical orthogonal design in which each $x_i \in \{-1, 1\}$ is an $N$-point exact $D$-optimal design for the first-order model if $|\mathbf{X}^{\mathrm{T}}\mathbf{X}| = N^p$. Therefore, we can define

$$D\text{-efficiency} = \left(\frac{|\mathbf{X}^{\mathrm{T}}\mathbf{X}|}{N^p}\right)^{1/p} \times 100 = \frac{|\mathbf{X}^{\mathrm{T}}\mathbf{X}|^{1/p}}{N} \times 100\,. \tag{1.4}$$

The quantity (1.4) is a lower bound on $D^*$-efficiency of a design, and sometimes it is not sharp. In other words, a gap between $D$- and $D^*$-efficiencies is sometimes not small (del Castillo, 2007).

2. **G-Optimality**

The $G$-optimality criterion, introduced by Smith (1918), minimizes the maximum of the scaled prediction variances (SPVs). Not only points in the designs, but all points in the design space $\mathcal{X}$, are used to calculate the SPV. The $G$ in the name stands for "global". For this criterion, we seek a design $\xi^*$ satisfying

$$\begin{aligned} \xi^* &= \arg\min_{\xi\in\Xi}\max_{\mathbf{x}\in\mathcal{X}} \mathrm{SPV}(\mathbf{x}), \\ &= \arg\min_{\xi\in\Xi}\max_{\mathbf{x}\in\mathcal{X}} N\mathbf{x}^{(m)^{\mathrm{T}}}(\mathbf{X}^{\mathrm{T}}\mathbf{X})^{-1}\mathbf{x}^{(m)}. \end{aligned}$$

A $G$-optimality criterion employs the minimax approach to assure that the design has no "weak" design points that have very poor prediction variance. It was originally used to obtain optimal designs for regression problems by Smith and later was called $G$-optimality by Kiefer and Wolfowitz (1959). The $G$-efficiency of a design is defined as

$$G\text{-efficiency} = \frac{p}{\max\limits_{\mathbf{x}\in\mathcal{X}} \mathrm{SPV}(\mathbf{x})} \times 100\,. \tag{1.5}$$

The numerator of the $G$-efficiency, $p$, is a lower bound for the maximum prediction variance. This is due to the fact that a sum of all diagonal elements $h_{ii}$ in the "hat" matrix, $\mathbf{X}(\mathbf{X}^{\mathrm{T}}\mathbf{X})^{-1}\mathbf{X}^{\mathrm{T}}$, equals $p$, so the average value of $\mathrm{SPV}(\mathbf{x})$ at the design points is $p$. This implies that $\max_{\mathbf{x}\in\mathcal{X}} \mathrm{SPV}(\mathbf{x}) \geq p$ (Myers et al., 2009). To have the $G$-efficiency of 100%, all design points will have the same leverage $h_{ii}$. Therefore, $G$-optimal designs tend to place all design points equidistant from the origin of the center of the design, on the boundary of $\mathcal{X}$, and those design points should have about the same leverage (del Castillo, 2007). Moreover, under the assumption of homoscedasticity, a $D$-optimal design is also a $G$-optimal design (Kiefer and Wolfowitz, 1960).

3. **A-Optimality**

   The $A$-optimality criterion, introduced by Chernoff (1953), seeks to minimize the trace of the inverse of the information matrix, $(\mathbf{X}^{\mathrm{T}}\mathbf{X})^{-1}$, or equivalently to minimize the average variance of the parameter estimates. The $A$ in the name stands for "average". Thus, for this criterion, we seek a design $\xi^*$ satisfying

$$\begin{aligned} \xi^* &= \arg\min_{\xi \in \Xi} \operatorname{trace}[\mathbf{M}^{-1}(\xi)], \\ &= \arg\min_{\xi \in \Xi} \operatorname{trace}[N(\mathbf{X}^{\mathrm{T}}\mathbf{X})^{-1}], \end{aligned}$$

   and the $A$-efficiency of design $\xi$ is defined as

$$A\text{-efficiency} = \frac{p}{\operatorname{trace}[\mathbf{M}^{-1}(\xi)]} \times 100, \tag{1.6}$$

   where the numerator of $A$-efficiency, $p$, is the trace of a hypothetical orthogonal design for a first-order model.

4. **IV-Optimality**

   The $IV$-optimality criterion seeks to minimize the average scaled prediction variance throughout the design space $\mathcal{X}$. The $IV$ in the name stands for "integrated variance". Thus, for this criterion, we seek an $N$-point design $\xi^*$

satisfying

$$\begin{aligned}\xi^* &= \arg\min_{\xi\in\Xi} \frac{1}{A}\int_{\mathcal{X}} \mathrm{SPV}(\mathbf{x})\, d\mathbf{x},\\ &= \arg\min_{\xi\in\Xi} \frac{N}{A}\,\mathrm{trace}\left[(\mathbf{X}^{\mathrm{T}}\mathbf{X})^{-1}\int_{\mathcal{X}} \mathbf{x}^{(m)^{\mathrm{T}}}\mathbf{x}^{(m)}\, d\mathbf{x}^{(m)}\right],\end{aligned}$$

where $A$ is the volume of the space $\mathcal{X}$. Usually, original factor values are coded to be in $[-1,+1]$ for all $k$ factors, so $\mathcal{X} = [-1,1]^k$ and $A = 2^k$. The $IV$-efficiency of design $\xi$ is defined as

$$IV\text{-efficiency} = \frac{A}{N\,\mathrm{trace}\left[(\mathbf{X}^{\mathrm{T}}\mathbf{X})^{-1}\int_{\mathcal{X}} \mathbf{x}^{(m)^{\mathrm{T}}}\mathbf{x}^{(m)}\, d\mathbf{x}^{(m)}\right]}. \tag{1.7}$$

In practice, $IV$-criterion is not often a choice used to construct an optimal design, but it is merely a mean of comparing designs constructed by other criteria (Atkinson et al., 2007).

Borkowski (2003b) used a genetic algorithm to generate $N$-point small exact $D$-, $A$-, $G$-, $IV$-optimal designs for $k = 1$ to 3 and $N = 3$ to 16 depending on $k$. The author gave a catalog of optimal designs in which many designs had not been found in the literature. Some existing optimal designs found in Atkinson and Donev (1992), Box and Draper (1974), Crary et al. (1992), Haines (1987), and Hartley and Rudd (1969) have been slightly improved.

## 3.7. Mixture Designs

Unlike the usual response surface designs previously discussed, a mixture experiment is an experiment in which the response is only a function of the proportions of the components or factors in the mixture. The percentages of the components must sum to 100%, so an increase in one component proportion will decrease one or more of the remaining component proportions. The mixture design was first discussed in Quenouille (1953) and systematically introduced by Scheffé (1958, 1963). Comprehensive books on data analyses of mixture experiments and optimal mixture designs can be found in Cornell (2002), Smith (2005), and Sinha et al. (2014).

Let $\mathbf{x}^{\mathrm{T}} = (x_1, x_2, \ldots, x_q)$ denote a vector of $q$ mixing components. If $0 \leq x_i \leq 1$ for $i = 1, 2, \ldots, q$, then the mixture design space is a simplex given by

$$\mathcal{X} = \{\mathbf{x} | x_i \geq 0,\, i = 1, 2, \ldots, q,\, \sum_{i=1}^{q} x_i = 1\}\,.$$

With the constraint $\sum_{i=1}^{q} x_i = 1$, the first-order model $E(y) = \beta_0 + \sum_{i=1}^{q} \beta_i x_i$ can be written as $E(y) = \sum_{i=1}^{q} \beta_i^* x_i$ where $\beta_i^* = \beta_0 + \beta_i$, and the latter form is called the canonical or Scheffé form of the first-order mixture model. Likewise, the second-order or quadratic model becomes

$$E(y) = \sum_{i=1}^{q} \beta_i^* x_i + \sum_{i=1}^{q} \sum_{\substack{j=1 \\ j>i}}^{q} \beta_{ij}^* x_i x_j\,, \tag{1.8}$$

where $\beta_i^* = \beta_0 + \beta_i + \beta_{ii}$ and $\beta_{ij}^* = \beta_{ij} - \beta_{ii} - \beta_{jj}$ for $i, j = 1, 2, \ldots, k, j > i$. Equation (1.8) is a result of multiplying $\beta_0$ by $\sum_{i=1}^{q} x_i = 1$ and replacing $\sum_{i=1}^{q} x_i^2$ by $\sum_{i=1}^{q} x_i (1 - \sum_{j=1, j\neq i}^{q} x_j)$ in equation (1.1).

The simplest mixture design proposed by Scheffé(1958) is called a simplex lattice design (SLD). The SLD consists of all possible combinations of $q$ proportions whose values are equally-spaced. The $i$th component has the possible proportion values:

$$x_i = 0, \frac{1}{m}, \frac{2}{m}, \ldots, \frac{m-1}{m}, 1, \text{ for } i = 1, 2, \ldots, q\,.$$

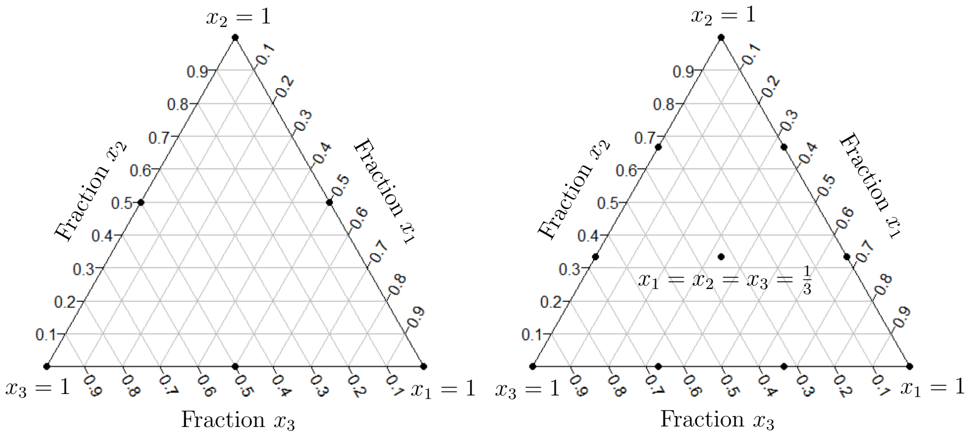



Figure 1.3: Simplex lattice designs for $q = 3$, $m = 2$ (left) and 3 (right).

We use a notation SLD$\{k, m\}$ for the SLD in $k$ components with $m+1$ equally spaced proportions for each component. For example, a SLD$\{3, 2\}$ is comprised of the points:

$$(1, 0, 0), (0, 1, 0), (0, 0, 1), (\frac{1}{2}, \frac{1}{2}, 0), (\frac{1}{2}, 0, \frac{1}{2}), (0, \frac{1}{2}, \frac{1}{2}).$$

Three vertex points $(1, 0, 0), (0, 1, 0), (0, 0, 1)$ are called the "pure blends" which contribute to the estimation of the coefficient $\beta_i^*$ in equation (1.8), and three two-component mixtures at the midpoints of the three edges are called "binary blends" which are required for estimating $\beta_{ij}^*$ in equation (1.8). The SLDs are graphically displayed by R packages mixexp (Lawson, 2014) and plotrix (Lemon et al., 2014). Figure 1.3 shows the SLD$\{3, 2\}$ (left) and SLD$\{3, 3\}$ (right). Note that SLD$\{3, 2\}$ does not have any interior points while SLD$\{3, 3\}$ has one simplex centroid $(1/3, 1/3, 1/3)$ inside the design space.

The second type of mixture design is called a simplex centroid design. A $q$-component simplex centroid design consists of $2^q - 1$ distinct design points, and it is actually a set of $t$ nonzero coordinates in a $q$-dimensional coordinate system. They are in the form of

$$(\frac{1}{t}, \frac{1}{t}, \dots, \frac{1}{t}, 0, 0, \dots, 0),\ (\frac{1}{t}, \frac{1}{t}, \dots, 0, \frac{1}{t}, 0, 0, \dots, 0),\ \dots,\ (0, 0, \dots, 0, \frac{1}{t}, \frac{1}{t}, \dots, \frac{1}{t})\ ,$$

where $t = 1, 2, \dots, q$. For example, the 4-component simplex centroid design has a total of 15 design points:

$$\begin{aligned}
&(1,0,0,0), (0,1,0,0), (0,0,1,0), (0,0,0,1),\\
&(\frac{1}{2}, \frac{1}{2}, 0, 0), (\frac{1}{2}, 0, \frac{1}{2}, 0), (\frac{1}{2}, 0, 0, \frac{1}{2}), (0, \frac{1}{2}, \frac{1}{2}, 0, 0), (0, \frac{1}{2}, 0, \frac{1}{2}, ), (0, 0, \frac{1}{2}, \frac{1}{2}),\\
&(\frac{1}{3}, \frac{1}{3}, \frac{1}{3}, 0), (\frac{1}{3}, \frac{1}{3}, 0, \frac{1}{3}), (\frac{1}{3}, 0, \frac{1}{3}, \frac{1}{3}), (0, \frac{1}{3}, \frac{1}{3}, \frac{1}{3}), (\frac{1}{4}, \frac{1}{4}, \frac{1}{4}, \frac{1}{4}).
\end{aligned}$$

The last type of mixture designs is an *axial design*. Unlike simplex lattice or simplex centroid designs, the axial design does not have points on the vertices, edges, and faces, but it only contains points inside the simplex. The $N = q$ axial design has design points of the form

$$((1 + (q-1)\Delta)/q, (1-\Delta)/q, \dots, (1-\Delta)/q)\ ,$$

and their permutations, $-1/(q-1) < \Delta < 1$ (Sinha et al., 2014). For example, the 4-component axial design with a choice of $\Delta = 0.3$ contains design points $(0.55, 0.15, 0.15, 0.15)$, $(0.15, 0.55, 0.15, 0.15)$, $(0.15, 0.15, 0.55, 0.15)$, and $(0.15, 0.15, 0.15, 0.55)$. For more details on generalized axial designs, refer to Sinha et al. (2014).

In addition to constraints that all component proportions are nonnegative and sum up to 100%, there may be constraints on the individual component proportions.

These are upper- and/or lower-bound constraints which have the form

$$0 \leq L_i \leq x_i \leq U_i \leq 1 \ , \ i = 1, 2, \ldots, q.$$

The constraints will reflect the feasible space for the mixture experiment. If some or all imposed constraints are lower-bound restrictions, the shape of mixture space is still a simplex. The resulting sub-region space can be transformed into a pseudo-component space in which all component values take values on 0 to 1 (Cornell, 2002), and the standard method of analysis for simple lattice designs can be then applied to mixture designs with such pseudo-components. This pseudo-component transformation, introduced by Kurotori (1966), is called the $L$-pseudocomponents and defined as

$$x_i^{'} = \frac{x_i - L_i}{1 - L},$$

where $L = \sum_{I=1}^{q} L_i < 1$.

In the presence of upper-bound constraints, the feasible region may not be a simplex. For example, a three-component mixture with an only upper-bound constraint $x_1 \leq U_1$ has a region of isosceles trapezoid shape. In this case, a computer-generated design is an alternative. In some cases, upper-bound constraints give a design space which is a simplex. For a discussion of mixture designs with constraints, see Cornell (2002) and Myers et al. (2009). We now only introduce the mixture experiment as it will appear again in Chapter 5.

## 4. Missing Observations in Literature

The first published research on missing values in a response surface design is probably by Draper (1961). He provided formulas to estimate missing values in three-factor second-order rotatable response surface designs with zero to six center runs. From 1960 to 1980, many statisticians studied the robustness of experimental designs against missing observations from different perspectives.

Box and Draper (1975) proposed a criterion to measure the sensitivity to wild observations, one of 12 good design properties listed by Box (1968). Their measure is the sum of squares of diagonal elements of the "hat" matrix, $\mathbf{X}(\mathbf{X}^{\mathrm{T}}\mathbf{X})^{-1}\mathbf{X}^{\mathrm{T}}$.

Ghosh (1979) introduced the maximum number of arbitrary observations, which can be lost and all parameters can still be estimated, to measure the robustness of a design to missing trials. We will call this the $t_{\max}$ criterion in the dissertation. The $t_{\max}$ criterion was later applied to other designs by MacEachern et al. (1995), Whittinghill (1998), and Tanco et al. (2013). Ghosh also proposed robust optimal balanced resolution $V$ plans for $2^k$ factorials, $k = 4, 5, \ldots, 8$, under the aforementioned situation but also remaining a resolution $V$ plan (Ghosh, 1980).

MacEachern et al. (1995) considered the estimability criterion as it applied to factorial experiments. The method for finding $t_{\max}$ was provided for factorial designs. The author also showed that for fitting a second-order model for $k \geq 3$,

(i) if $\alpha = \sqrt{k}$, $t_{\max}(\mathbf{D}) = \min\{n_c - 1, 3\}$;

(ii) if $\alpha \neq \sqrt{k}$, $t_{\max}(\mathbf{D}) = \min\{n_c + 1, 3\}$,

where $\alpha$ is axial distance and $\mathbf{D}$ is the model matrix of a $k$-factor central composite design with $n_c \geq 1$. We can interpret $t_{\max}(\mathbf{D}) = \min\{n_c + 1, 3\}$ that, for example, if $n_c = 1$ and we lose more than three runs, some parameters will not be estimated. Details of proofs of their theorems are found in the technical report (MacEachern et al., 1993).

Whittinghill (1998) investigated the robustness against missing observations of Box-Behnken designs with a specific number of center points and found that given $\mathbf{X}$

is the model matrix, $t_{\max}(\mathbf{X}) = 1$ for $k = 3, 7$; $t_{\max}(\mathbf{X}) = 2$ for $k = 4$; $t_{\max}(\mathbf{X}) = 3$ for $k = 5, 6, 9, 10, 12, 16$; and $t_{\max}(\mathbf{X}) = 10$ for $k = 11$.

Tanco et al. (2013) studied the robustness of three-level response surface designs against missing observations, and also proposed a new robust criterion called *probability of estimability*. The idea is related to the $t_{\max}$ criterion but provides more information about the probability to estimate all parameters with the largest possible number of missing design observations. That is, Tanco's $t_{max}$ is the largest number of missing observations while having the model be estimable with a probability $(1 - \alpha)$. Suppose there are $\binom{N}{t}$ possible design sub-matrices whose $t$ rows are removed and $\mathbf{X}_{t,j}$ denotes the $j$th $(n-t) \times p$ design sub-matrix of $\mathbf{X}$, $j = 1, 2, \ldots, \binom{N}{t}$. Tanco et al. (2013) proposed their criterion as

$$t_{\max}(1-\alpha) = \max\left\{t : 1 \leq t \leq N - p \text{ and } Pr\left(\text{Model is not estimable} \mid \mathbf{X}_t\right) \leq \alpha\right\},$$

where $\alpha$ is an upper bound on the following equation:

$$Pr\left(\text{Model is not estimable}|\mathbf{X}_t\right) = \frac{\sum_{j=1}^{\binom{N}{t}} I\left[|\mathbf{X}_{t,j}^{\mathrm{T}}\mathbf{X}_{t,j}| = 0\right]}{\binom{N}{t}}. \tag{1.9}$$

Typical values of $\alpha$ are .01 and .05. Since calculating an exact quantity (1.9) is too computationally time-consuming, the author estimated equation (1.9) by using the Monte-Carlo method.

Herzberg and Andrews (1976) proposed measures of robustness which are variations of the generalized variance criterion and the minimization of the maximum variance criterion. The authors wrote the maximum likelihood equation of a linear model in a term of $\mathbf{X}^{\mathrm{T}}\mathbf{D}^2\mathbf{X}$ where the matrix $\mathbf{D}^2$ is a diagonal matrix with diagonal elements $\{d_{ii}^2\}$. The missing observations are modeled by using the function:

$$d_{ii}^2 = \begin{cases} 0 & \text{with probability } p(\mathbf{x}_i); \\ 1 & \text{with probability } 1 - p(\mathbf{x}_i), \end{cases}$$

where $p(\mathbf{x}_i)$ is the probability of losing an observation located at $\mathbf{x}_i$. The value $d_{ii}^2$ can be zero for an outlier if it is rejected when estimating parameters (Herzberg and Andrews, 1976). The authors also defined a terminology of "probability of breakdown" of a design as the probability of $|\mathbf{X}^{\mathrm{T}}\mathbf{D}^2\mathbf{X}|$ being zero, i.e., $P(|\mathbf{X}^{\mathrm{T}}\mathbf{D}^2\mathbf{X}| = 0)$. This occurs when a sufficient number of observations are lost and not all parameters are estimable. It is postulated that the smaller the value of $P(|\mathbf{X}^{\mathrm{T}}\mathbf{D}^2\mathbf{X}| = 0)$, the more robust the design is against a missing value. Another measure by Herzberg and Andrews was $E(|\mathbf{X}^{\mathrm{T}}\mathbf{D}^2\mathbf{X}|)$. This measure can be described as the average precision to be expected from a design. Andrews and Herzberg (1979) also proposed a measure of design efficiency:

$$AH = \frac{1}{N}\frac{E(|\mathbf{X}^{\mathrm{T}}\mathbf{D}^2\mathbf{X}|^{1/p})}{|\mathbf{M}|^{1/p}},$$

where $\mathbf{M}$ is the Fisher information matrix of the $D$-optimal design. They compared this quantity to a measure of design efficiency given by Atkinson (1973),

$$A = \frac{1}{N}\frac{|\mathbf{X}^{\mathrm{T}}\mathbf{X}|^{1/p}}{|\mathbf{M}|^{1/p}}\ .$$

The larger the $A$ value is, the more robust the design is. However, they did not provide a method to construct the robust designs. The author also established the relationship between the reduced determinant with one missing design point and the determinant with no missing design points:

$$\frac{|\mathbf{X}^{\mathrm{T}}\mathbf{X}|_{\text{Reduce}}}{|\mathbf{X}^{\mathrm{T}}\mathbf{X}|} = 1 - h_{jj},$$

where $h_{jj}$ is the $j$th diagonal of matrix $\mathbf{X}(\mathbf{X}^{\mathrm{T}}\mathbf{X})^{-1}\mathbf{X}^{\mathrm{T}}$, also known as the leverage. The relationships between $|\mathbf{X}^{\mathrm{T}}\mathbf{X}|_{\text{Reduce}}$ with two or three missing design points and $|\mathbf{X}^{\mathrm{T}}\mathbf{X}|_{\text{Full}}$ were also discussed in Andrews and Herzberg (1979).

Ghosh (1982a) defined two measures, $I_1(\mathbf{a})$ and $I_2(\mathbf{a})$, of the information contained in a missing observation $\mathbf{a}$ as

$$I_1(\mathbf{a}) = \mathbf{a}^{\mathrm{T}}(\mathbf{X}^{\mathrm{T}}\mathbf{X})^{-1}\mathbf{a} \quad \text{and} \quad I_2(\mathbf{a}) = \frac{\mathbf{a}^{\mathrm{T}}(\mathbf{X}^{\mathrm{T}}\mathbf{X})^{-2}\mathbf{a}}{1 - \mathbf{a}^{\mathrm{T}}(\mathbf{X}^{\mathrm{T}}\mathbf{X})^{-1}\mathbf{a}},$$

where $\mathbf{a}^{\mathrm{T}}$ is a missing row in $\mathbf{X}$. For robust designs, the value of $I_1(\mathbf{a})$ will be between zero and one, and if the least information is contained in $\mathbf{a}$, $I_1(\mathbf{a})$ will be close to zero. In addition, Ghosh (1982b) observed that in robust designs, some observations are more informative than others, thus the loss in efficiency will be substantially larger if the most informative observation is missing. Ghosh, accordingly, suggested not collecting the least informative observations in the saturated or near-saturated designs in the beginning, but the most informative observations should be collected first.

Srivastava et al. (1991) extended the study of Ghosh (1982c) to several types of designs, e.g., balanced incomplete block, Youden square, and rotatable central composite designs when there is a single missing observation.

Akhtar and Prescott (1986) considered a loss due to a single missing observation in central composite designs. Note that the loss for these authors means the relative loss of efficiency in terms of $|\mathbf{X}^{\mathrm{T}}\mathbf{X}|$, equivalent to the $D$-optimality criterion. They proposed the maximum loss, denoted by

$$\ell_{max} = \max(\ell_f, \ell_a, \ell_c), \tag{1.10}$$

where $\ell_f, \ell_a$, and $\ell_c$ are the relative losses due to a single missing factorial, axial, or center point, respectively. The axial point distance, $\alpha$, from the center point, is varied so that the minimum of the maximum $\ell_{max}$ was found. The values of $\alpha$ for rotatable, outlier robust, and minimax loss central composite designs for $k = 2, 3, 4, 5$ with two center points were tabulated in Akhtar and Prescott (1986). In our experience, the minimax loss criterion, equation (1.10), used in CCDs does not necessarily give a very good design. For example, the choice of axial distance due to Akhtar and Prescott's approach for $k = 5$ with two center runs is 0.7045, but this robust design has only the $D$-efficiency of 33.812%. With a rotatable $\alpha$, the CCD with two center runs has the $D$-efficiency as high as 85.996%, which increases by 52% compared to the minimax loss central composite design. However, the criterion due to Akhtar and Prescott had influenced the research of Akram (1993), Lal et al. (2001) and Ahmad et al. (2012).

Akram (1993) discussed the robustness of several types of CCDs, e.g., cuboidal, spherical, orthogonal, rotatable, minimum variance, and Box and Draper outlier-robust designs, against three missing observations by applying Akhtar and Prescott's criterion. The authors also identified the influential points based on all possible combinations of factorial, axial, or center points that make $\mathbf{X}^{\mathrm{T}}\mathbf{X}$ singular. For example, for a large CCD, the largest loss occurs if two of three missing observations are axial points located on the same axis with any third axial or factorial point. However, no optimal designs are discussed, and the robust designs are based only on the existing CCDs.

Lal et al. (2001) investigated the robustness of experimental designs for estimating a subset of parameters in a linear model against missing observations. They showed that the design which is robust under a homoscedastic model is also robust under the heteroscedastic model and with correlated data. Their work, in general, focused on block designs.

Ahmad et al. (2012) proposed new augmented pairs minimax loss designs (APM) which are more robust against a single missing observation. This is considered as an improved Morris (2000) design together with the minimax loss criterion approach, introduced by Akhtar and Prescott (1986). The authors compared APM designs with CCDs, small composite designs, and Morris designs.

Hackl (1995) discussed the problem of an optimal allocation of design points where the trials may fail with non-zero probability. Given that $1 - p_i$ is the probability of being missing at point $\mathbf{x}_i$ and $r$ observations were collected after conducting an $N$-trial experimentation, $r \leq N$, the expected loss in estimating $\boldsymbol{\beta}$ for an $N$-trial design $\xi_u$ with potential missing trials is

$$D_{\xi_u}(\hat{\beta}) = \sum_{s=1}^{N} \frac{1}{s} \sum_{j \in J_s} p_{s,j}^{(N)} [\mathbf{M}(\xi_{s,j}^{(N)})]^{-1},$$

where $J_s$ is the set of all possible subsets of size $s$ in $\mathcal{X}(\xi_u)$ and the weight for the design $\xi_{s,j}^{(N)}$ is the probability:

$$p_{s,j}^{(N)} = \left( \prod_{i \in I_{s,j}^{(a)}(\xi_u)} p_i \right) \left( \prod_{i \in I_{s,j}^{(m)}(\xi_u)} (1 - p_i) \right),$$

where $I_{s,j}^{(a)}$ and $I_{s,j}^{(m)}$ are the available and missing subsets of responses, respectively. The author applied the aforementioned ideas to find an exact $D$-optimal design for the quadratic model $Y = \beta_0 + \beta_1 x + \beta_2 x^2 + \epsilon$ when there are failing trials. The optimal designs were found by comparing all possible design candidates, but closed-form formulas were not provided because of the complexity of the problem (Imhof et al., 2002).

Imhof et al. (2002) discussed that with potentially failing trials, the observed Fisher information matrix without a constant term is

$$I^O(\xi, \beta) = \sum_{i=1}^{n} \frac{n_i}{N} \frac{\partial f(x_i, \beta)}{\partial \beta} \frac{\partial f(x_i, \beta)^{\mathrm{T}}}{\partial \beta}, \tag{1.11}$$

where $n_i$ is the number of observations actually observed at point $\mathbf{x}_i$ and $\sum_{i=1}^{n} n_i = N$. The quantity $n_i$ is random, thus $I^O(\xi, \beta)$ is also random. If the response probability equals one for all points in $\mathcal{X}$, equation (1.11) will be the same as (1.3). Imhof et al. (2002) used the expected information matrix, $E\left[I^O(\xi, \beta)\right]$, to compare designs where the expectation takes over the response probabilities at design points in $\xi$. The expected information matrix is

$$J(\xi, \beta) = \int p(x) \frac{\partial f(x, \beta)}{\partial \beta} \frac{\partial f(x, \beta)^{\mathrm{T}}}{\partial \beta} \, d\xi(x) \, .$$

If $\Phi$ is a desirable optimality criterion, the $\Phi$-optimal design is found by maximizing $\Phi\left(J(\xi, \beta)\right)$. The $D$-optimal design for the polynomial model, $Y = \beta_0 + \sum_{i=1}^{m} \beta_i x^i$ , was found by analytically maximizing the determinant $|J(\xi, \beta)|$ where $p(x) = \kappa/(x - \theta)$, $\theta \in \mathbb{R} - \mathcal{X}$ and $\kappa > 0$. In their paper, only one independent variable was discussed because the problem was too complex to find the closed-form formula for the weight at each design point for multiple independent variables.

Imhof et al. (2004) continued working with the same criterion as Imhof et al. (2002) but used the Michaelis-Menten model, a non-linear model, with a broad class of response probability functions, e.g., $p_1(x, \theta) = (\theta + x)/(1 + x)$ and $p_2(x, \theta) =$

$[\theta + (b - x)]/[1 + (b - x)]$, where $0 \leq \theta \leq 1$. They also studied the robustness of the $D$-optimal designs when the response probability function is completely mis-specified.

## 5. Problem Statements and Outlines

Even though an experiment is carefully planned, some observations may be lost during the process of collecting data or may be suspicious in some way. For example, some responses might later be found to be wrong and could also be considered as missing data. MacEachern et al. (1995) mentioned that missing observations can be the result from many causes, for example, the loss of experimental units, cancellation of runs that take too long to achieve, and miscoded data where their correct values are non-trackable. In chemical industrial process, a certain combination of chemical levels may be highly volatile, and so the response is unlikely to be collectible, or the equipment may malfunction and the response is lost. In ecological studies, an arbitrary treatment in an experimental plot can be eaten or destroyed by animals (Robinson and Anderson-Cook, 2010). In the literature of missing values, there is evidence that missing observations can even occur in well-planned experiments. The risk of losing observations usually cannot be ignored in practice. Thus, it might be preferable to use designs less than optimal according to some design criteria but robust to missing data (Akhtar and Prescott, 1986).

It is known that as the number of design points increases, the precision of an approximate model will be improved, but many studies concentrate, instead, on reducing the number of design points (John, 1999). When small response surface designs are used, the effects of missing points may be substantial. The ability to estimate all parameters could be completely lost, the variances of predicted responses could be incredibly large in a certain part of an experimental region, and the generalized variance of parameter estimates could also be high. Not only small designs, but also some designs having many runs relative to the number of model parameters to be estimated are also susceptible to the aforementioned effects due to a loss of data. In an optimal design aspect, designs will usually not be optimal if (1) some missing values exist, (2) some observations are outliers, or (3) distribution of errors departs from normality (Herzberg and Andrews, 1976). The concepts of optimality, however, are appropriate for design comparisons when the number of observations is valid as advertised (Imhof et al., 2004).

Most published research on missing design data can be categorized into three groups: (1) those providing measures of robustness against missing observations, i.e., Andrews and Herzberg (1979), Ghosh (1979), Herzberg and Andrews (1975, 1976), MacEachern et al. (1995), Srivastava et al. (1991), Tanco et al. (2013); (2) those studying the loss due to missing observations in central composite designs and its variations, i.e., Ahmad and Gilmour (2010), Akhtar and Prescott (1986), Akram (1993), Herzberg and Andrews (1976), Whittinghill (1998); and (3) those constructing of robust designs, i.e., Hackl (1995), Imhof et al. (2002, 2004). Only the last category incorporated the construction of robust designs for fitting second-order models. They analytically found approximate optimal designs, whose theoretically optimal weights can be irrational numbers, but because of mathematical complexity only one factor is considered and the probability of missing data is needed to be known beforehand which might not be realistic.

It is clear that many issues regarding missing data in RSM have not been addressed or explored. The problems and corresponding objectives addressed in this dissertation are as follows.

1. The effects of missing data for CCDs and BBDs have been only studied in terms of the $t_{\max}$ criterion and $|\mathbf{X}^{\mathrm{T}}\mathbf{X}|$. The $k$-factor CCDs with a different number of center points can have the same $t_{\max}$ (MacEachern et al., 1995), so a measure giving more information is required. We propose a new measure of robustness against a missing response and apply it to CCDs, HSCDs, PBCDs, BBDs, hybrid designs, and some small exact alphabetic optimal designs. In addition, the impact of a missing point will be observed via the fraction of design space (FDS) plots, variance dispersion graphs (VDGs), and contours of SPVs. These issues will be in Chapter 2.

2. Both FDS plots and VDGs can be very useful to show the influence of missing points, but a reliable R package that can produce those plots is still needed. Moreover, no R packages that made a contour of SPVs have been found, so we submitted a new R package to do so. The algorithm used to generate uniformly distributed random points inside a $k$-dimensional sphere of radius $R$ and on the surface of a $k$ dimensional hypercube will also be described in Chapter 2.

3. The behaviors of $D$-, $A$-, $G$-, and $IV$-efficiencies with a missing response in CCDs are not known when the values of $\alpha$ are varied. The CCDs with one center run and different values of axial distance will be studied when one missing response occurs. The precision of predictions of resulting CCDs will be also examined. These issues are in Chapter 3.

4. There are no $n$-point $k$-factor optimal robust exact designs which can be employed without knowing the probability of missing data function. We will develop the existing optimality criteria and use them to construct the robust exact designs against one missing value. We assume that small optimal exact designs being created are typically used in the final stage of RSM in which

all important factors are discovered, and the experimental region is thoroughly studied. Furthermore, we do assume that the probabilities of the response values being collected are the same for all design points. Thus, the missing data occur under the mechanism of missing completely at random (MCAR). This type of mechanism of missingness is *ignorable*. For more details in types of missing data, refer to Rubin (1976), Little and Rubin (2002), and Allison (2001). This topic will be studied in Chapter 4.

5. None of the existing literature discussed missing data problems in mixture experiments. The impact of a missing response in this context will be explored, and also the optimal robust exact mixture designs will be constructed via the point-exchange algorithm with the modified $D$-, $A$-, $G$-, and $IV$-optimality criteria. This topic is presented in Chapter 5.

6. So far, we assume a missing observation might happen in a future experiment, and thus we find the robust designs to fit the second-order model with the minimum loss in a desirable optimality criterion when a missing response actually happens. Suppose, however, a researcher decides to use a certain experimental design with a randomized run order, but when collecting the data, a missing point occurs in the $i$th experimental run. Instead of continuing to collect the rest of data as initially planned, a new set of design points is constructed based on a certain optimality criterion. This augmented design is then used to collect the remaining responses. This idea will be referred to as "adaptive" experimentation. This will be discussed in Chapter 6.

# CHAPTER 2

# ROBUSTNESS OF RESPONSE SURFACE DESIGNS

In this chapter, the sensitivity of small second-order response surface designs will be studied through the loss of the $D$-efficiency. Also, the R package "VdgRsm" has been developed to make variance dispersion graphs (VDGs), fraction of design space (FDS) plots, and contours of scaled prediction variances (SPVs) to see the impact of a missing point on prediction variances. Methods for generating $N$ points on a surface of a $k$-dimensional sphere of radius $r$ and on a surface of a $k$-dimensional cube will be described. At the end of this chapter, three examples will be given that describe how to investigate the impact of a missing response in response surface designs via VDGs, FDS plots, and contours of SPVs.

## 1. Robustness of Response Surface Designs to One Missing Response

MacEachern et al. (1995) showed that $k$-factor CCDs with $n_c \geq 1$ and axial distance of $\alpha = \sqrt{k}$ have $t_{\max} = \min\{n_c - 1, 3\}$ and those with $n_c \geq 1$ and $\alpha \neq \sqrt{k}$ have $t_{\max} = \min\{n_c + 1, 3\}$. For example, the 2-factor CCD with $n_c = 1, \alpha = 1$ and 2-factor CCD with $n_c = 3, \alpha = \sqrt{2}$ will have the same $t_{\max}$ of two. One might think the latter design should have been more robust to missing data than the former because it has more design points. However, this is not straightforward because the sensitivity of CCDs is related to both $n_c$ and $\alpha$. As a supplement to the $t_{\max}$ criterion, we need a measure to tell us how the $D$-efficiency changes when there is one missing point. A design having a small change in the $D$-efficiency when one missing point happens is said to be a robust design in terms of the $D$-efficiency.

We will study the robustness of designs via newly proposed measures that will now be described. Suppose the original information matrix $\mathbf{X}^{\mathrm{T}}\mathbf{X}$ is $N \times p$ where $N$ and $p$ are the number of observations and parameters in a second-order model, respectively. After removing the $i$th point, the corresponding information matrix is $\mathbf{X}_{-i}^{\mathrm{T}}\mathbf{X}_{-i}$, and the true $D$-efficiency of a design can be approximated by a lower bound $D$-efficiency defined as

$$D_{-i} = \frac{|\mathbf{X}_{-i}^{\mathrm{T}}\mathbf{X}_{-i}|^{1/p}}{N-1} \times 100, \tag{2.1}$$

where $i = 1, 2, \ldots, N$ and $N - 1 \geq p$. The minimum of $D_{-i}$ will depict the worst case scenario of losing the most "sensitive" observation and is defined as

$$\text{Min } D = \min_{1 \leq i \leq N} \{D_{-i}\}. \tag{2.2}$$

We propose a maximum relative loss in $D$-efficiency of design $\xi_N$ as

$$\text{Max } \ell(\xi_N) = \frac{D\text{-efficiency} - \text{Min } D}{D\text{-efficiency}} \times 100, \tag{2.3}$$

where $D$-efficiency is defined as (1.4). Both Max $\ell(\xi_N)$ and Min $D$ represent the worst case. To assess how the $D$-efficiency changes when one arbitrary run is missing, we first define a *leave-m-out* $D$-efficiency as

$$D^{(m)} = \frac{\sum_{t \in T_m} D_t}{\binom{N}{m}}, \tag{2.4}$$

where $T_m$ is a set of all possible subsets of $N - m$ design points and $D_t$ is the $D$-efficiency of subset design $t \in T_m$. In particular, when $m = 1$, $D^{(1)}$ is the average of $D$-efficiencies of all possible designs having one missing point. We can then use $D^{(1)}$

to calculate the average relative loss in $D$-efficiency defined as

$$\text{Avg } \ell(\xi_N) = \frac{D\text{-efficiency} - D^{(1)}}{D\text{-efficiency}} \times 100\,. \tag{2.5}$$

If Avg $\ell(\xi_N)$ is relatively close to Max $\ell(\xi_N)$, all design points are essentially equally important. If this is not a case, some points are more important than the others. The Avg $\ell(\xi_N)$ measure is useful when we compare the robustness of two or more designs against one missing value because it is based on the $D$-efficiency which is often used to compare designs with different sample sizes. The Avg $\ell(\xi_N)$ cannot replace the $t_{\max}$ criterion but supplements it as they each give different information. Note that the $t_{\max}$ criterion gives us the maximum number of arbitrary observations which can be lost, and all parameters are still estimable.

The Max $\ell(\xi_N)$, Min $D$, and Avg $\ell(\xi_N)$ will be calculated for CCDs, HSCDs, PBCDs, BBDs, hybrid designs, and exact $D$-, $A$-, $IV$-, and $G$-optimal designs.

### 1.1. Robustness of CCDs ($k = 2, 3, 4$)

The number of center runs, $n_c$, and values of axial distance, $\alpha$, are varied for CCDs. If $\alpha = 1$, such a design is called the face-centered composite design (FCD), and if $\alpha$ equals the fourth root of the number of factorial runs, the corresponding CCD is called the *rotatable* CCD. Table 2.1 summarizes the maximum and average relative loss of the $D$-efficiency for CCDs with different values of $\alpha$ and $n_c$ for $k = 2$, 3, and 4.

Inspection of Table 2.1 reveals that the Avg $\ell$ of $k$-factor designs with the same $\alpha$ decreases as $n_c$ increases. Also, the Avg $\ell$ tends to be low for CCDs having high values of $t_{\max}$. When considering $k$-factor CCDs, $k = 2, 3, 4$ with $\alpha = 1$, as $n_c$ increases, the Max $\ell$, Min $D$, and Avg $\ell$ only slightly change. In general, increasing the number

Table 2.1: The Avg $\ell(\xi_N)$, Max $\ell(\xi_N)$, and Min $D$ of CCDs.

| $k$ | $\alpha$ | $n_c$ | $N$ | $t_{\max}$ | Avg $\ell(\xi_N)\%$ | Max $\ell(\xi_N)\%$ | Min $D$ |
|---|---|---|---|---|---|---|---|
| 2 | 1 | 1 | 9 | 2 | 7.344 | 14.371 | 39.581 |
| | | 2 | 10 | 3 | 6.026 | 14.863 | 38.125 |
| | | 3 | 11 | 3 | 5.214 | 15.455 | 36.215 |
| | $\sqrt{2}$ | 1 | 9 | 0 | 15.081 | 100.000 | 0.000 |
| | | 2 | 10 | 1 | 4.719 | 5.645 | 59.911 |
| | | 3 | 11 | 2 | 4.025 | 6.589 | 57.690 |
| 3 | 1 | 1 | 15 | 2 | 4.863 | 8.659 | 40.844 |
| | | 2 | 16 | 3 | 4.416 | 8.997 | 39.131 |
| | | 3 | 17 | 3 | 4.069 | 9.309 | 37.452 |
| | $\sqrt[4]{8}$ | 1 | 15 | 2 | 5.259 | 31.364 | 47.155 |
| | | 2 | 16 | 3 | 3.388 | 4.526 | 65.870 |
| | | 3 | 17 | 3 | 3.085 | 4.896 | 64.297 |
| | $\sqrt{3}$ | 1 | 15 | 0 | 9.797 | 100.000 | 0.000 |
| | | 2 | 16 | 1 | 3.370 | 4.262 | 68.425 |
| | | 3 | 17 | 2 | 3.068 | 4.636 | 66.803 |
| 4 | 1 | 1 | 25 | 2 | 2.159 | 3.050 | 43.165 |
| | | 2 | 26 | 3 | 2.039 | 3.201 | 41.916 |
| | | 3 | 27 | 3 | 1.938 | 3.340 | 40.700 |
| | 2 | 1 | 25 | 0 | 5.669 | 100.000 | 0.000 |
| | | 2 | 26 | 1 | 1.804 | 1.896 | 75.800 |
| | | 3 | 27 | 2 | 1.695 | 2.041 | 74.881 |

of center runs does not much improve the robustness of CCDs with $\alpha = 1$. In most cases, with the exception of the rotatable or near-rotatable designs with $n_c = 1$, the Max $\ell$ increases as $n_c$ increases due to that fact that adding center runs results in decreasing the $D$-efficiency. When $\alpha$ is near or equal to $\sqrt{k}$, designs are not very robust to one missing point. The $\mathbf{X}^{\mathrm{T}}\mathbf{X}$ matrix of CCDs with $n_c = 1$ and $\alpha = \sqrt{k}$ will be singular if one center point happens to be missing, and those designs will have the Max $\ell$ of 100% and Min $D$ of 0. Hence, we suggest including two center runs when CCDs with $\alpha = \sqrt{k}$ are employed. The third center run, in general, does not appreciably change the values of the Max $\ell$, Min $D$, or Avg $\ell$.

1.2. Robustness of HSCDs ($k$ = 2, 3, 4)

Like CCDs, the number of center runs, $n_c$, and values of axial distance, $\alpha$, are varied for HSCDs. However, the rotatable values of $\alpha$ for $k = 2, 3$, and 4 are $\sqrt[4]{2} \approx 1.189$, 2, and $\sqrt[4]{8} \approx 1.682$, respectively. The Avg $\ell(\xi_N)$, Max $\ell(\xi_N)$, and Min $D$ of HSCDs are summarized in Table 2.2.

Table 2.2: The Avg $\ell(\xi_N)$, Max $\ell(\xi_N)$, and Min $D$ of HSCDs.

| $k$ | $\alpha$ | $n_c$ | $N$ | Avg $\ell(\xi_N)$% | Max $\ell(\xi_N)$% | Min $D$ |
|---|---|---|---|---|---|---|
| 2 | 1 | 1 | 7 | 25.816 | 100.000 | 0.000 |
| | | 2 | 8 | 10.960 | 15.219 | 25.454 |
| | | 3 | 9 | 9.313 | 16.543 | 23.830 |
| | $\sqrt[4]{2}$ | 1 | 7 | 25.959 | 100.000 | 0.000 |
| | | 2 | 8 | 11.082 | 17.027 | 33.977 |
| | | 3 | 9 | 9.420 | 18.323 | 31.809 |
| | $\sqrt{2}$ | 1 | 7 | 26.403 | 100.000 | 0.000 |
| | | 2 | 8 | 11.462 | 19.189 | 45.354 |
| | | 3 | 9 | 9.753 | 20.450 | 42.460 |
| 3 | 1 | 1 | 11 | 21.056 | 30.014 | 20.000 |
| | | 2 | 12 | 16.543 | 27.561 | 19.487 |
| | | 3 | 13 | 14.055 | 26.641 | 18.602 |
| | $\sqrt[4]{4}$ | 1 | 11 | 14.373 | 15.515 | 37.321 |
| | | 2 | 12 | 11.865 | 14.912 | 36.364 |
| | | 3 | 13 | 10.485 | 15.018 | 34.713 |
| | $\sqrt{3}$ | 1 | 11 | 21.146 | 100.000 | 0.000 |
| | | 2 | 12 | 11.350 | 16.789 | 48.298 |
| | | 3 | 13 | 10.282 | 17.367 | 46.105 |
| 4 | 1 | 1 | 17 | 13.677 | 17.503 | 24.229 |
| | | 2 | 18 | 11.849 | 16.703 | 23.376 |
| | | 3 | 19 | 10.688 | 16.822 | 22.334 |
| | $\sqrt[4]{8}$ | 1 | 17 | 9.308 | 12.204 | 46.162 |
| | | 2 | 18 | 8.200 | 11.506 | 45.501 |
| | | 3 | 19 | 7.546 | 11.402 | 44.151 |
| | 2 | 1 | 17 | 13.734 | 100.000 | 0.000 |
| | | 2 | 18 | 7.575 | 11.987 | 56.613 |
| | | 3 | 19 | 7.100 | 12.258 | 54.933 |

For $k = 2$, adding the second center run considerably improves the robustness of HSCDs against one missing point, and designs with $n_c = 1$ all have Max $\ell$ of 100% regardless of values of $\alpha$. For $k = 3$ and 4, most designs have Avg $\ell$ between 8 and 14% except for 3-factor HSCDs. The designs with $\alpha = \sqrt{k}$, of course, will suffer from singularity of $\mathbf{X}^{\mathrm{T}}\mathbf{X}$ if the center run is lost. Like CCDs, adding a third center run in any HSCDs does not much reduce the Avg $\ell$ and Max $\ell$, or increase the Min $D$. In conclusion, we recommend including two center runs for any $\alpha$ for $k = 2$ and 3, and for $k = 4$ one center run can be practical except for $\alpha = 2$ for which two center runs are needed to avoid singularity.

### 1.3. Robustness of PBCDs ($k = 5$, 6)

Because PBCDs and HSCDs are the same for $k = 3, 4$ and 6, only PBCDs for $k = 5$ and 6 are considered. Those are near-saturated designs, and it is interesting to observe how sensitive they are to a missing run. The number of factorial points for $k = 5$ and 6 are 12 and 16, respectively. As shown in Table 1.2, factorial points are chosen from particular columns of PBDs to form PBCDs in a way that the $D$-criterion is maximized.

From Table 2.3, PBCDs with $\alpha = 1$ have larger Avg $\ell$'s than those with rotatable $\alpha$ or $\alpha = \sqrt{k}$. Except for PBCDs with $\alpha = \sqrt{k}$, the second center run does not much improve the Max $\ell$ and Min $D$, thus one center run is an efficient choice for 5-factor PBCDs. For 6-factor PBCDs with the same $n_c$, as $\alpha$ increases from 1 to 2, the Avg $\ell$ or Max $\ell$ decreases by almost 50%. If $\alpha$ can be set by the experimenter, then $\alpha = 2$ is preferable over $\alpha = 1$ for $k = 6$.

Table 2.3: The Avg $\ell(\xi_N)$, Max $\ell(\xi_N)$, and Min $D$ of PBCDs.

| $k$ | $\alpha$ | $n_c$ | $N$ | Avg $\ell(\xi_N)\%$ | Max $\ell(\xi_N)\%$ | Min $D$ |
|---|---|---|---|---|---|---|
| 5 | 1 | 1 | 23 | 15.523 | 28.205 | 17.934 |
| | | 2 | 24 | 13.873 | 26.394 | 17.730 |
| | | 3 | 25 | 12.773 | 25.499 | 17.323 |
| | $\sqrt[4]{12}$ | 1 | 23 | 9.302 | 14.621 | 41.738 |
| | | 2 | 24 | 8.329 | 13.865 | 41.263 |
| | | 3 | 25 | 7.763 | 13.654 | 40.315 |
| | $\sqrt{5}$ | 1 | 23 | 10.770 | 100.000 | 0.000 |
| | | 2 | 24 | 7.143 | 10.713 | 53.120 |
| | | 3 | 25 | 6.814 | 10.868 | 51.900 |
| 6 | 1 | 1 | 29 | 18.622 | 24.575 | 19.227 |
| | | 2 | 30 | 16.392 | 23.062 | 19.029 |
| | | 3 | 31 | 15.024 | 22.287 | 18.663 |
| | 2 | 1 | 29 | 10.597 | 12.907 | 46.876 |
| | | 2 | 30 | 9.390 | 12.112 | 46.394 |
| | | 3 | 31 | 8.741 | 11.840 | 45.502 |
| | $\sqrt{6}$ | 1 | 29 | 11.345 | 100.000 | 0.000 |
| | | 2 | 30 | 7.675 | 9.097 | 60.209 |
| | | 3 | 31 | 7.400 | 9.198 | 59.051 |

1.4. Robustness of Hybrid Designs ($k = 3, 4, 6$)

The hybrid designs R416A and R416B do not need a center run to be added to study the robustness against one missing value because the number of design points is one greater than the number of parameters in a second-order model. On the contrary, both R628A and R628B designs are saturated and need one or more center runs to study the robustness. Note that designs R311A, R311B, R416C, and R628A originally have one center run included. In this study, the original design point $\mathbf{x}'_i$, $i = 1, 2, \ldots, N$, in a $k$-factor hybrid design is scaled to be on $k$-dimensional sphere by the following formula:

$$\mathbf{x}_i = \sqrt{k}\frac{\mathbf{x}'_i}{\|\mathbf{x}'_i\|} = \sqrt{k}\frac{\mathbf{x}'_i}{\sqrt{\sum_{j=1}^{k} x'^2_{ij}}},$$

Table 2.4: The Avg $\ell(\xi_N)$, Max $\ell(\xi_N)$, and Min $D$ of hybrid designs.

| $k$ | Design | $n_c$ | $N$ | Avg $\ell(\xi_N)$% | Max $\ell(\xi_N)$% | Min $D$ |
|---|---|---|---|---|---|---|
| 3 | R310 | 1 | 11 | 44.604 | 78.055 | 9.207 |
| | | 2 | 12 | 39.401 | 77.576 | 8.971 |
| | | 3 | 13 | 35.678 | 77.455 | 8.564 |
| | R311A | 1 | 11 | 21.659 | 100.000 | 0.000 |
| | | 2 | 12 | 12.091 | 17.325 | 54.909 |
| | | 3 | 13 | 10.960 | 17.899 | 52.416 |
| | R311B | 1 | 11 | 20.877 | 96.123 | 2.753 |
| | | 2 | 12 | 11.426 | 15.803 | 58.727 |
| | | 3 | 13 | 10.351 | 16.388 | 56.061 |
| 4 | R416A | 0 | 16 | 48.943 | 100.000 | 0.000 |
| | | 1 | 17 | 9.626 | 15.497 | 59.167 |
| | | 2 | 18 | 8.543 | 15.541 | 58.320 |
| | | 3 | 19 | 7.984 | 15.716 | 56.589 |
| | R416B | 0 | 16 | 49.017 | 91.861 | 6.062 |
| | | 1 | 17 | 18.983 | 40.266 | 43.919 |
| | | 2 | 18 | 17.351 | 39.348 | 43.290 |
| | | 3 | 19 | 16.187 | 39.072 | 42.005 |
| | R416C | 1 | 16 | 52.334 | 100.000 | 0.000 |
| | | 2 | 17 | 44.537 | 100.000 | 0.000 |
| | | 3 | 18 | 41.856 | 100.000 | 0.000 |
| 6 | R628A | 2 | 29 | 83.040 | 100.000 | 0.000 |
| | | 3 | 30 | 67.179 | 100.000 | 0.000 |
| | | 4 | 31 | 77.375 | 100.000 | 0.000 |
| | R628B | 1 | 29 | 11.790 | 14.129 | 65.521 |
| | | 2 | 30 | 11.075 | 13.984 | 64.847 |
| | | 3 | 31 | 10.615 | 13.993 | 63.600 |

where $x_{ij}$ is the value of the $j$th factor in the $i$th observation. The Avg $\ell(\xi_N)$, Max $\ell(\xi_N)$, and Min $D$ are presented in Table 2.4.

Inspection of Table 2.4 reveals that, in general, among three-factor hybrid designs, the R311B seems to be the most robust to a missing run as its values of Avg $\ell$ are the lowest. When considering three-factor designs having the same $N$ for $N = 11, 12$, and 13, the R310 with $n_c = 1$ has the highest Min $D$ when $N = 11$, and the R311B has the highest Min $D$ for $N = 11$ and 12. Thus, the R311A seems to be the least

Table 2.5: The Avg $\ell(\xi_N)$, Max $\ell(\xi_N)$, and Min $D$ of BBDs.

| $k$ | $n_c$ | $N$ | Avg $\ell(\xi_N)$% | Max $\ell(\xi_N)$% | Min $D$ |
|---|---|---|---|---|---|
| 3 | 1 | 13 | 12.945 | 100.000 | 0.000 |
| | 2 | 14 | 5.287 | 6.248 | 35.345 |
| | 3 | 15 | 4.804 | 6.727 | 34.178 |
| | 4 | 16 | 4.445 | 7.141 | 32.831 |
| 4 | 1 | 25 | 5.669 | 100.000 | 100.000 |
| | 2 | 26 | 1.804 | 1.896 | 25.005 |
| | 3 | 27 | 1.695 | 2.041 | 24.702 |
| | 4 | 28 | 1.617 | 2.176 | 24.247 |
| 5 | 1 | 41 | 3.247 | 100.000 | 0.000 |
| | 2 | 42 | 0.887 | 0.887 | 17.292 |
| | 3 | 43 | 0.848 | 0.943 | 17.209 |
| | 3 | 44 | 0.821 | 0.997 | 17.041 |

robust to a missing value. For $k = 4$, when comparing designs with the same $N$, the R416A is considered to be the most robust because it has the lowest Avg $\ell$ and the lowest Max $\ell$, and the highest Min $D$ for all $N$'s except for $N = 16$. For $k = 6$, the R628B is obviously superior to the R628A for all $N$'s.

## 1.5. Robustness of BBDs ($k$ = 3, 4, 5)

As discussed in Chapter 1, Section 3.5, the BBDs are naturally spherical, and design points are equidistant from the center run. At least one center run is required to avoid singularity, so designs with one center run all have the Max $\ell$ of 100% as presented in Table 2.5. When $n_c > 1$, the BBDs are very robust to a missing run as their Avg $\ell$ and Max $\ell$ are very low, between 1 and 6%. Adding the third center run slightly decreases the Avg $\ell$, thus having two center runs is sufficient to make the BBD robust against a missing value.

## 1.6. Robustness of Optimal Designs ($k = 2, 3$)

The optimal designs in this study are catalogued in Borkowski (2003b). The Avg $\ell(\xi_N)$, Max $\ell(\xi_N)$, and Min $D$ were calculated for small exact D-, A-, G-, and IV-optimal designs as summarized in Table 2.6.

Table 2.6: The Avg $\ell(\xi_N)$, Max $\ell(\xi_N)$, and Min $D$ of small exact optimal designs.

| $k$ | Design | $N$ | Avg $\ell(\xi_N)\%$ | Max $\ell(\xi_N)\%$ | Min $D$ |
|---|---|---|---|---|---|
| 2 | Exact $D$-optimal | 7 | 22.742 | 44.161 | 25.144 |
| | | 8 | 11.478 | 26.236 | 33.648 |
| | | 9 | 7.344 | 14.372 | 39.581 |
| | | 10 | 5.461 | 14.327 | 39.400 |
| | | 11 | 4.084 | 13.895 | 39.739 |
| | | 12 | 3.065 | 13.583 | 40.310 |
| | Exact $A$-optimal | 7 | 70.303 | 100.000 | 0.000 |
| | | 8 | 16.178 | 42.399 | 23.972 |
| | | 9 | 7.344 | 14.371 | 39.581 |
| | | 10 | 6.026 | 14.863 | 38.125 |
| | | 11 | 5.214 | 15.455 | 36.215 |
| | | 12 | 4.276 | 16.698 | 35.051 |
| | Exact $G$-optimal | 7 | 26.698 | 100.000 | 0.000 |
| | | 8 | 10.455 | 16.958 | 36.953 |
| | | 9 | 6.926 | 12.073 | 38.149 |
| | | 10 | 5.046 | 8.759 | 39.574 |
| | | 11 | 3.783 | 6.912 | 40.354 |
| | | 12 | 2.932 | 5.933 | 39.127 |
| | Exact $IV$-optimal | 7 | 70.303 | 100.000 | 0.000 |
| | | 8 | 15.732 | 36.014 | 26.183 |
| | | 9 | 8.587 | 20.954 | 33.144 |
| | | 10 | 6.026 | 14.863 | 38.125 |
| | | 11 | 5.214 | 15.455 | 36.215 |
| | | 12 | 4.631 | 16.006 | 34.290 |

Table 2.6 (continued)

| $k$ | Design | $N$ | Avg $\ell(\xi_N)$% | Max $\ell(\xi_N)$% | Min $D$ |
|---|---|---|---|---|---|
| 3 | Exact $D$-optimal | 11 | 35.020 | 100.000 | 0.000 |
| | | 12 | 9.664 | 13.404 | 38.956 |
| | | 13 | 7.051 | 17.385 | 38.326 |
| | | 14 | 5.606 | 11.377 | 41.056 |
| | | 15 | 4.579 | 11.535 | 40.719 |
| | | 16 | 3.858 | 11.205 | 38.944 |
| | Exact $A$-optimal | 11 | 31.419 | 60.818 | 16.020 |
| | | 12 | 13.546 | 28.130 | 30.313 |
| | | 13 | 13.772 | 52.042 | 19.314 |
| | | 14 | 5.497 | 8.317 | 42.453 |
| | | 15 | 4.863 | 8.659 | 40.844 |
| | | 16 | 4.564 | 9.775 | 39.273 |
| | Exact $G$-optimal | 11 | 15.774 | 26.197 | 30.817 |
| | | 12 | 10.882 | 33.403 | 27.875 |
| | | 13 | 7.042 | 15.620 | 38.561 |
| | | 14 | 5.497 | 8.317 | 42.453 |
| | | 15 | 4.640 | 8.535 | 41.922 |
| | | 16 | 4.564 | 9.775 | 39.273 |
| | Exact $IV$-optimal | 11 | 28.068 | 51.303 | 19.951 |
| | | 12 | 22.946 | 52.907 | 18.571 |
| | | 13 | 13.772 | 52.042 | 19.314 |
| | | 14 | 8.942 | 32.901 | 26.765 |
| | | 15 | 5.183 | 9.995 | 39.445 |
| | | 16 | 4.702 | 10.395 | 37.807 |

Inspection of Table 2.6 reveals that for $k = 2$, the Avg $\ell$ and Max $\ell$ considerably decrease when $N$ increases from 7 to 8 regardless of the optimality criterion. The 7-point $A$-, $G$-, and $IV$-optimal designs are rather sensitive to a missing point because the corresponding Max $\ell$ can be 100%. Among two-factor optimal designs, the exact $G$-optimals, for most of $N$'s, have the lowest Avg $\ell$ and Max $\ell$. However, when $N \geq 9$, the $D$-, $A$-, $G$-, and $IV$-optimal designs are not much different in terms of the Avg $\ell$, Max $\ell$, or Min $D$. For three-factor designs with the same $N$, robustness to a missing is rather different depending on the criterion. For example, when an 11-point design is used, the $G$-optimal design is obviously superior to the others, but for $N = 12$, the $D$-optimal design is preferable. However, as $N$ increases, the Avg $\ell$ and Max $\ell$ slightly decrease regardless of the design criterion being used. For example, for $A$-optimal designs, when $N \geq 14$, all robustness criteria do not change much.

## 2. The Package "VdgRsm"

The variance dispersion graph (VDG), introduced by Giovannitti-Jensen and Myers (1989), is a plot of the maximum, minimum, and average of SPVs for points on a sphere against the corresponding radius of the sphere. It is used to depict the comprehensive behavior of prediction variances throughout a region. Myers et al. (1992) showed that using the $D$-optimality criterion alone can be misleading if prediction is of interest. Trinca and Gilmour (1999) introduced the difference VDG (DVDG) that can be used to choose a design in a particular circumstance. Borkowski (1995) analytically derived functions for finding the maximum, minimum, and average spherical variances for CCDs and BBDs. Rozum and Myers (1991) expanded the VDG to a cuboidal region.

Zahran et al. (2003) addressed a weakness of the VDG by proposing a new graphical method called the Fraction of Design Space (FDS) plot; this cannot displace the VDG but rather supplements it. Given that the SPVs are calculated throughout a design space, the FDS plot is a plot of the fraction of design space that is less than or equal to the given SPV. Let $\nu$ be any given SPV, $k$ be the number of factors, and $\Psi$ be the total volume of the design region. The FDS is defined as

$$FDS = \frac{1}{\Psi} \underset{A}{\int \cdots \int} dx_k \ldots dx_1,$$

where $A = \{(x_1, x_2, \ldots, x_k) : SPV(\mathbf{x}) < \nu\}$. Only one R package called "Vdgraph" (Lawson, 2012) is able to make VDGs and FDS plots, but only designs in a spherical region are allowed. Moreover, we found that the Vdgraph package has an error in making the VDG for some designs. Examples include a five-factor CCD with $n_c = 5$ and $\alpha = \sqrt[4]{32}$ and a two-factor CCD with $n_c = 2$ and $\alpha = \sqrt{2}$. These two designs are rotatable but the maximum SPVs are not the same as the average SPVs for some values of $\alpha$ in the output obtained from the Vdgraph package.

Accordingly we developed and submitted the R package called "VdgRsm" to the Comprehensive R Archive Network (CRAN) in 2014. The VdgRsm package is applicable for designs in spherical and cuboidal regions, and both VDGs and FDS plots are available (Srisuradetchai and Borkowski, 2014). The radius in a cuboidal region is calculated in a usual way but restricted to design points in the cube. For example, a two-factor FCD has only 4 of its design points, $(\pm 1, \pm 1)$, having a radius of $\sqrt{2}$, but the number of design points with radius of $\sqrt{2}$ in a rotatable two-factor design is infinite.

The VDGs of the rotatable five-factor CCD with $n_c = 4$ produced by the Vdgraph (left) and VdgRsm (right) R packages are illustrated in Figure 2.1. Because the maximum, average, and minimum of SPVs are the same for each radius, three lines will completely overlap as in the right panel in Figure 2.1. In 2015, the VdgRsm package included a function that can generate contour plots of SPVs and these will be presented in the next section.

In our R package, uniformly distributed random numbers are generated which are mainly used in calculating the SPV. Figure 2.2 shows an example of $1,500$ uniformly distributed points in a circle of radius $\sqrt{2}$ representing a design region. The algorithm for generating points uniformly inside a $k$-dimensional hypersphere of radius $R$ is the following:

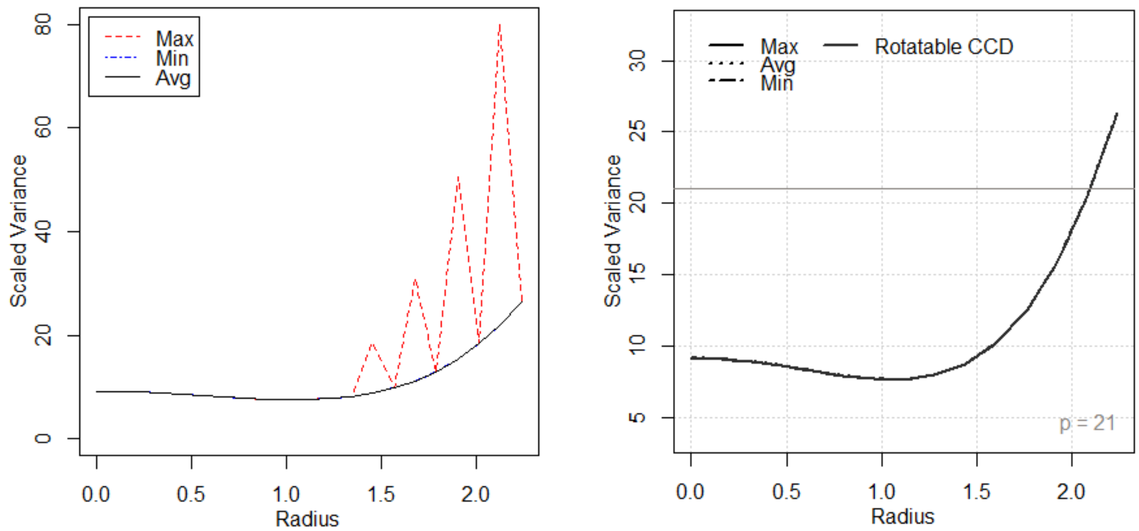



Figure 2.1: Examples of VDGs produced by the R package Vdgraph (left) and Vd-gRsm (right).

1. Determine a radius $R$ for the hypersphere;

2. Generate a vector of $k$ random variables $\mathbf{x}^{\mathrm{T}} = (x_1, x_2, \ldots, x_k)$ where $x_i$ comes from a standard normal distribution;

3. Find a unit vector $\mathbf{z}$ whose the $i$th element is

$$z_i = \frac{x_i}{\sqrt{x_1^2 + x_2^2 + \ldots + x_k^2}} = \frac{x_i}{||x||},$$

   where $i = 1, 2, \ldots, k$. Then a vector $\mathbf{z}^{\mathrm{T}} = \left(\frac{x_1}{||x||}, \frac{x_2}{||x||}, \ldots, \frac{x_k}{||x||}\right)$ is on the surface of a unit $k$-hypersphere. The point $\mathbf{z}$ will be uniformly distributed because the distribution of point $\mathbf{x}^{\mathrm{T}} = (x_1, x_2, \ldots, x_k)$ depends only on the distance from the origin and not direction, so projecting it to a unit sphere makes it uniformly distributed (Knuth, 1997). The vector $z_i$ would tell us a direction;

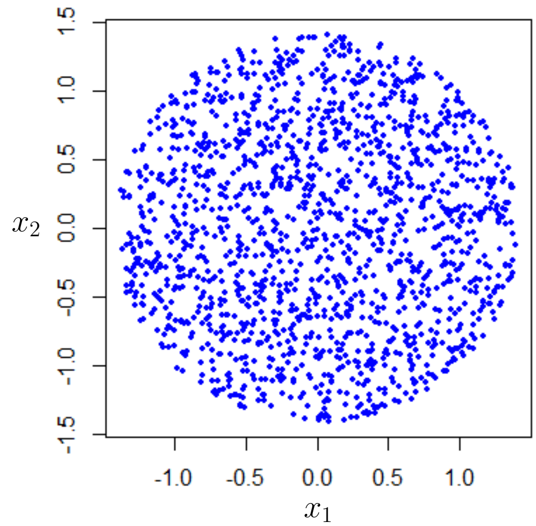



Figure 2.2: Uniformly random points within a circle of radius $\sqrt{2}$.

4. Let $D$ be the distance between the origin point and a point of radius $r$ in a $k$-dimensional hypersphere of radius $R$, $0 \leq r \leq R$, and $Pr(D \leq r) = (r/R)^k$. From the probability integral transformation, we will generate a uniform random number $U$, between 0 and 1, and then solve for $r$ to satisfy $Pr(D \leq r) = u$. Thus, $r = RU^{1/k}$. Multiply vector $\mathbf{z}$ by the radius $r = RU^{1/k}$ to produce the point $(rz_1, rz_2, \ldots, rz_k)$ uniformly distributed inside a $k$-dimensional sphere of radius $R$ (Fishman, 1996);

5. Repeat steps 2 to 4 for $M$ times in order to generate $M$ points.

The previous procedures are used to generate design points for constructing VDGs and FDS plots in both spherical and cuboidal regions in the VdgRsm package. For the cuboidal region, points that lie outside a hypercube will be removed. However, it is not natural to make use of a hypersphere when the design is cuboidal (Myers et al., 2009). Thus, in our package we also have a VDG in which radii are calculated from nested cubes. Figure 2.3 shows an example of nested cubes in $[-1, +1]^2$.

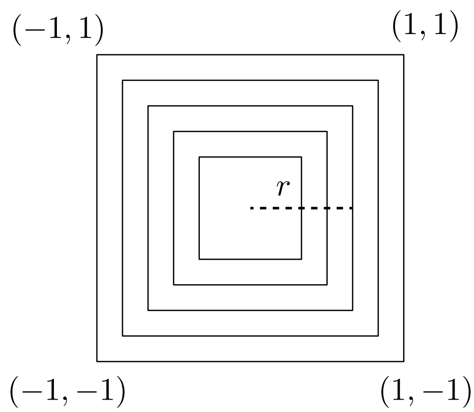



Figure 2.3: Nested cubes in a cuboidal region.

We proposed a simple procedure to generate $M$ points uniformly on a surface of a $k$-dimensional hypercube of radius $r$:

1. Generate $k-1$ random numbers $x_1, x_2, \ldots, x_{k-1}$ independently from $\mathrm{U}[-r, r]$;

2. Sample one number, $x_k$, from the set $\{-r, r\}$ to form a point $(x_1, x_2, \ldots, x_{k-1}, x_k)$;

3. Randomly shuffle elements in the vector $(x_1, x_2, \ldots, x_{k-1}, x_k)$;

4. Repeat steps 1 to 3 for $M$ times to generate $M$ points on a surface of a $k$-dimensional hypercube of radius $r$.

For example, to generate 10 points on a surface of a unit 3-dimensional hypercube, we first generate a $10\times3$ matrix $\mathbf{X}^*$ in which the first two columns are random numbers from $U[-1, 1]$ and the third column contains numbers randomly selected from the set $\{-1, 1\}$, and then shuffle elements in each row as presented in matrix $\mathbf{X}$ below. Figure 2.4 illustrates a plot of $10,000$ on the surface of a cube.

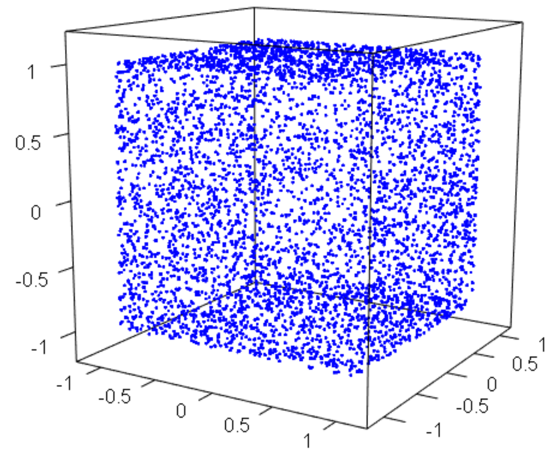



Figure 2.4: $10,000$ uniformly distributed points on the surface of a unit cube.

$$\mathbf{X}^* = \begin{pmatrix} 0.04983 & 0.79590 & 1 \\ -0.37260 & -0.72400 & 1 \\ -0.99480 & 0.42490 & -1 \\ -0.64740 & -0.57840 & -1 \\ 0.91110 & -0.46950 & 1 \\ -0.86870 & 0.42130 & -1 \\ -0.00251 & -0.09916 & -1 \\ 0.03096 & -0.70700 & -1 \\ -0.23320 & 0.14960 & 1 \\ -0.23080 & 0.26660 & -1 \end{pmatrix} \longrightarrow \mathbf{X} = \begin{pmatrix} 1.00000 & 0.79590 & 0.04983 \\ 1.00000 & -0.72400 & -0.37260 \\ -0.99480 & 0.42490 & -1.00000 \\ -0.64740 & -0.57840 & -1.00000 \\ 1.00000 & 0.91110 & -0.46950 \\ 0.42130 & -0.86870 & -1.00000 \\ -0.00251 & -1.00000 & -0.09916 \\ 0.03096 & -0.70700 & -1.00000 \\ -0.23320 & 1.00000 & 0.14960 \\ -1.00000 & -0.23080 & 0.26660 \end{pmatrix}.$$

## 3. Impact of a Missing Value

In Section 1, the robustness of several designs was discussed with respect to the loss $D$-efficiency which is related to the generalized variance of estimates in the second-order model. However, if the prediction variance is of primary interest, the Avg $\ell(\xi_N)$, Max $\ell(\xi_N)$, and Min $D$ cannot provide such information. When the Max $\ell > 0$

($\mathbf{X}_{-i}^{\mathrm{T}}\mathbf{X}_{-i}$ is not singular), the VDGs and FDS plots are helpful to demonstrate the effects of a missing point on prediction variances throughout a design region. We will next present examples of the use of VDGs, FDS plots, and contours of SPVs to assess the impact of a missing response. All plots are produced by the VdgRsm package (Srisuradetchai and Borkowski, 2014).

## 3.1. Example of a CCD in a Spherical Region

Suppose we use a 10-point rotatable CCD with two center runs for fitting a second-order model. Using Equation (1.4), its $D$-efficiency is 63.496% and scaled prediction variance function can be calculated from (1.2). However, we used the prediction variance function formula which was analytically derived by Borkowski (1995) to obtain

$$\begin{aligned} \mathrm{SPV}(\mathbf{x}) &= 10\left[\frac{1}{2} - \frac{3}{8}(x_1^2 + x_2^2) + \frac{7}{32}(x_1^2 + x_2^2)^2\right]; \\ &= 10\left[\frac{1}{2} - \frac{3}{8}r^2 + \frac{7}{32}r^4\right], \end{aligned}$$

where $r = \sqrt{x_1^2 + x_2^2}$. Suppose the factorial point $(-1, -1)$ is missing. The information matrices of the original design and the design with a missing factorial point denoted as $\mathbf{X}^{\mathrm{T}}\mathbf{X}$ and $\mathbf{X}_{-1}^{\mathrm{T}}\mathbf{X}_{-1}$ are, respectively,

$$\mathbf{X}^{\mathrm{T}}\mathbf{X} = \begin{array}{c} \begin{matrix} 1 & x_1 & x_2 & x_1^2 & x_2^2 & x_1x_2 \end{matrix} \\ \begin{pmatrix} 10 & 0 & 0 & 8 & 8 & 0 \\ 0 & 8 & 0 & 0 & 0 & 0 \\ 0 & 0 & 8 & 0 & 0 & 0 \\ 8 & 0 & 0 & 12 & 4 & 0 \\ 8 & 0 & 0 & 4 & 12 & 0 \\ 0 & 0 & 0 & 0 & 0 & 4 \end{pmatrix} \end{array} \begin{matrix} 1 \\ x_1 \\ x_2 \\ x_1^2 \\ x_2^2 \\ x_1x_2 \end{matrix},$$

and

$$\mathbf{X}_{-1}^{\mathrm{T}}\mathbf{X}_{-1} = \begin{array}{c} \begin{matrix} 1 & x_1 & x_2 & x_1^2 & x_2^2 & x_1x_2 \end{matrix} \\ \begin{pmatrix} 9 & 1 & 1 & 7 & 7 & -1 \\ 1 & 7 & -1 & 1 & 1 & 1 \\ 1 & -1 & 7 & 1 & 1 & 1 \\ 7 & 1 & 1 & 11 & 3 & -1 \\ 7 & 1 & 1 & 3 & 11 & -1 \\ -1 & 1 & 1 & -1 & -1 & 3 \end{pmatrix} \end{array} \begin{matrix} 1 \\ x_1 \\ x_2 \\ x_1^2 \\ x_2^2 \\ x_1x_2 \end{matrix}.$$

With $(-1, -1)$ missing, all odd moments in the information matrix are nonzero, and as discussed in Chapter 1, Section 2.2, we can see that the design with a missing $(-1, -1)$ is not as rotatable as the original design because the maximum, minimum, and average of SPVs are not the same in each $r$. Also, all estimated coefficients of the design with the missing point are correlated as the off-diagonal elements in $\mathbf{X}_{-1}^{\mathrm{T}}\mathbf{X}_{-1}$ are nonzero. The number of nonzero convariances increases from $3/15 \times 100\% = 20\%$ to 100% when point $(-1, -1)$ is lost.

A missing point also causes a higher scaled prediction variance as illustrated in Figure 2.5. Without a missing point, SPVs vary from approximately 3.35 to 6.25,

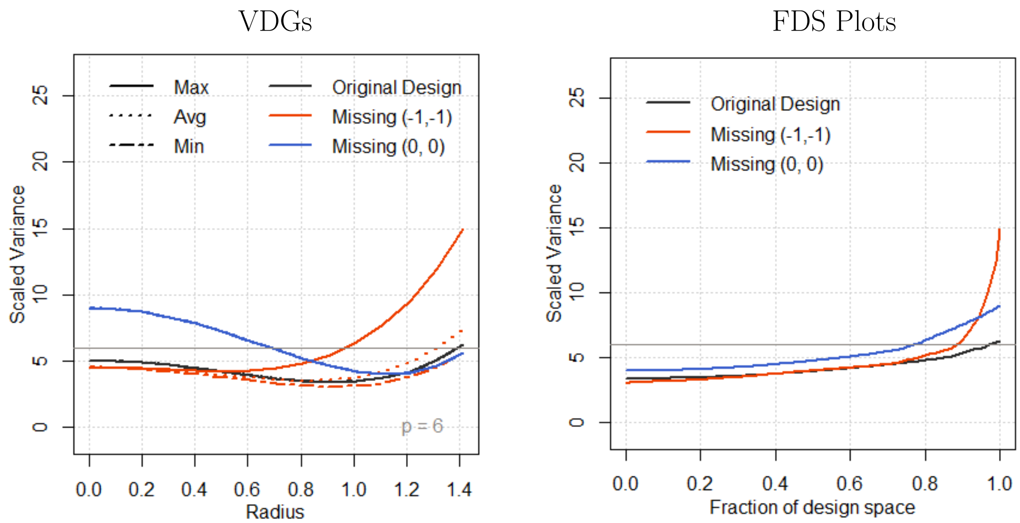



Figure 2.5: The VDGs (left) and FDS plots (right) for the rotatable CCD without missing points, with missing point $(-1, -1)$, and with missing point $(0, 0)$.

and the highest SPV occurs at $r = \sqrt{2}$. When $(-1, -1)$ is missing, the average SPVs (ASPVs) are similar to those of the original design for all radii. The maximum SPVs (MaxSPVs) of the design with a missing $(-1, -1)$ become larger than those of the original design after $r \approx .5$. The MaxSPV increases as high as 15 at $r = \sqrt{2}$. The FDS plot of the original design shows that almost 100% of the design region has SPVs $< 6$, which means the design is near $G$-optimal. With $(-1, -1)$ missing, the percentage of a design space with SPVs $< 6$ decreases to about 89%. Also, the $G$-efficiency decreases from $6/6.25 \times 100 = 96\%$ to $6/15 \times 100 = 40\%$.

As presented in Figure 2.5, the impact of a missing point on SPVs depends on the type of a missing point. With a missing $(0, 0)$, the design is still rotatable but the precision of prediction at or near the design center is rather poor. The SPVs are higher than those of the original design when $0 \leq r \lessapprox 1.2$. The corresponding FDS plot indicates that approximately 76% of the design region has the SPVs $< 6$, the $G$-optimal value.

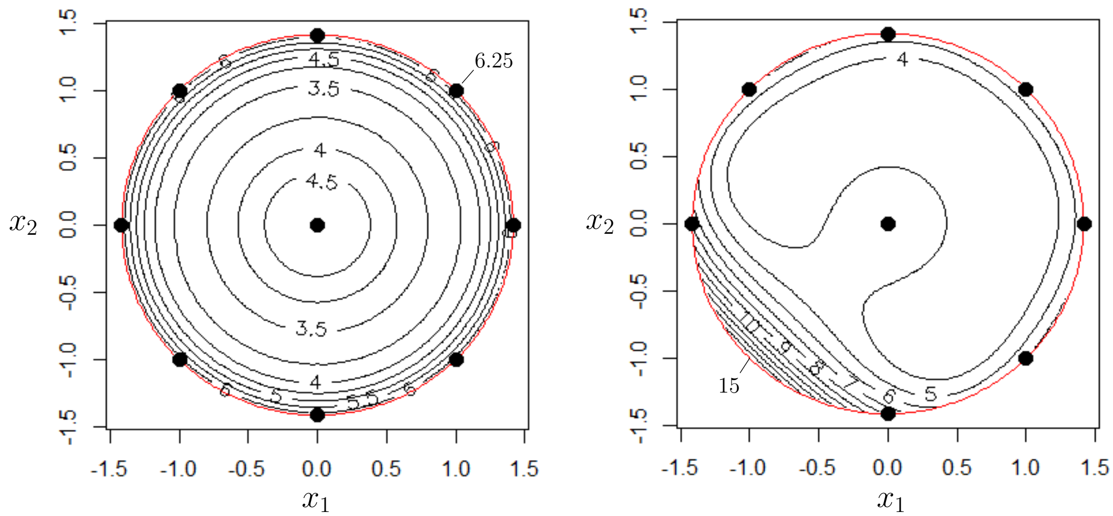



Figure 2.6: Contours of SPVs of the CCD (left) and design with missing $(-1, -1)$ (right). Solid circles represent the design points.

However, because the VDG and FDS plots cannot locate an area whose precisions of predictions are poor, we need a contour plot to show the "weak" area in a design region. Figure 2.6 gives contours of SPVs for the original design (left) and the design with missing $(-1, -1)$ (right). It is not surprising that the area around the missing point $(-1, -1)$ has higher SPVs because no responses are collected there. At point $(-1, -1)$, the SPV is 15, the highest SPV.

We have given the example of the two-factor rotatable CCD with $n_c = 2$ whose the Avg $\ell$ and Max $\ell$ are 4.719% and 5.645% as summarized in Table 2.1. The design is rather robust to a missing point in terms of the $D$-efficiency, but this is only one aspect. A missing point also affects the rotatability and orthogonality of the design which can be assessed via the information matrix. The contour plot shows the "weak" part of the design space, and how rotatability can be seriously affected.

## 3.2. Example of a HSCD in a Cuboidal Region

Suppose we use an eight-point two-factor HSCD having two center runs in a cuboidal region for fitting a second-order model. Using Equation (1.4), its $D$-efficiency is 30.023%, and from Table 2.2 the Avg $\ell$ and Max $\ell$ are 10.960% and 15.219%, respectively. It is not a rotatable design, and some parameter estimates are correlated. The SPV function in product form is in (2.6), and we can see that only 8 of 15 parameter estimates are not correlated. Suppose the axial point $(1, 0)$ is missing. In the updated information matrix, the number of uncorrelated parameter estimates is reduced to 6 of 15. Thus, a missing point does not affect the property of orthogonality very much.

$$\mathrm{SPV}(\mathbf{x}) = (1, x_1, x_2, x_1^2, x_2^2, x_1x_2) \begin{pmatrix} 4 & 0 & 0 & -4 & -4 & 4 \\ 0 & 8/3 & -4/3 & 0 & 0 & 0 \\ 0 & -4/3 & 8/3 & 0 & 0 & 0 \\ -4 & 0 & 0 & 8 & 4 & -8 \\ -4 & 0 & 0 & 4 & 8 & -8 \\ 4 & 0 & 0 & -8 & -8 & 16 \end{pmatrix} \begin{pmatrix} 1 \\ x_1 \\ x_2 \\ x_1^2 \\ x_2^2 \\ x_1x_2 \end{pmatrix} \qquad (2.6)$$

Figure 2.7 presents the VDG for the HSCD with and without a missing point. A calculation of the average SPV (ASPV), minimum SPV (MinSPV), and maximum SPV (MaxSPV) is restricted to the points on the surface of nested hypercubes with vertices $(\pm r, \pm r, \pm r)$ for $0 \leq r \leq 1$. The VDG shows that the ASPVs of both designs are about the same until $r \approx .4$, and then ASPVs of the HSCD with a missing $(1, 0)$ become larger than those of the original design. The MaxSPV can be as high as 142.66 when $r = 1$ in the design with missing $(1, 0)$ while the highest MaxSPV of the original design is only 57.19. From the FDS plot, approximately 65% of a design space of the design with missing $(1, 0)$ has the SPV $< 6$, and when compared to the original design, the missing $(1, 0)$ causes about 10% reduction in the fraction of the design space with SPV values $< 6$.

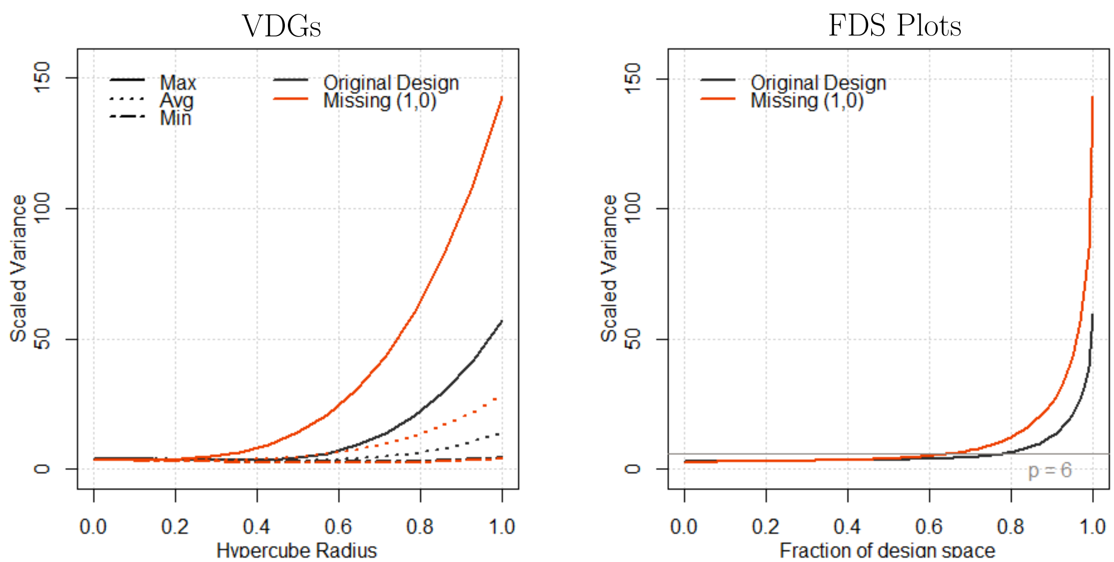



Figure 2.7: The VDGs (left) and FDS plots (right) for HSCDs without missing points and with missing point $(1, 0)$.

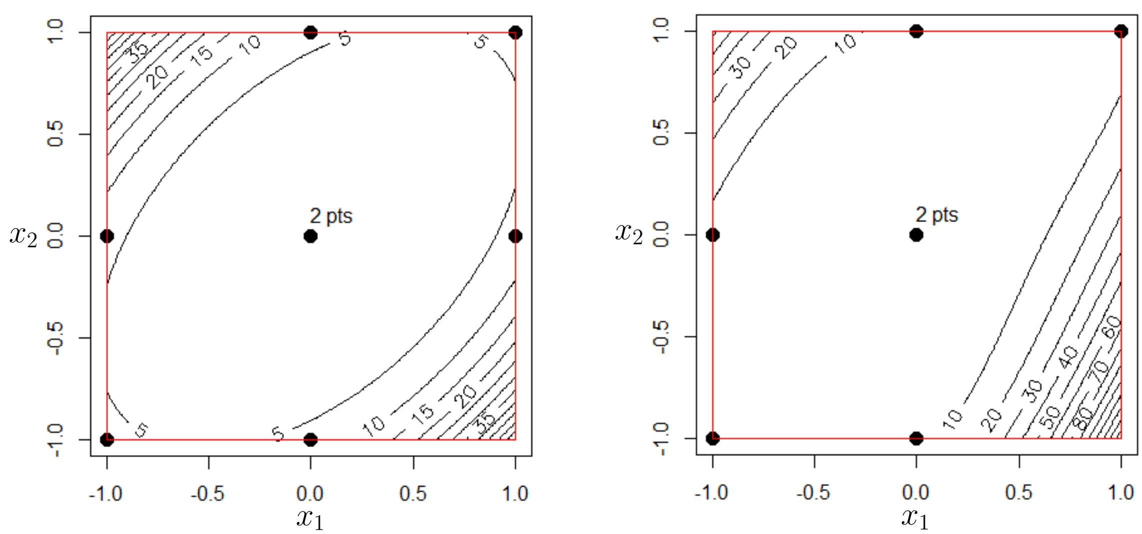



Figure 2.8: Contours of SPVs of HSCDs without missing points (left) and with missing point $(1, 0)$ (right).

Figure 2.8 shows contours of SPVs of the original HSCD (left) and design with missing $(1, 0)$. Again, the HSCD is not rotatable as the contour lines are not circular. Originally, the HSCD does not include points $(-1, 1)$ and $(1, -1)$, so the SPV will be high in the area near those design points. With a missing $(1, 0)$, the design now has two neighboring points where a response is not collected, thus the area with poor prediction is expanded.

### 3.3. Example of an Exact $D$-Optimal Design in a Cuboidal Region

Suppose we use a 7-point exact $D$-optimal design catalogued in Borkowski (2003b) for fitting a second-order model. Its $D$-efficiency is 45.029%, and the Avg $\ell$ and Max $\ell$ are 22.742% and 44.161%, respectively. This design is considered a robust design comparing to the exact $A$-, $G$-, and $IV$-optimal designs with the same sample size because it has the lowest Avg $\ell$ and Max $\ell$ as listed in Table 2.6. However, the $D$-optimal design might not be robust in terms of prediction which will now be observed.

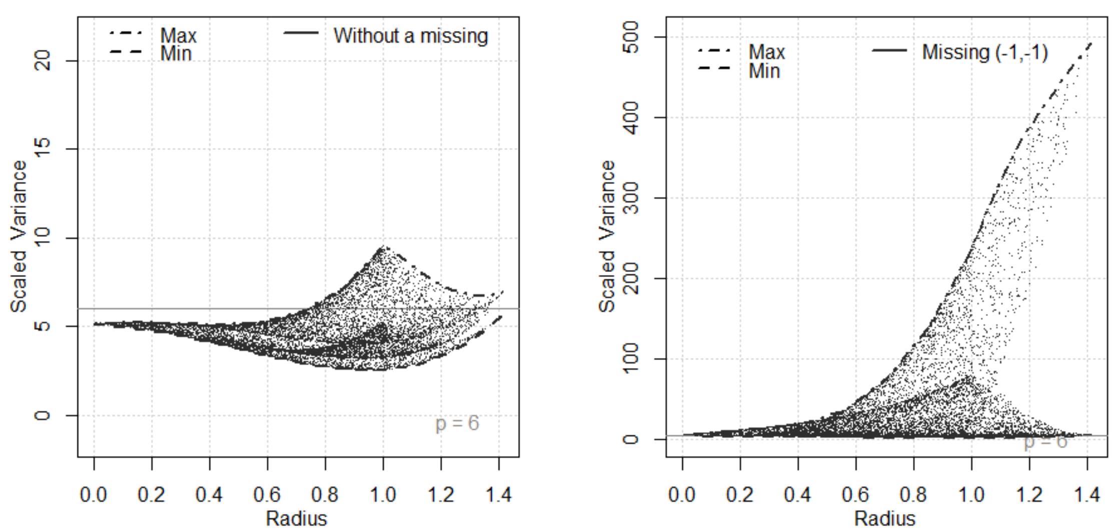



Figure 2.9: The VDGs for the 7-point $D$-optimal exact design without missing points (left) and with missing $(-1, -1)$ (right).

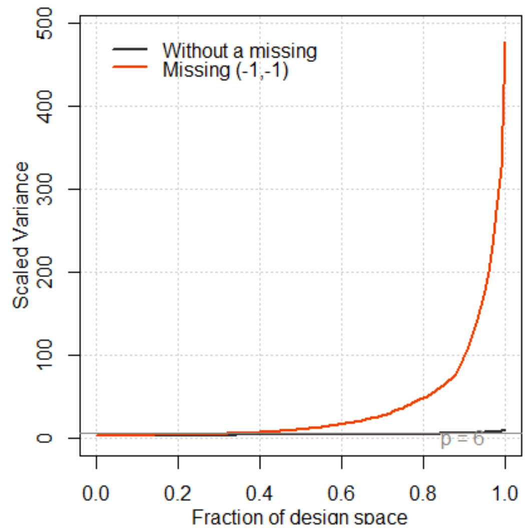



Figure 2.10: The FDS plots for the 7-point $D$-optimal exact design without missing points and with missing $(-1, -1)$.

Suppose point $(-1, -1)$ is missing. The resulting 6-point design has a $D$-efficiency of 25.144%. The VDGs of the original design and the design with $(-1, -1)$ missing are illustrated in Figure 2.9. The SPVs of the original design were between 2.5 and 9.5 which is a considerably narrower interval compared to that of the design with $(-1, -1)$ missing having SPVs between 6 and 493. The randomly generated design points provide us with information about the distribution of SPVs across radii. This is an option in the VdgRsm package. Notice that not many generated design points were found as $r \to \sqrt{2}$ because the hyperarcs shrink for $r > 1$ when restricted to a hypercube.

Figure 2.10 shows the FDS plot. With a missing point $(-1, -1)$, more than 80% of the design space has SPV greater than the $G$-optimal value of 6. We can say that the missing point results in a very poor prediction in most design region. Figure 2.11 illustrates the contours of SPVs before and after having a missing $(-1, -1)$. As shown in Figure 2.11 (right), there is an open region near point $(-1, -1)$ where no

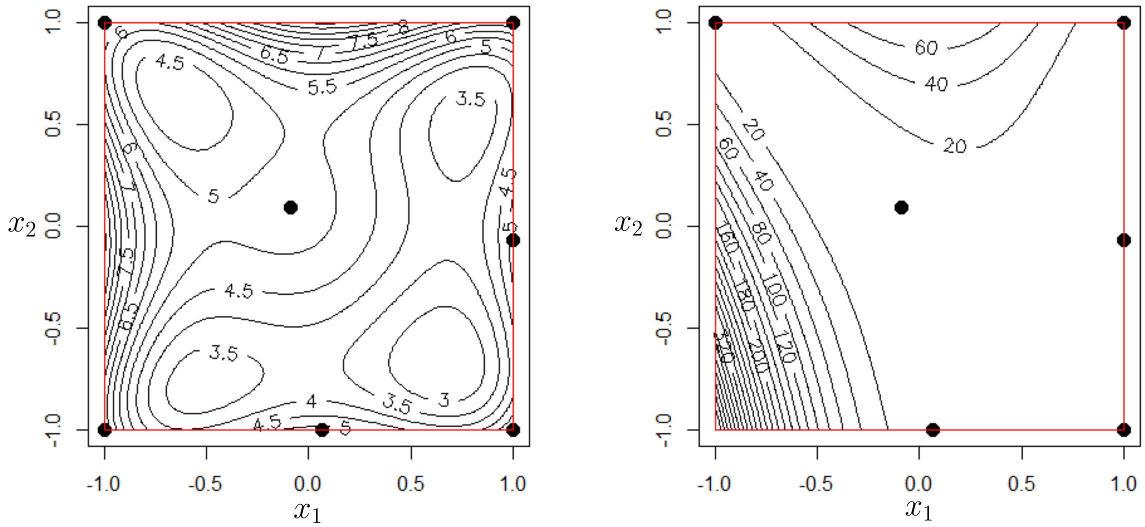



Figure 2.11: Contours of SPVs of the 7-point$D$-optimal exact design without missing points (left) and with missing $(-1, -1)$ (right).

response is collected, and, thus the SPVs are extremely high near that point. Overall, the 7-point exact $D$-optimal design is not considered to be a robust design against a missing point.

# CHAPTER 3

# ROBUST COMPOSITE DESIGNS IN A HYPERSPHERE

## 1. Motivations

Some experiments can be expensive and experimental units can be limited, thus designs with one replication (also called unreplicated), such as unreplicated factorial or fractional factorial designs, are widely used. Methods of analysis for these designs have been widely studied in the literature, e.g., Box and Meyer (1986), Lenth (1989), Kenneth and Richard (1991), Juan and Pefña (1992), Loh (1992), Schneider et al. (1993), and Venter and Steel (1996). Hamada and Balakrishnan (1998) gave comprehensive reviews on the existing methods and compared them using simulation studies. The ability to estimate $n-1$ contrasts in certain $n$-run experiments has caused these unreplicated designs to receive attention. In RSM, the CCDs without replicated factorial and axial points are generally used because all effects in the second-order model can be estimated, and for $k \geq 5$, many attempts to reduce the number of factorial points are found in the literature, e.g., Box and Wilson (1951), Box and Hunter (1957), Hartley (1959), Westlake (1965), Box et al. (2005), Draper and Lin (1996). The number of replicated center runs influences the SPVs and also provides an estimate of pure error. In some situations, one or two center points are enough, but in certain circumstances, more center runs are suggested (Myers et al., 2009). Draper (1982) compared approaches for selecting the number of center points in the second-order response surface designs. These approaches are due to Box and Hunter (1957), Box and Draper (1963), Box and Draper (1975), Lucas (1974, 1976, 1977), and Draper (1982), and will referred to as BH57(a)-(b), BD63, BD75, LU76, and DP82, respectively. Note that Box and Hunter (1957) provided two methods to select $n_c$. Furthermore, for $k = 2$ to 4, factorial and axial points are unreplicated, and for $k = 5$, half fractional factorial points are used in Draper (1982). The results show that for $k = 2, 3, 4$, with a single replicate of factorial and axial points and $\alpha = \sqrt{k}$ or $\sqrt[4]{n_f}$, the $n_c$'s recommended in BH57(b), BD75, LU76, and DP82 are from two to four center runs; for $k = 5$, with half fractional factorial points and $\alpha = 2$, the suggested $n_c$'s in BH57(b), BD63, BD75, and DP82 are from zero to two. However, for $k = 2$, when $\alpha = 1$, BH57(b), BD75, and DP82 require zero or one center run; for $k = 3$, BH57(a), BD75 and DP82 also require zero or one center run; for $k = 4$ and 5, BD75 and DP82 do not need a center run. Lucas (1976) compared the central composite designs with one, two, and three center runs, and the $D$-efficiencies are close. Adding the second center run, however, will give a large increase in the $G$-efficiency.

From the literature review, the CCDs for $k = 2, 3, 4$ with $\alpha = 1$ do not require a center point while for the rotatable or near-rotatable CCD, two to four center runs are recommended. For half-fractional factorial rotatable CCDs for $k = 5$ and 6, the recommended $n_c$ can even be zero due to the BD75 method (Box and Draper, 1975). The use of only one replicate of the center point could be due to a very expensive experiment or the experimenters' intention. However, if the only center run is missing or uncollectible in spherical CCDs, the $\mathbf{X}^{\mathrm{T}}\mathbf{X}$ matrix will be singular. Thus, it can be risky to have only one center run in rotatable CCDs. In this chapter, given that a single-replicated CCD is used in experimentation, we will find the optimal or "robust" $\alpha$ where if a factorial, axial, or center run happens to be missing in the future, a desirable alphabetic optimality criterion is still maximized. To find such an $\alpha$, the maximin criterion is applied to the existing optimality criteria. The behavior of $D$-, $A$-, $G$-, $IV$-efficiencies will be also studied for the following situations: (1) without a missing point; (2) one missing factorial point; (3) one missing axial point; and (4) a missing center run. The maximin $D$-, $A$-, $G$-, $IV$-efficiencies will be calculated and the corresponding axial distance, $\alpha$, will be searched numerically.

## 2. Singularity of CCDs without a Center Point

When a spherical CCD with $n_c = 1$ is used in experimentation, the axial distance, $\alpha$, equals $\sqrt{k}$. In this case, the center run is mandatory. If a missing response happens in the center run, the information matrix $\mathbf{X}^{\mathrm{T}}\mathbf{X}$ will be singular. Thus, replications of center points are recommended, if possible. We will now prove that the CCD with $\alpha = \sqrt{k}$ needs at least one center run to avoid singularity.

*Proof* The information matrix $\mathbf{X}^{\mathrm{T}}\mathbf{X}$ of an $N$-point $k$-factor spherical CCD with a single replication of factorial and axial points and $n_c$ center points is

$$
\mathbf{X}^{\mathrm{T}}\mathbf{X} =
\begin{array}{c}
\begin{array}{ccccccccccccc}
\scriptstyle 0 & \scriptstyle 1 & \scriptstyle \cdots & \scriptstyle k & \scriptstyle 1 & \scriptstyle 2 & \scriptstyle \cdots & \scriptstyle k & \scriptstyle 1 & \scriptstyle 2 & \scriptstyle \cdots & \scriptstyle \binom{k}{2}
\end{array} \\
\left(\begin{array}{ccccccccccccc}
N & 0 & \cdots & 0 & M & M & \cdots & M & 0 & 0 & \cdots & 0 \\
0 & M & \cdots & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots & \vdots & \vdots & & \vdots & \vdots & \vdots & & \vdots \\
0 & 0 & \cdots & M & 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 \\
M & 0 & \cdots & 0 & A & F & \cdots & F & 0 & 0 & \cdots & 0 \\
\vdots & \vdots & & \vdots & F & A & \ddots & \vdots & \vdots & \vdots & & \vdots \\
 & & & & \vdots & \ddots & \ddots & F & 0 & 0 & \cdots & 0 \\
M & 0 & \cdots & 0 & F & \cdots & F & A & 0 & 0 & \cdots & 0 \\
0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 & F & 0 & \cdots & 0 \\
\vdots & \vdots & & \vdots & \vdots & \vdots & & \vdots & 0 & F & \ddots & \vdots \\
0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 & \vdots & \ddots & \ddots & 0 \\
0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 & 0 & \cdots & 0 & F
\end{array}\right)
\end{array}
\begin{array}{c}
\\ \scriptstyle 0 \\ \scriptstyle 1 \\ \scriptstyle \vdots \\ \scriptstyle k \\ \scriptstyle 1 \\ \scriptstyle 2 \\ \scriptstyle \vdots \\ \scriptstyle k \\ \scriptstyle 1 \\ \scriptstyle 2 \\ \scriptstyle \vdots \\ \scriptstyle \binom{k}{2}
\end{array} ,
$$

where $N = 2^k + 2k + n_c$, $M = 2^k + 2k$, $A = 2^k + 2k^2$, and $F = 2^k$. Without center runs, $N = 2^k + 2k$. As we are interested in a rank of matrix $\mathbf{X}^{\mathrm{T}}\mathbf{X}$, switching columns and/or rows does not change the rank of matrix $\mathbf{X}^{\mathrm{T}}\mathbf{X}$. Hence, after switching rows and columns, $\mathbf{X}^{\mathrm{T}}\mathbf{X}$ can be written as:

$$\mathbf{X}^{\mathrm{T}}\mathbf{X} = \begin{array}{ccc|ccccc|cccc|c}
\scriptstyle 1 & \scriptstyle \dots & \scriptstyle k & \scriptstyle 0 & \scriptstyle 1 & \scriptstyle 2 & \scriptstyle \dots & \scriptstyle k & \scriptstyle 1 & \scriptstyle 2 & \scriptstyle \dots & \scriptstyle \binom{k}{2} & \\
M & \dots & 0 & 0 & 0 & 0 & \dots & 0 & 0 & 0 & \dots & 0 & \scriptstyle 1 \\
\vdots & \ddots & \vdots & \vdots & \vdots & \vdots & & \vdots & \vdots & \vdots & & \vdots & \scriptstyle \vdots \\
0 & \dots & M & 0 & 0 & 0 & \dots & 0 & 0 & 0 & \dots & 0 & \scriptstyle k \\
\hline
0 & \dots & 0 & N & M & M & \dots & M & 0 & 0 & \dots & 0 & \scriptstyle 0 \\
0 & \dots & 0 & M & A & F & \dots & F & 0 & 0 & \dots & 0 & \scriptstyle 1 \\
\vdots & & \vdots & M & F & A & \ddots & \vdots & \vdots & \vdots & & \vdots & \scriptstyle 2 \\
 & & & \vdots & \vdots & \ddots & \ddots & F & 0 & 0 & \dots & 0 & \scriptstyle \vdots \\
0 & \dots & 0 & M & F & \dots & F & A & 0 & 0 & \dots & 0 & \scriptstyle k \\
\hline
0 & \dots & 0 & 0 & 0 & 0 & \dots & 0 & F & 0 & \dots & 0 & \scriptstyle 1 \\
\vdots & \vdots & & \vdots & \vdots & \vdots & & \vdots & 0 & F & \ddots & \vdots & \scriptstyle 2 \\
0 & 0 & \dots & 0 & 0 & 0 & \dots & 0 & \vdots & \ddots & \ddots & 0 & \scriptstyle \vdots \\
0 & 0 & \dots & 0 & 0 & 0 & \dots & 0 & 0 & \dots & 0 & F & \scriptstyle \binom{k}{2}
\end{array} .$$

The above matrix is a diagonal block matrix consisting of three diagonal elements which are square matrices with different dimensions. The ranks of the first and third diagonal block matrices are:

$$\mathrm{rank}\begin{pmatrix} M & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & M \end{pmatrix} = k, \quad \text{and} \quad \mathrm{rank}\begin{pmatrix} F & 0 & \dots & 0 \\ 0 & F & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \dots & 0 & F \end{pmatrix} = \binom{k}{2}.$$

Without center points, $N = M = 2^k + 2k$. So, the second diagonal block matrix is

$$\begin{array}{c} \begin{matrix} \scriptstyle 0 & \scriptstyle 1 & \scriptstyle 2 & \scriptstyle \dots & \scriptstyle k \end{matrix} \\ \begin{pmatrix} 2^k+2k & 2^k+2k & 2^k+2k & \dots & 2^k+2k \\ 2^k+2k & 2^k+2k^2 & 2^k & \dots & 2^k \\ 2^k+2k & 2^k & 2^k+2k^2 & \ddots & \vdots \\ \vdots & \vdots & \ddots & \ddots & 2^k \\ 2^k+2k & 2^k & \dots & 2^k & 2^k+2k^2 \end{pmatrix} \begin{matrix} \scriptstyle 0 \\ \scriptstyle 1 \\ \scriptstyle 2 \\ \vdots \\ \scriptstyle k \end{matrix} \end{array} .$$

After inspecting the above matrix, the first column is found to be an average of the rest of the columns:

$$C_0 = \frac{1}{k}C_1 + \frac{1}{k}C_2 + \ldots + \frac{1}{k}C_k \,,$$

where $C_i$ is the $(i+1)$th column in the matrix. Thus, this $(k+1) \times (k+1)$ matrix has a rank of $k$. Because the rank of a block diagonal matrix equals the sum of ranks of the diagonal matrices, $\text{rank}(\mathbf{X}^{\mathrm{T}}\mathbf{X}) = k + k + \binom{k}{2}$, one less than the number of parameters. But, if there are $n_c$ center runs with $N = 2^k + 2k + n_c$, the first column will not be a linear combination of the other $k$ columns. Therefore, a center run is essential for spherical CCDs.

## 3. Modified Alphabetic Optimality Criteria

In this section, the alphabetic optimality criteria are modified to assess the sensitivity of designs to a single missing point. They can be also used as criteria to construct robust designs, which will be discussed in Chapter 4.

## 3.1. Variations of the $D$-Efficiency

We have discussed the modification of the $D$-efficiency in Chapter 2, Section 1, but for completeness we will mention it again here. Given that the original information matrix $\mathbf{X}^{\mathrm{T}}\mathbf{X}$ is $N \times p$ where $N$ and $p$ are the number of observations and parameters in a second-order model, respectively. After removing the $i$th point, the corresponding information matrix is $\mathbf{X}^{\mathrm{T}}_{-i}\mathbf{X}_{-i}$ and its $D$-efficiency is

$$D_{-i} = \frac{|\mathbf{X}^{\mathrm{T}}_{-i}\mathbf{X}_{-i}|^{1/p}}{N-1} \times 100,$$

where $i = 1, 2, \ldots, N$. It is important to remember that the denominator $N-1$ of $D_{-i}$ equals $|\mathbf{X}^{\mathrm{T}}\mathbf{X}|^{1/p}$ assuming an exact $(N-1)$-point $D$-optimal design for the first-order model. Thus, $D_{-i}$ is a lower bound of the actual $D$-efficiency of the design with the $i$th missing point.

The minimum of $D_{-i}$ can reflect the worst case scenario of having one missing response and is defined as:

$$\text{Min } D = \min_{1 \le i \le N} \{D_{-i}\}.$$

The determinant of matrix $|\mathbf{X}^{\mathrm{T}}\mathbf{X}|$ was proven to increase as the $\alpha$ increases regardless of the number of center points (Lucas, 1974). Also, we define a *leave-m-out* $D$-efficiency as:

$$D^{(m)} = \frac{\sum_{t \in T_m} D_t}{\binom{N}{m}},$$

where $T_m$ is the set of all possible subset designs of size $N-m$ and $D_t$ is the $D$-efficiency of subset design $t \in T_m$. For any $m$, $D^{(m)}$ is the average of the $D$-efficiencies of all possible designs with $m$ missing responses.

## 3.2. Variations of the $A$-Efficiency

With the $i$th point missing, the corresponding $A$-efficiency is

$$A_{-i} = \frac{p}{\text{trace}[(N-1)(\mathbf{X}_{-i}^{\mathrm{T}}\mathbf{X}_{-i})^{-1}]} \times 100\,,$$

and the minimum of $A_{-i}$ representing the worst case scenario of having one missing observation is defined as:

$$\text{Min } A = \min_{1 \le i \le N} \{A_{-i}\}\,.$$

Also, the *leave-m-out* $A$-efficiency is defined as:

$$A^{(m)} = \frac{\sum_{t \in T_m} A_t}{\binom{N}{m}},$$

where $A_t$ is the $A$-efficiency of subset design $t \in T_m$. For any $m$, $A^{(m)}$ is the average of $A$-efficiencies of all possible designs with $m$ missing points.

## 3.3. Variations of the $G$-Efficiency

With the $i$th point missing, the corresponding $G$-efficiency is

$$G_{-i} = \frac{p}{\max\limits_{\mathbf{x} \in \mathcal{X}}[(N-1)\mathbf{x}^{\mathrm{T}}(\mathbf{X}_{-i}^{\mathrm{T}}\mathbf{X}_{-i})^{-1}\mathbf{x}]} \times 100,$$

and the minimum of $G_{-i}$ representing the worst case scenario of having one missing observation is defined as:

$$\text{Min } G = \min_{1 \le i \le N} \{G_{-i}\}\,.$$

Also, a *leave-m-out* $G$-efficiency is defined as:

$$G^{(m)} = \frac{\sum_{t \in T_m} G_t}{\binom{N}{m}},$$

where $G_t$ is the $G$-efficiency of subset design $t \in T_m$. For any $m$, $G^{(m)}$ is the average of $G$-efficiencies of all possible designs with $m$ missing points.

## 3.4. Variations of the $IV$-Efficiency

With the $i$th missing point, the corresponding $IV$-efficiency is

$$IV_{-i} = \frac{A}{(N-1)\,\text{trace}\left[(\mathbf{X}_{-i}^{\mathrm{T}}\mathbf{X}_{-i})^{-1}\int_{\mathcal{X}} \mathbf{x}^{(m)\mathrm{T}}\mathbf{x}^{(m)}\, d\mathbf{x}^{(m)}\right]} \times 100\,,$$

where $A$ is the volume of the design with a missing trial. The minimum of $IV_{-i}$ represents the worst case scenario where a design with the $i$th missing response gives the lowest $IV$-efficiency. So, it is defined as:

$$\text{Min } IV = \min_{1 \le i \le N} \{IV_{-i}\}\,.$$

The *leave-m-out* $IV$-efficiency is defined as:

$$IV^{(m)} = \frac{\sum_{t \in T_m} IV_t}{\binom{N}{m}},$$

where $IV_t$ is the $IV$-efficiency of subset design $t \in T_m$. For any $m$, $IV^{(m)}$ is the average of $IV$-efficiencies of all possible designs with $m$ missing points.

Because the $IV$-criterion requires a calculation of integral $\int_{\mathcal{X}}$ SPV $(\mathbf{x})$, it can be tedious depending on the shape of a design space and the number of dimensions. Borkowski (2003a) compared two methods, using fixed and random set points, to estimate the average prediction variance (APV). The fixed-point-set method gives a poor approximation of the APV even though the number of evaluation points was increased to $21^k$, $k = 3$, 4, and 5. Instead, a set of randomly selected points gives an estimate close to the exact value. Using the random points is an example of a Monte-Carlo integration approximation which we will discuss below.

Suppose the SPV($\mathbf{x}$) has $k$ dimensions, and we want to estimate the integral of SPV($\mathbf{x}$) over $\mathcal{X} \in \mathbb{R}^k$. The basic approximation is

$$\int_{\mathcal{X}} \mathrm{SPV}(\mathbf{x})\, d\mathbf{x} \approx A(\overline{\mathrm{SPV}}) = \hat{V}, \tag{3.1}$$

where $\overline{\mathrm{SPV}} = \sum_{i=1}^{M} \mathrm{SPV}(\mathbf{x}_i)/M$ is the sample mean of the SPV($\mathbf{x}_i$) values, $A$ is the volume of the design space $\mathcal{X}$, and $M$ is the number of points uniformly generated in $\mathcal{X}$. The standard error of estimate $\hat{V}$ is

$$\mathrm{s.e.}(\hat{V}) = \frac{A}{\sqrt{M}} \times \sqrt{\frac{\sum_{i=1}^{M} \mathrm{SPV}^2(\mathbf{x}_i) - M\,\overline{\mathrm{SPV}}^2}{M-1}}.$$

Notice that the standard error of the estimate $\hat{V}$ will decrease as $M$ increases.

## 4. Min-$D$ Robust Composite Designs

As discussed in Chapter 3, Section 2, the moment matrix of the CCD with $n_c = 1$ and $\alpha = \sqrt{k}$ in a hypersphere can be singular if only one center run is missing. Assuming only one center run is used in an experiment, we will find the $\alpha$ that maximizes the Min $D$ for $k$-factor CCDs, $k = 2$, 3, and 4. Because of the structure of CCDs, a missing observation can only occur as a factorial, axial, or center point.

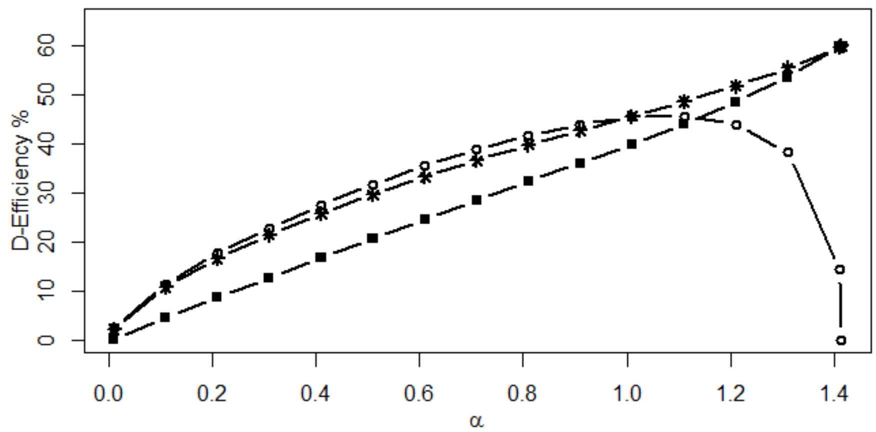



Figure 3.1: $D$-efficiencies of two-factor CCDs having a missing response: solid squares for a missing factorial, stars for a missing axial, and open circles for a missing center run.

## 4.1. Two-Factor Min-$D$ CCD

The behaviors of $D$-efficiencies of two-factor CCDs with a single missing point over different values of $\alpha$ are illustrated in Figure 3.1. When $\alpha < 1.143$, the missing factorial point causes the greatest reduction in $D$-efficiencies, but after $\alpha = 1.143$, the $D$-efficiency decreases rapidly if the center run is lost. This critical $\alpha = 1.143$ value will be referred to as $\alpha_{\text{crit}}$.

A comparison of the $D$-efficiency and Min $D$ of the two-factor CCDs is presented in Figure 3.2. It is well known that the $D$-efficiency increases as $\alpha$ increases (Lucas, 1974), but this is not true for the Min $D$. The highest Min $D$ of 45.408% occurs at $\alpha_{\text{crit}}$. The CCD with $\alpha_{\text{crit}}$ will subsequently be called the robust design. Notice that when $\alpha < \alpha_{\text{crit}}$, the difference between $D$- and Min $D$-efficiencies is less than 10%, but for after $\alpha > \alpha_{\text{crit}}$, the difference increases very quickly. The $D$-efficiency of the robust design will decrease only slightly from 50.781 to 45.408 if a factorial or center point is missing. As shown in Figure 3.2, although the spherical CCD ($\alpha = \sqrt{2}$) has $D$-efficiency as high as 62.854, there is a risk to having its $D$-efficiency drop to zero if

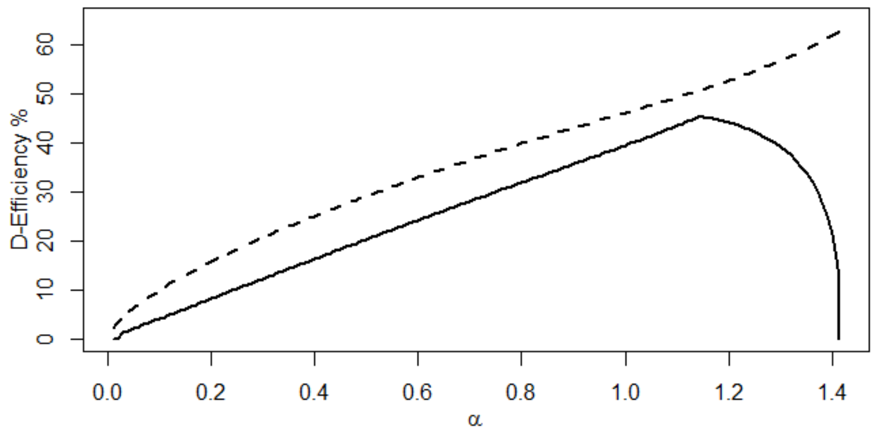



Figure 3.2: The $D$-efficiency and Min $D$ of two-factor CCDs: solid line for Min $D$'s and dashed line for $D$-efficiencies.

the center run is lost. We will soon examine the precision of predictions of the robust design.

Figure 3.3 shows contours of SPVs of the robust design with different types of a missing run. Figures (a), (b), (c), and (d) correspond to the robust design without any missing runs, and designs with $(-1, -1)$, $(-\alpha_{\text{crit}}, 0)$, $(0, 0)$ missing, respectively. Although the robust designs with a missing factorial or center run have the same $D$-efficiency, their precisions for predictions are different and depend on a location of a point for prediction. The maximum SPVs of the designs with a missing $(-1, -1)$, $(-\alpha_{\text{crit}}, 0)$, and $(0, 0)$ are 23.5, 18, and 23.7, respectively.

### 4.2. Three-Factor Min-$D$ CCD

Analogous to Figure 3.1 for a two-factor CCD, Figure 3.4 illustrates the behaviors of $D$-efficiencies for three-factor CCDs with a single missing point over different values of $\alpha$. For this case, $\alpha_{\text{crit}} = 1.466$. The plot reveals with $\alpha < \alpha_{\text{crit}}$, three missing types cause about the same reduction in $D$-efficiencies, but a missing factorial run would give the lowest $D$-efficiency. Like the two-factor Min-$D$ CCD, for $\alpha > \alpha_{\text{crit}}$, the $D$-efficiency decreases rapidly and drops to zero if the response at the center point is lost.

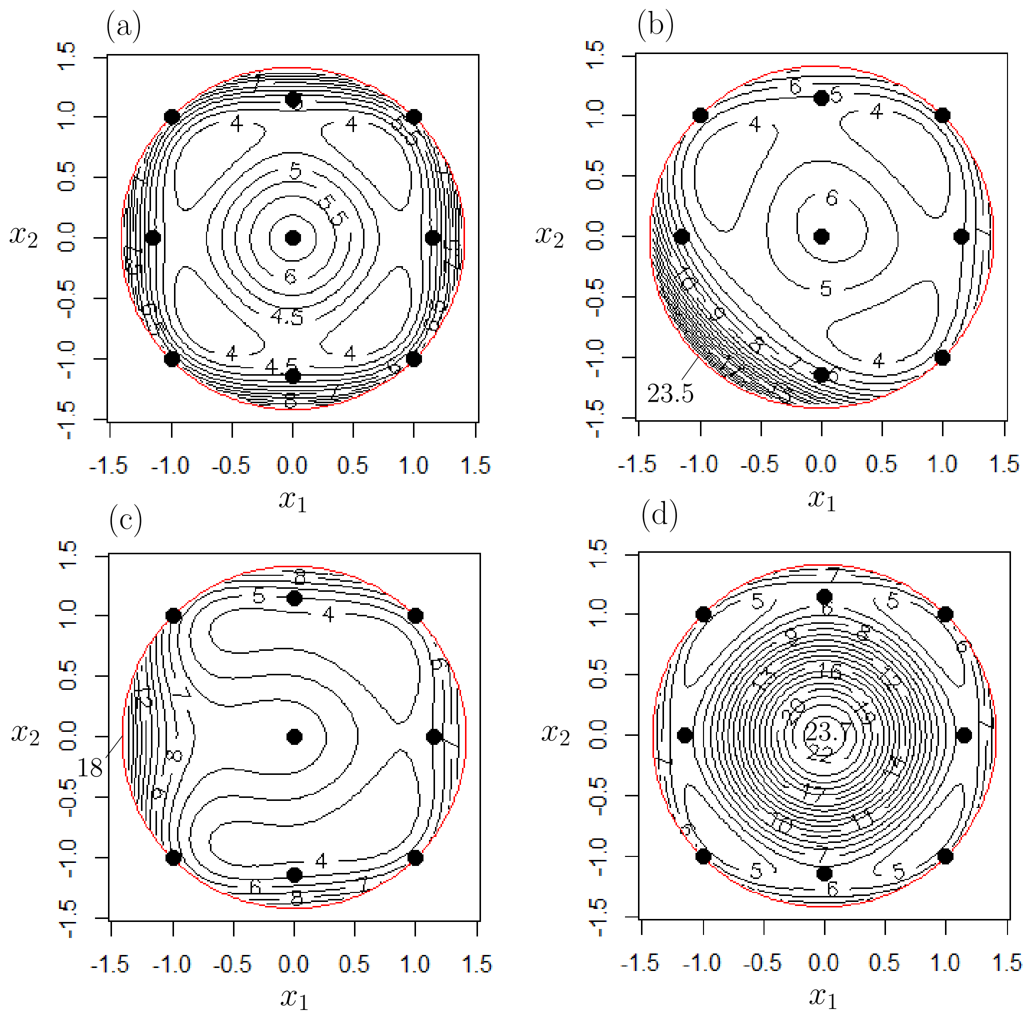



Figure 3.3: Contours of SPVs of the two-factor robust exact CCD based on the Min $D$: (a) without a missing response; (b) a missing factorial point; (c) a missing axial point; and (d) a missing center point. Solid circles represent the design points.

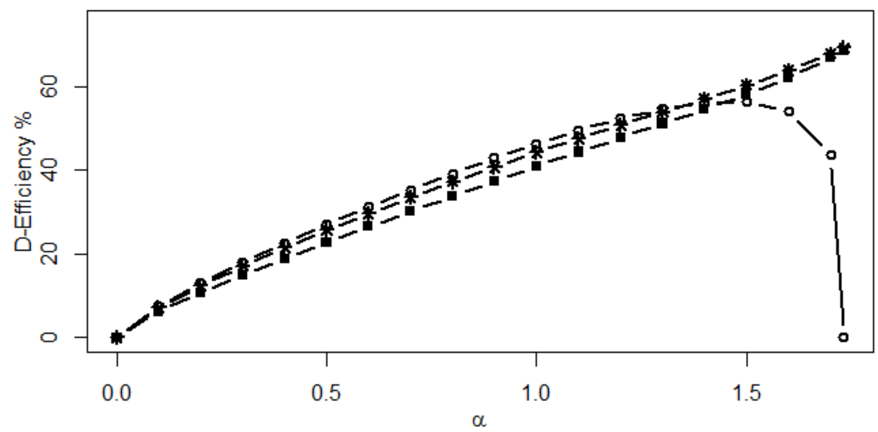



Figure 3.4: $D$-efficiencies of three-factor CCDs having a missing response: solid squares for a missing factorial, stars for a missing axial, and open circles for a missing center run.

A comparison of the $D$-efficiency and Min $D$ of three-factor CCDs is illustrated in Figure 3.5. The conclusions are similar to those for the two-factor case except the highest Min $D$ is 56.396%. The $D$-efficiency and Min $D$ of CCDs with $\alpha < \alpha_{\text{crit}}$ are not much different, but for $\alpha > \alpha_{\text{crit}}$, the Min $D$ will drop to zero at $\alpha = \sqrt{3}$. The $D$-efficiency of the robust CCD will decrease only slightly from 60.2363 to 56.396 if the factorial or center point is missing. The spherical CCD will have a $D$-efficiency as high as 71.13, but this is not very a robust design if there is still a chance to lose a response at the center run. Figure 3.6 (a) shows a comparison of VDGs of robust designs without a missing run, with a missing factorial run, and with a missing center run which, hereafter, are referred to as $\xi$, $\xi_f$, and $\xi_c$, respectively. Inspection of the VDG reveals that the SPV of $\xi_c$ can be as high as 40 at the center of the design and decreases as $r$ increases until $r \approx 1.5$. The missing factorial run does not change the average scaled prediction variance (ASPV) much as it is close to that of $\xi$. Also, the MinSPVs of $\xi$ and $\xi_f$ are about the same for all radii. Notice that design $\xi$ is not far from a rotatable design, and its maximum SPV is only 14.87 and occurs at $(\pm r, 0, 0)$,

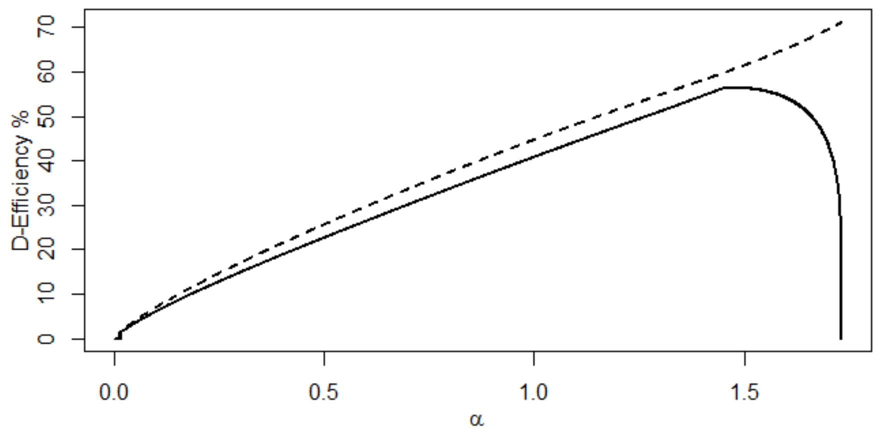
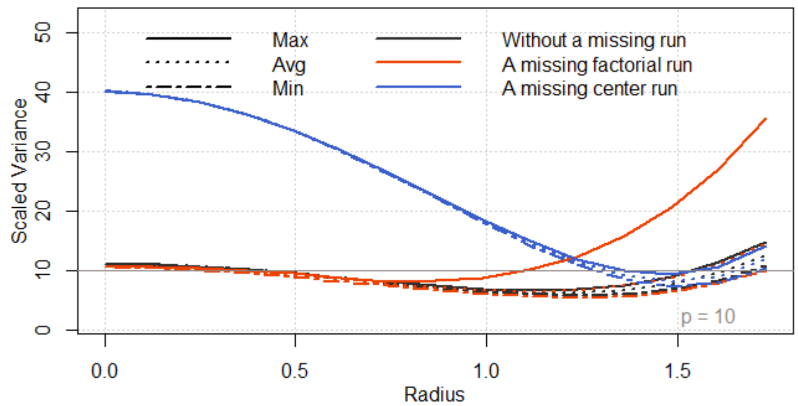


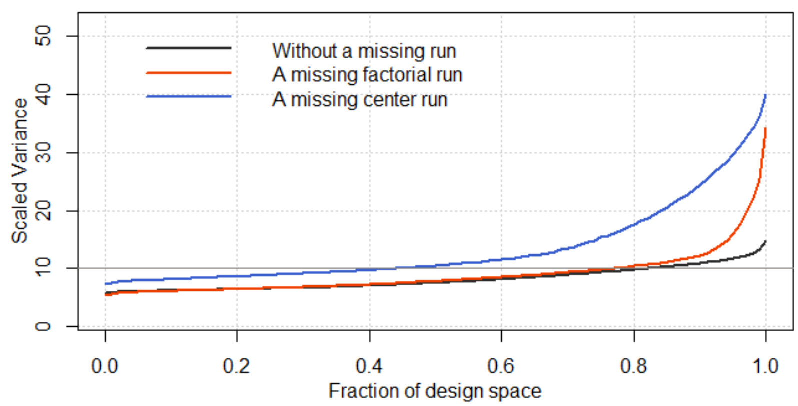

Figure 3.5: The $D$-efficiency and Min $D$ of three-factor CCDs: solid line for Min $D$'s and dashed line for $D$-efficiencies.

$(0, \pm r, 0)$, or $(0, 0, \pm r)$, $r = \sqrt{3}$. This is due to the fact that $\xi$ has an axial point distance $< \sqrt{3}$, so no data are collected at those points. Figure 3.6 (b) shows the FDS plots of $\xi$, $\xi_f$, and $\xi_c$. Less than 50% of a design region of $\xi_c$ has a SPV less than 10, which is the $G$-optimal value, and designs $\xi$ and $\xi_f$, respectively, have about 77% and 83% of the design space with SPVs less than the $G$-optimal value.

The VDGs of the robust and spherical designs are illustrated in Figure 3.7(a). Because axial points of the robust design are closer to the center of the design than those of the spherical design, when $r \lessapprox 1.25$, the VDG is lower for the robust design. While for $r \gtrapprox 1.25$, the MaxSPVs are larger, and the ASPV is slightly larger for the robust design than that of the spherical design. Figure 3.7 (b) shows the FDS plots. The percentages of the design space having SPVs of less than 10 in both designs are about the same.



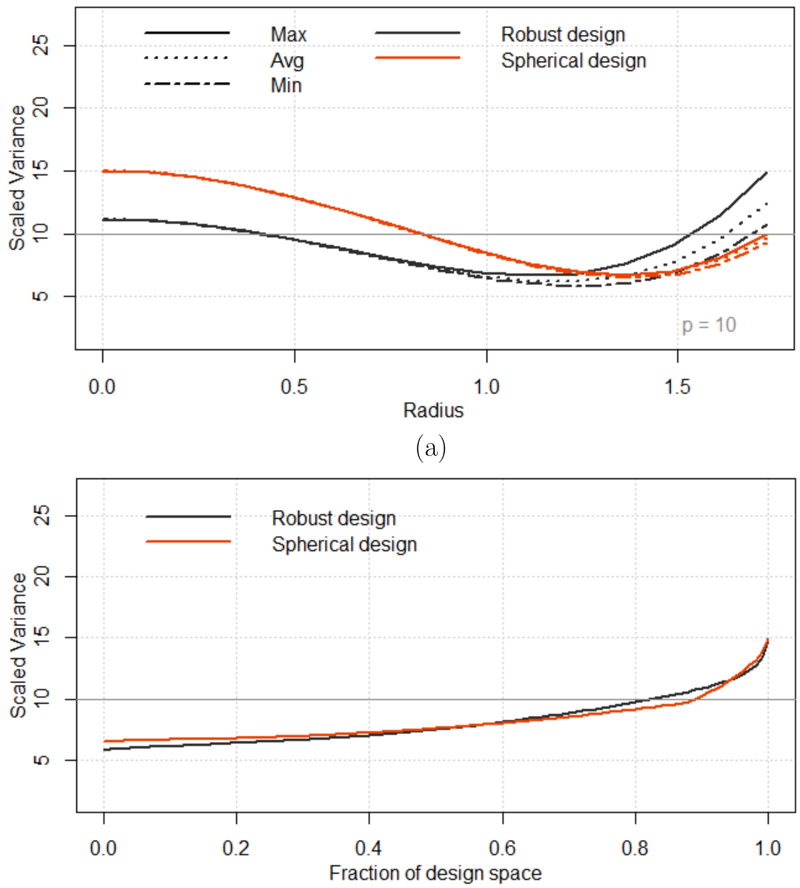

(a)




(b)

Figure 3.6: The VDGs (a) and FDS plots (b) of three-factor robust CCDs based on the Min $D$ without a missing run (black line), with a missing factorial run (red line), and with a missing center run (blue line).

In conclusion, the robust design uses $\alpha = 1.466$ and has a $D$-efficiency of 60.263 if there is no missing run. The spherical design has a $D$-efficiency of 71.13, but it can be zero if the center run is missing. When the robust design is used, the lowest possible $D$-efficiency is 56.396, and SPVs are just slightly larger than those of the spherical design at design points near the spherical axial points, e.g., $(\sqrt{3}, 0, 0)$.




(a)



(b)

Figure 3.7: The VDGs (a) and FDS plots (b) of the three-factor spherical CCD and robust CCD based on the Min $D$.

## 4.3. Four-Factor Min-$D$ CCD

The behaviors of $D$-efficiencies of four-factor CCDs with a single missing point over different values of $\alpha$ are similar to the three-factor Min-$D$ except with $\alpha_{\text{crit}} = 1.767$ and maximum $\alpha = \sqrt{4} = 2$. It is illustrated in Figure 3.8. Because the number of design points is much greater than the number of parameters, the changes in the $D$-efficiency due to any of the missing types are about the same. However, the $D$-efficiency drops quickly to zero as $\alpha \to 2$ if the center run is missing.

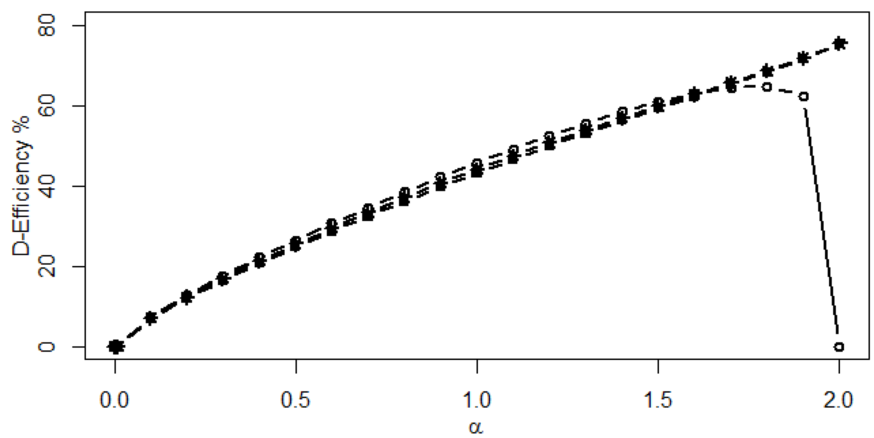



Figure 3.8: $D$-efficiencies of four-factor CCDs having a missing response: solid squares for a missing factorial, stars for a missing axial, and open circles for a missing center run.

In Figure 3.9, the highest Min $D$ is 64.786% for the robust design with $\alpha = \alpha_{\text{crit}}$. Unlike the two- or three-factor CCDs, when $\alpha < \alpha_{\text{crit}}$, the differences between the $D$-efficiencies and Min $D$'s are very small, so the effect of a missing run can be ignored. When $\alpha > \alpha_{\text{crit}}$, the $D$-efficiency decreases quickly to zero if the center run is missing. For the robust design, the $D$-efficiency is 68.638 and will drop to its minimum of 64.786 if the center point is missing. The spherical CCD, however, has a $D$-efficiency of 76.727, but there is a risk of dropping to zero if the center run is lost. Thus, using $\alpha$ of 1.767 makes the design more robust to a missing trial in a spherical region.

Figure 3.10 (a) shows comparisons of VDGs of robust CCDs. The patterns for $\xi$, $\xi_f$, and $\xi_c$ are similar to those of the three-factor Min-$D$ CCD except the change in inflection occurs at $r = 1.8$, and the maximum SPV $\approx 81.288$. Also, the SPVs are very close between $\xi_f$ and $\xi$ for $r < 1.8$ while the MinSPVs are about the same for all radii. Notice that design $\xi$ is close to being rotatable with a maximum SPV $\approx 21.15$, and occurs at $(\pm r, 0, 0, 0)$, $(0, \pm r, 0, 0)$, $(0, 0, \pm r, 0)$, and $(0, 0, 0, \pm r)$, $r = \sqrt{k} = 2$. This is analogous to the three-factor case in Section 4.2. In Figure 3.10 (b), the FDS

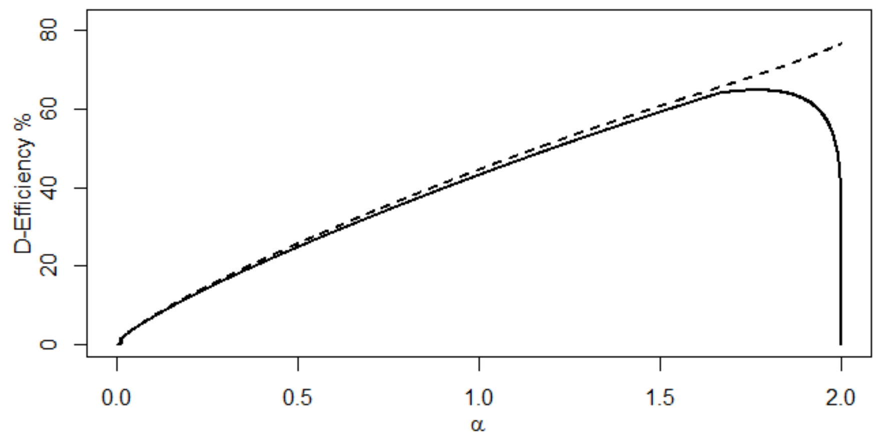
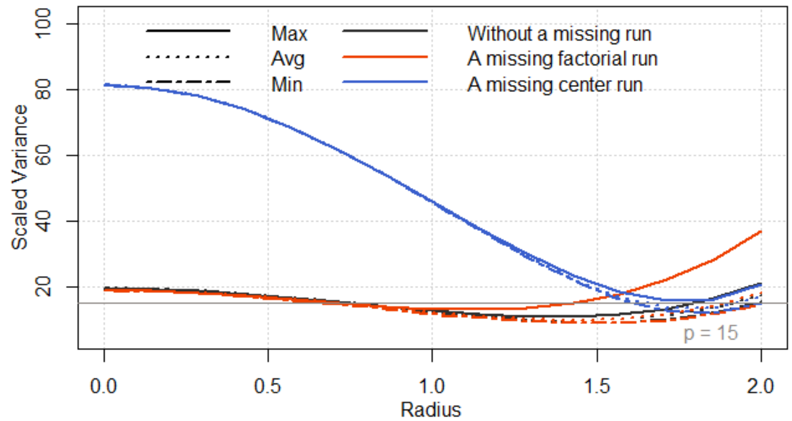


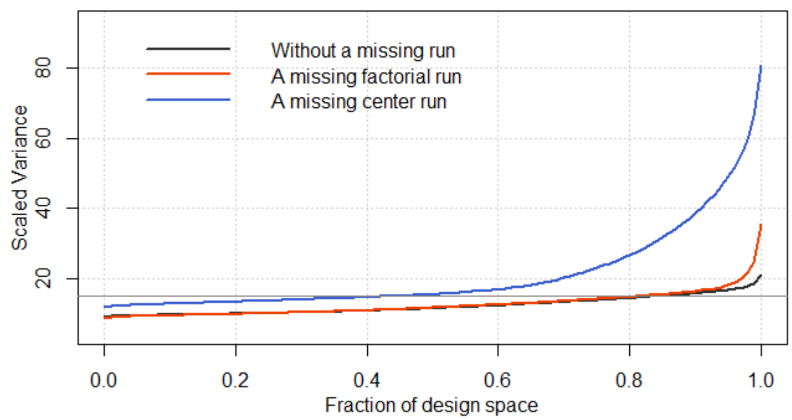

Figure 3.9: The $D$-efficiency and Min $D$ of four-factor CCDs: solid line for Min $D$'s and dashed line for $D$-efficiencies.

plots show that for $\xi_c$, less than 45% of the design region has the SPV $< 15$, but designs $\xi$ and $\xi_f$ have about 85% of the design space with SPVs $< 15$.

The VDGs of the robust and spherical designs are similar to those of the three-factor VDGs in Figure 3.7(a) except with the inflection point being $\approx 1.5$. The VDGs are lower in the robust design for $r \lessapprox 1.5$ while the MaxSPVs are larger in the robust design for $r \gtrapprox 1.5$. When $r \gtrapprox 1.62$, the ASPVs of the robust design are slightly larger compared to those of the spherical design. The FDS plots in Figure 3.11 (b) show that for the robust design, approximately 85% of the design region has SPVs $< 15$ (the $G$-optimal value) while it is about 92% for the spherical design.



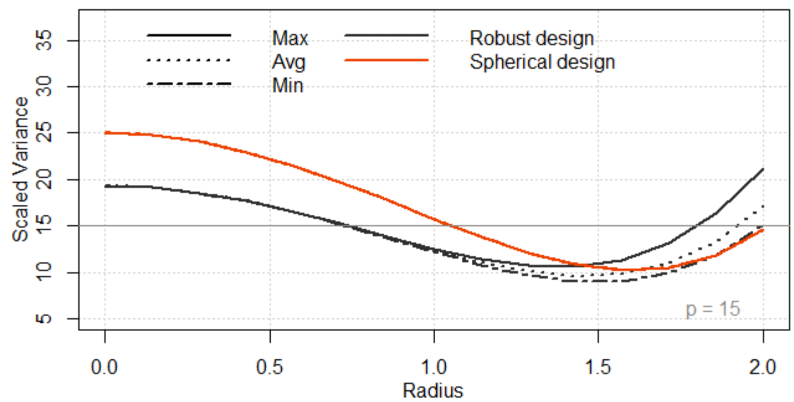

(a)



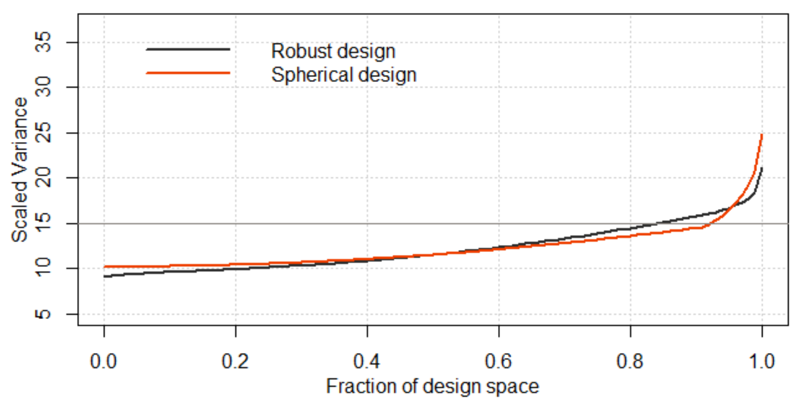

(b)

Figure 3.10: The VDGs (a) and FDS plots (b) of four-factor robust CCDs based on the Min $D$ without a missing run (black line), with a missing factorial run (red line), and with a missing center run (blue line).

In conclusion, if the robust design is used and the center run is missing, although the information matrix is not singular, researchers should be aware of very poor predictions of points near or at the center of the design. If there is no missing run, the robust design (CCD with $\alpha = 1.767$) has $D$-efficiency of 68.638, and the SPVs are, in general, slightly higher than those of the spherical CCD.




(a)




(b)

Figure 3.11: The VDGs (a) and FDS plots (b) of the four-factor spherical CCD and robust CCD based on the Min $D$.

## 5. Min-$A$ Robust Composite Designs

Previously discussed in Section 2, the moment matrix of the spherical CCD with $n_c = 1$ can be singular if only one center run is missing. In this section, the $\alpha$ that maximizes the Min $A$ of CCDs with $n_c = 1$ will be searched numerically. Because of the structure of CCDs, a missing observation can only occur as a factorial, axial, or center point.

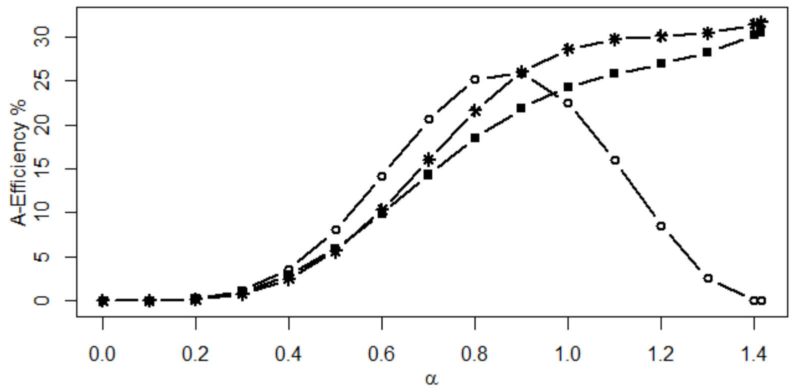



Figure 3.12: $A$-efficiencies of two-factor CCDs having a missing response: solid squares for a missing factorial, stars for a missing axial, and open circles for a missing center run.

## 5.1. Two-Factor Min-$A$ CCD

The behaviors of $A$-efficiencies for two-factor CCDs with a single missing point over different values of $\alpha$ are illustrated in Figure 3.12. When $\alpha < .6$, CCDs with a missing factorial or axial run have about the same $A$-efficiency, but when $.6 < \alpha < .974$, the missing factorial causes the greatest reduction in the $A$-efficiency. For $\alpha > .974$, the $A$-efficiency decreases quickly and drops to zero at $\alpha = \sqrt{2}$ if the response at the center run is lost. For this case, the critical $\alpha$ is .974, which will be referred to as $\alpha_{\text{crit}}$.

A comparison of the $A$-efficiency and Min $A$ of the two-factor spherical CCDs is illustrated in Figure 3.13. The highest Min $A$ of 23.71% occurs at $\alpha_{\text{crit}}$. The CCD with $\alpha = \alpha_{\text{crit}}$ will subsequently be called the robust design. As $\alpha$ increases from zero, the difference between the $A$-efficiency and Min $A$ increases. The $A$-efficiency of the robust design will decrease only slightly from 30.962 to 23.71 (Min $A$) if a factorial or center run is missing. The spherical CCD has an $A$-efficiency of 30.476, which is slightly less than that of the robust design.

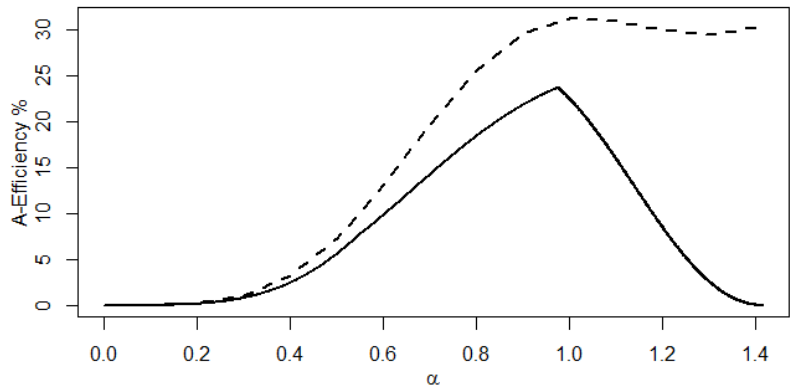



Figure 3.13: The $A$-efficiency and Min $A$ of two-factor CCDs: solid line for Min $A$'s and dashed line for $A$-efficiencies.

Figure 3.14 presents contours of SPVs of the robust design with different types of missing runs. Figures (a), (b), (c), and (d) correspond to the robust design without any missing runs, and designs with $(-1, -1)$, $(-\alpha_{\text{crit}}, 0)$, $(0, 0)$ missing, respectively. Although designs with a missing factorial or center run have the same $A$-efficiency, their precisions for predictions are different and depend on a location of the point for prediction. The maximum SPV of the designs having a missing $(-1, -1)$, $(-\alpha_{\text{crit}}, 0)$, and $(0, 0)$ are $35.2, 25.2$, and $13.6$, respectively.

## 5.2. Three-Factor Min-$A$ CCD

Analogous to Figure 3.12 for a two-factor CCD, Figure 3.15 illustrates the behaviors of $A$-efficiencies for three-factor CCDs with a single missing point over different values of $\alpha$. For this case, $\alpha_{\text{crit}} = 1.176$. For $\alpha \lessapprox \alpha_{\text{crit}}$, CCDs with a missing axial will the lowest $A$-efficiency, and for $\alpha \gtrapprox \alpha_{\text{crit}}$, the $A$-efficiencies of CCDs with a missing center run are the lowest and decrease quickly to zero.

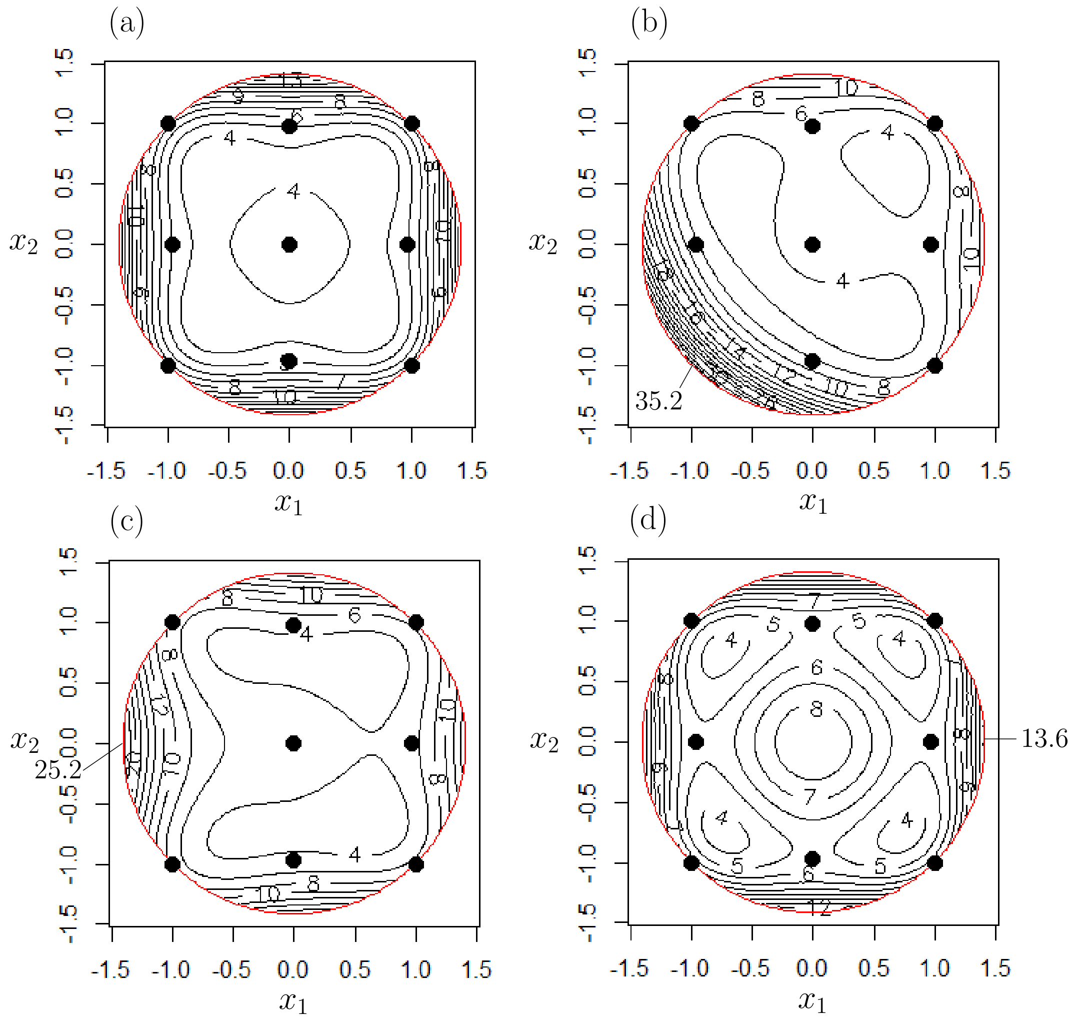



Figure 3.14: Contours of SPVs of the two-factor robust CCD based on the Min $A$: (a) without a missing response; (b) a missing factorial point; (c) a missing axial point; and (d) a missing center point. Solid circles represent the design points.

Figure 3.16 presents the behaviors of the $A$-efficiency and Min $A$ of the CCDs. The conclusions are similar to those for the two-factor case except the highest Min $A$ is 32.815%. The difference between the $A$-efficiency and Min $A$ of the spherical CCD with $\alpha < \alpha_{\text{crit}}$ is less than 5%. The $A$-efficiency of the robust design will decrease slightly from 37.218 to 32.815 if a factorial or center run is missing. The spherical CCD will have an $A$-efficiency of 32.401, which is slightly less than that of the robust

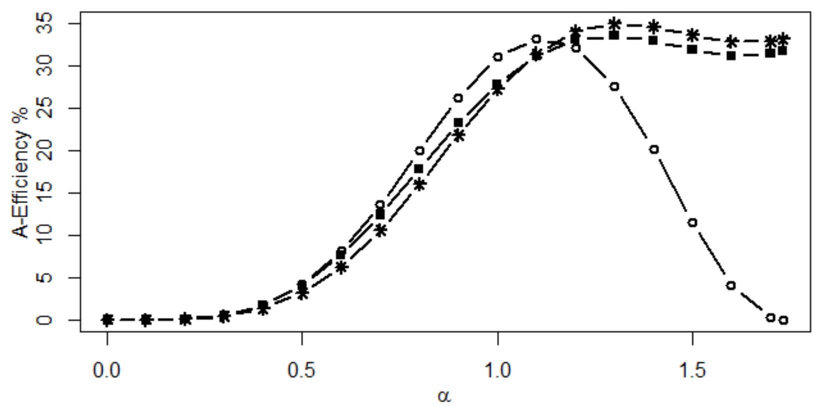



Figure 3.15: $A$-efficiencies of three-factor spherical CCDs having a missing response: solid squares for a missing factorial, stars for a missing axial, and open circles for a missing center run.

design, but its Min $A$ is zero. In this case, based on the $A$-efficiency and Min $A$, the robust CCD is superior to the spherical CCD.

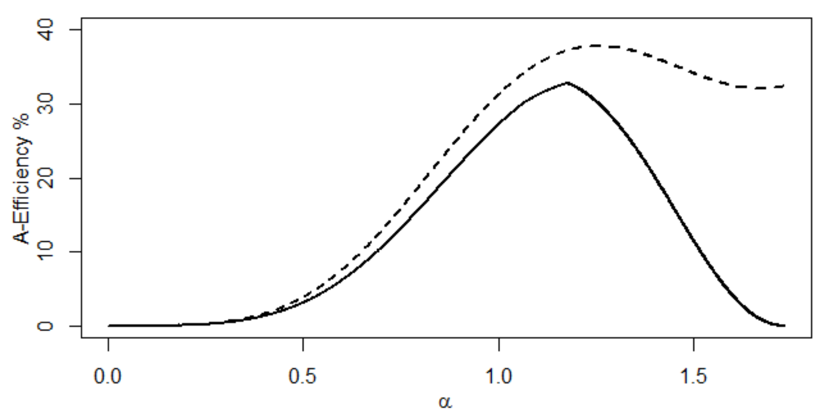



Figure 3.16: The $A$-efficiency and Min $A$ of three-factor CCDs: solid line for Min $A$'s and dashed line for $A$-efficiencies.

Figure 3.17 (a) shows a comparison of VDGs of $A$-optimal robust exact designs without a missing run, with a missing factorial run, and with a missing center run which, hereafter, are referred to as $\xi$, $\xi_f$, and $\xi_c$, respectively. Inspection of the VDG

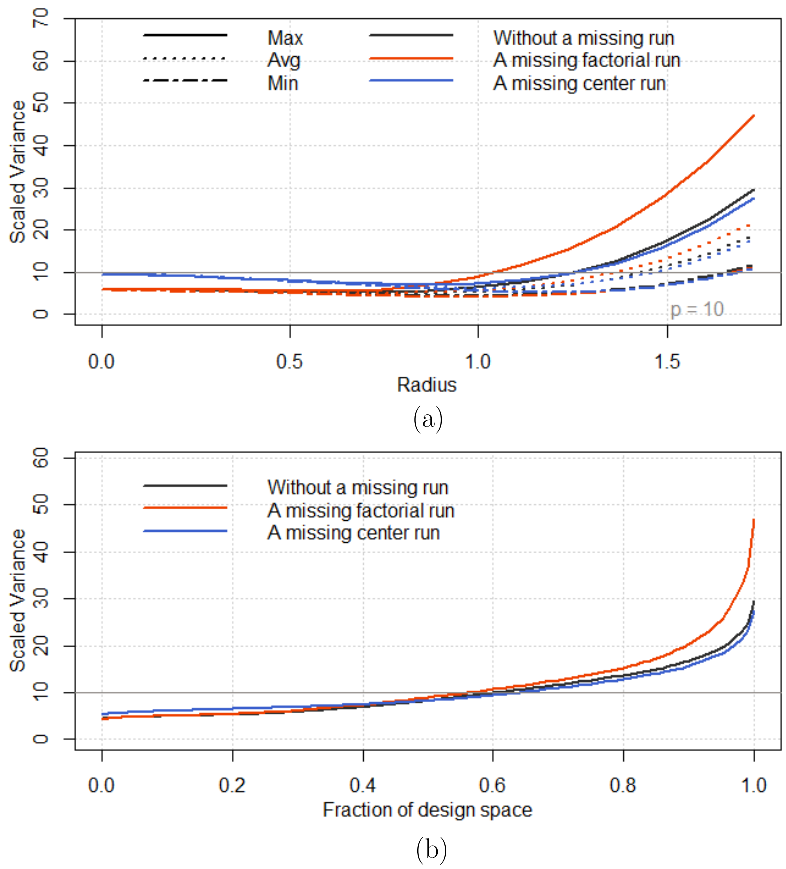



Figure 3.17: The VDGs (a) and FDS plots (b) of three-factor robust CCDs based on the Min $A$ without a missing run (black line), with a missing factorial run (red line), and with a missing center run (blue line).

reveals that the SPV of $\xi_f$ can be as high as 47.344 at $r = \sqrt{3}$. The missing center run does not change the ASPV much compared to that of $\xi$. The MinSPVs of $\xi$ and $\xi_f$ are about the same for all radii. Notice that even though the center run is lost, the SPVs of points near or at the center run are very low compared to the robust Min-$D$ CCD. Figure 3.17 (b) shows the FDS plots of $\xi$, $\xi_f$, and $\xi_c$. It is seen that all designs $\xi$, $\xi_f$, and $\xi_c$ have about the same percentage of the design space with SPVs $< 10$, the $G$-optimal value.

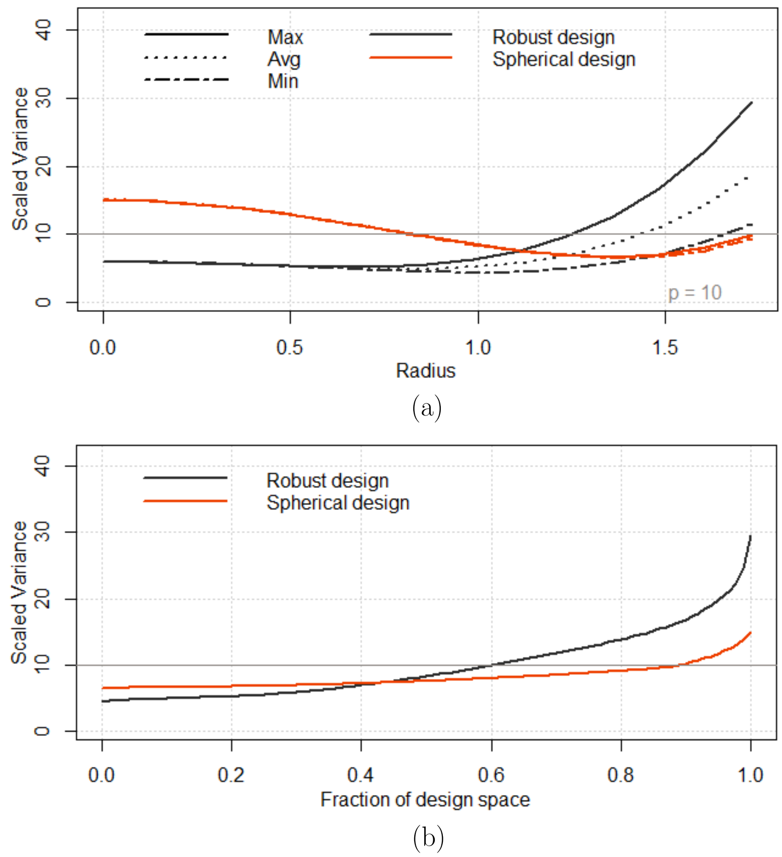



Figure 3.18: The VDGs (a) and FDS plots (b) of the three-factor spherical CCD and robust CCD based on the Min $A$.

Figure 3.18 (a) shows a comparison of VDGs of the robust and spherical CCDs. Because axial points of the robust design are closer to the center of the design than those of the spherical design, when $r \lessapprox 1.1$, the VDG is lower for the robust design. For $r \gtrapprox 1.25$, the MaxSPVs, as well as ASPVs, are larger for the robust design, and its maximum ASPV is 18.92 which is about 9 larger than the maximum SPV of spherical CCD. Figure 3.18 (b) shows the FDS plots. The percentage of the design space of the spherical CCD with SPVs $< 10$ is approximately 89% while it is only 60% for the robust design. Thus, even though the robust design has a higher $A$-efficiency, the precision of predictions is poor at the design space with $r \longrightarrow \sqrt{3}$.

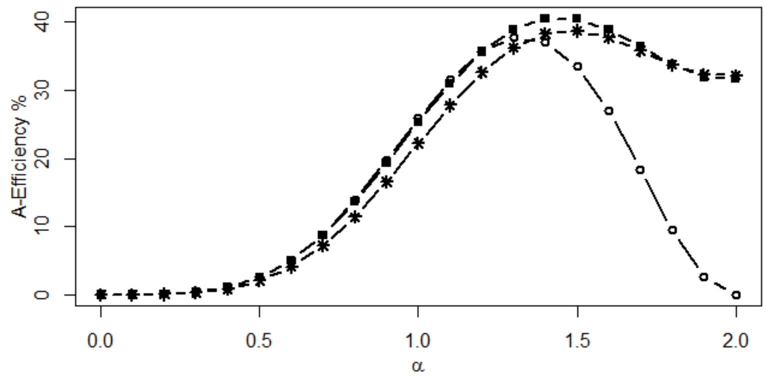



Figure 3.19: $A$-efficiencies of four-factor CCDs having a missing response: solid squares for a missing factorial, stars for a missing axial, and open circles for a missing center run.

## 5.3. Four-Factor Min-$A$ CCD

The behaviors of $A$-efficiencies for four-factor CCDs with a single missing point over different values of $\alpha$ are similar to the three-factor Min $A$ except with $\alpha_{\text{crit}} = 1.36$. They are illustrated in Figure 3.19. When $\alpha \lessapprox 1.2$, the CCDs with a missing factorial and with a missing center run have the about the same $A$-efficiency. Also, when $\alpha < \alpha_{\text{crit}}$, the missing axial run causes the greatest reduction in $A$-efficiencies, and when $\alpha > \alpha_{\text{crit}}$, the $A$-efficiency decreases quickly and drops to zero at $\alpha = 2$ if the center run is missing.

In Figure 3.20, the highest Min $A$ is 37.708% for the robust design with $\alpha = \alpha_{\text{crit}}$. When $\alpha < \alpha_{\text{crit}}$, the $A$-efficiency and Min $A$ are slightly different, and when $\alpha > \alpha_{\text{crit}}$, the Min $A$ drops quickly to zero if the center run is missing. For the robust design, the $A$-efficiency is 41.251 and will drop to its minimum of 37.708 if the axial or center run is missing. The spherical CCD, however, has an $A$-efficiency of 31.648, slightly less than that of the robust CCD.

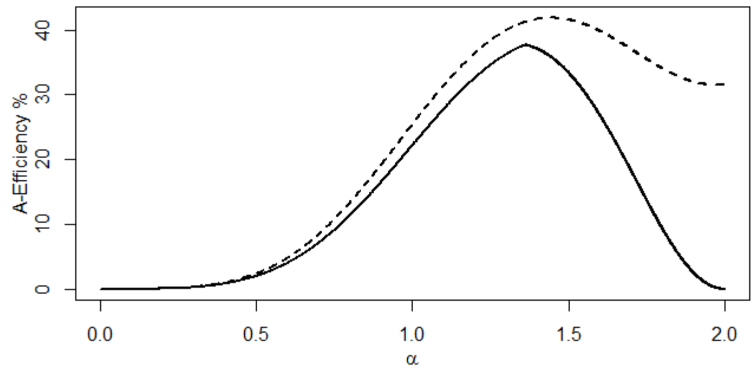



Figure 3.20: The $A$-efficiency and Min $A$ of four-factor CCDs: solid line for Min $A$'s and dashed line for $A$-efficiencies.

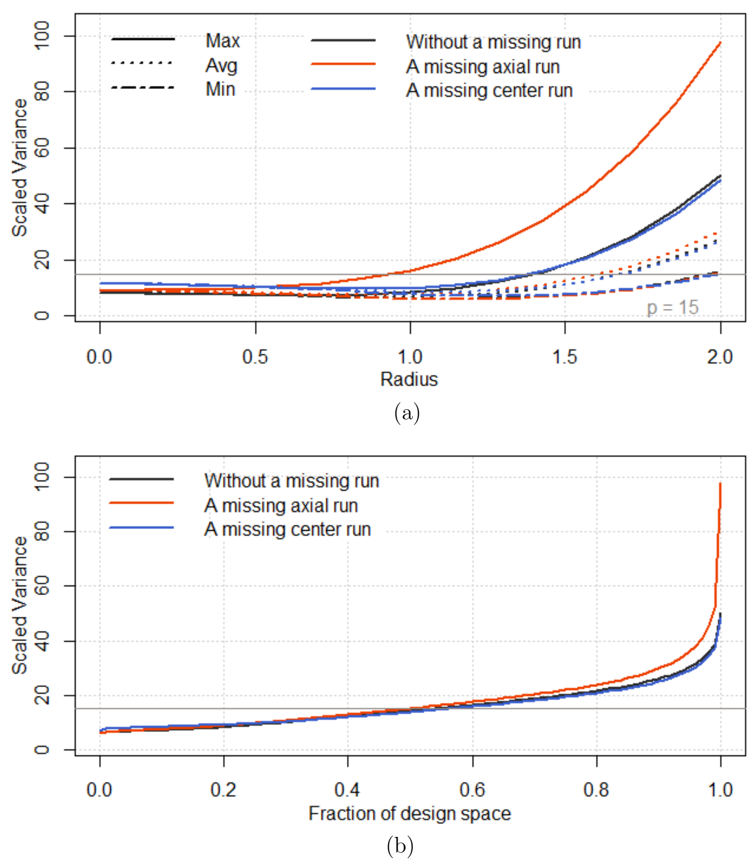



Figure 3.21: The VDGs (a) and FDS plots (b) of four-factor robust CCDs based on the Min $A$ without a missing run (black line), with a missing axial run (red line), and with a missing center run (blue line).

A comparison of VDGs of robust CCDs is presented in Figure 3.21 (a). The patterns for $\xi$, $\xi_a$, and $\xi_c$ are similar to those of the three-factor Min-$A$ CCD except the change in inflection occurs at $r \approx 1$, and the maximum SPV $\approx 97.568$. This maximum SPV of $\xi_a$ occurs at $(\pm r, 0, 0, 0)$, $(0, \pm r, 0, 0)$, $(0, 0, \pm r, 0)$, or $(0, 0, 0, \pm r)$, $r = 2$. However, the ASPVs, as well as MinSPVs, of $\xi_a$ are the about the same as those of $\xi$ for all radii. For $r \lessapprox 1$, SPVs are slightly larger in $\xi_c$ than in $\xi$, and for $r \gtrapprox 1$, the distributions of SPVs of $\xi$ and $\xi_c$ are similar. Figure 3.21 (b) shows the FDS plots of $\xi, \xi_a$, and $\xi_c$. The percentages of the design space with SPVs $< 15$ of $\xi, \xi_a$, and $\xi_c$ are about the same. Overall, if the robust CCD is employed, and a response at one of the axial points is lost, researchers should be aware of a very high SPV at that missing point.

A comparison of VDGs of the robust and spherical designs is presented in Figure 3.22 (a). Because axial points of the robust design are closer to the center of the design than those of the spherical design, for $r \lessapprox 1.2$, the VDGs are lower in the robust than in the spherical design. For $r \gtrapprox 1.47$, the MaxSPVs (also ASPVs) are larger in the robust design. Unlike the spherical design, the robust design is not near rotatable. The FDS plots in Figure 3.22 (b) show that for the robust design, approximately 55% of the design region has SPVs $< 15$ (the $G$-optimal value) while it is about 92% for the spherical design. In this case, although the robust has a higher $A$-efficiency, approximately 10% of the design region has very high SPV values (more than 30), thus the prediction for some points near the edge of the design region, e.g., $(0, \pm 2, 0, 0)$, should be avoided.

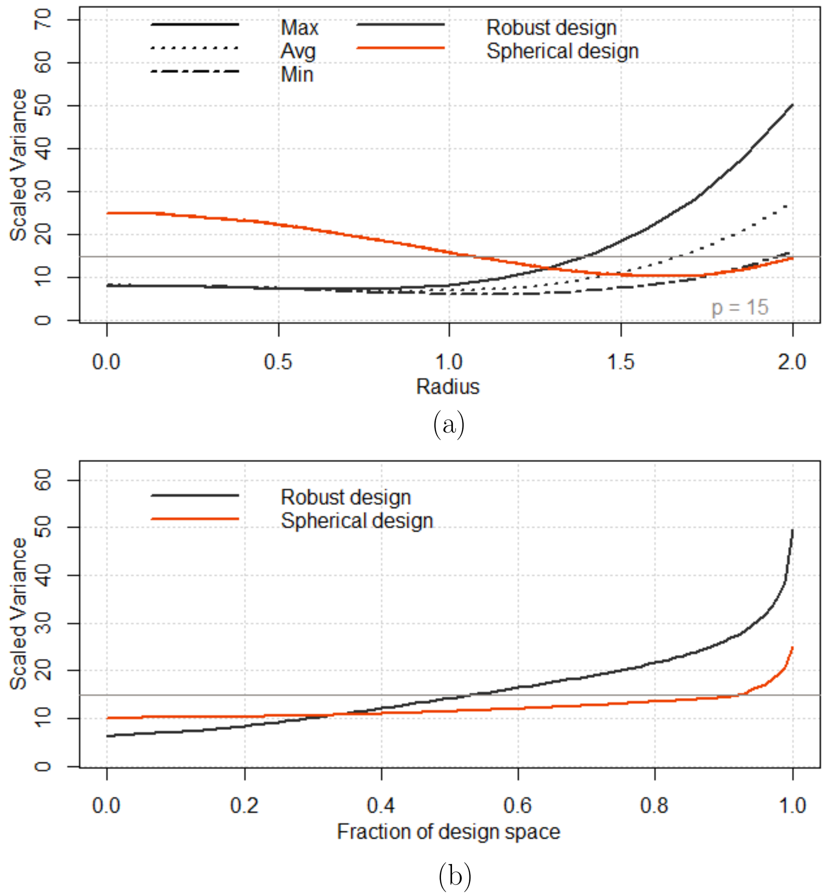



Figure 3.22: The VDGs (a) and FDS plots (b) of the four-factor spherical CCD and robust CCD based on the Min $A$.

## 6. Min-$G$ Robust Composite Designs

The moment matrix of the spherical CCD with $n_c = 1$ can be singular if the only center run is missing. Therefore, the $\alpha$ that maximizes the Min $G$ will be searched numerically. Because of the structure of CCDs, a missing observation can only occur as a factorial, axial, or center point.

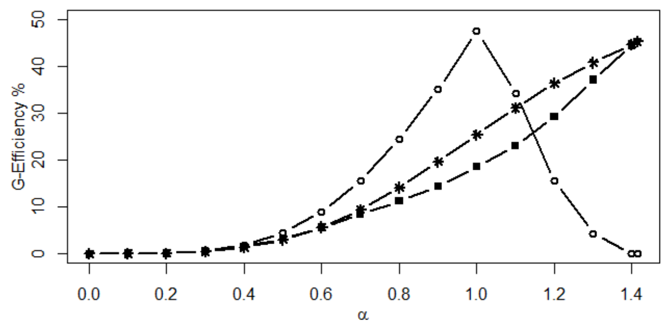



Figure 3.23: $G$-efficiencies of two-factor CCDs having a missing response: solid squares for a missing factorial, stars for a missing axial, and open circles for a missing center run.

## 6.1. Two-Factor Min-$G$ CCD

The behaviors of $G$-efficiencies for two-factor CCDs with a single missing point over different values of $\alpha$ are illustrated in Figure 3.23. For $0.7 < \alpha < 1.142$, the factorial points are more important than the other points because losing one of them causes the greatest reduction in the $G$-efficiency. For $\alpha > 1.142$, if the center run is missing, the $G$-efficiency will quickly decrease to zero. The $\alpha = 1.142$ will be referred to as $\alpha_{\text{crit}}$. In Figure 3.24, a comparison of the $G$-efficiencies and Min $G$ of the two-factor CCDs with different values of $\alpha$ is presented. The highest Min $G$ of 25.483% occurs at $\alpha_{\text{crit}}$. The CCD with $\alpha_{\text{crit}}$ will subsequently be called the robust design. Note that $\alpha_{\text{crit}}$ is very close to $\alpha_{\text{crit}}$ obtained from the Min $D$ criterion. Comparing to Figure 3.2, it is obvious that a missing value has more impact on the $G$-efficiency than the $D$-efficiency. When $\alpha > \alpha_{\text{crit}}$, the Min $G$ decreases and equals zero at $\alpha = \sqrt{2}$. The $G$-efficiency of the robust design will decrease appreciably from 61.882 to 25.485 if a factorial or center run is lost. The spherical CCD has $G$-efficiency of 66.671, slightly larger than that of the robust design, but the Min $G$ of the spherical design can be zero.

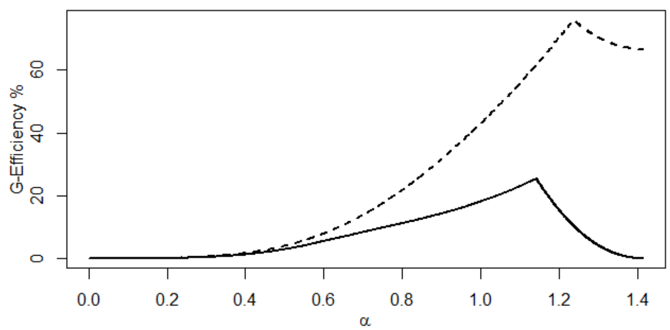



Figure 3.24: The $G$-efficiency and Min $G$ of two-factor CCDs: solid line for Min $G$'s and dashed line for $G$-efficiencies.

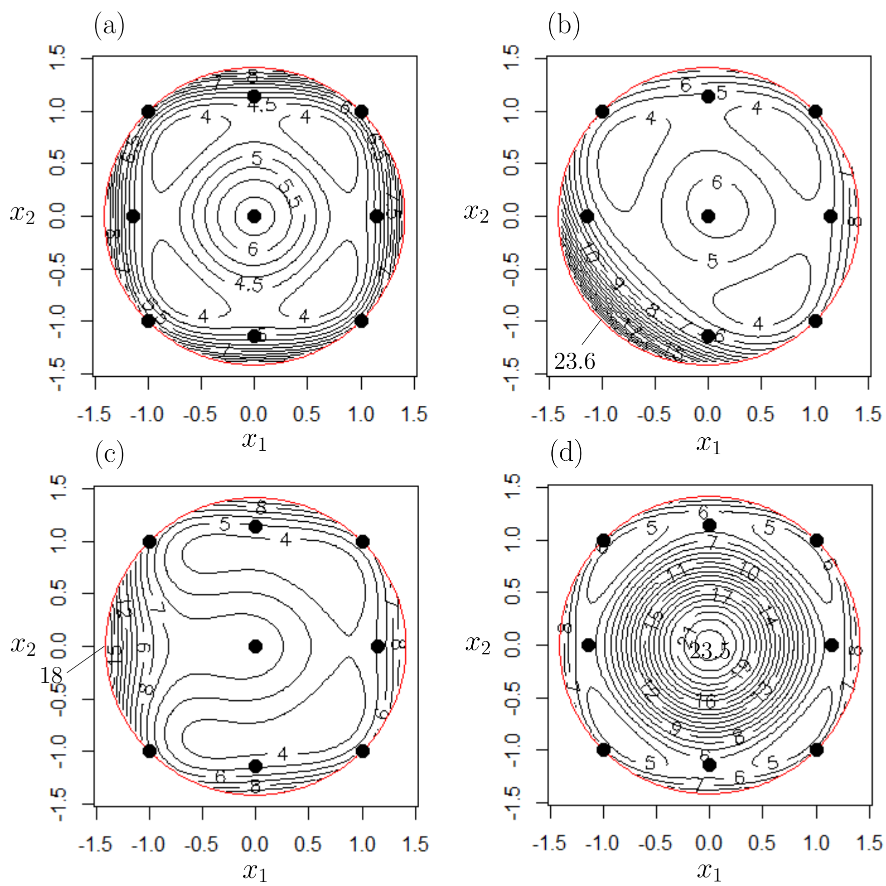



Figure 3.25: Contours of SPVs of the two-factor robust CCD based on the Min $G$: (a) without a missing response; (b) a missing factorial point; (c) a missing axial point; and (d) a missing center point. Solid circles represent the design points.

Contours of SPVs of the robust design with different types of a missing run are illustrated in Figure 3.25. Figures (a), (b), (c), and (d) correspond to the robust design without any missing runs, and designs with $(-1,-1)$, $(-\alpha_{\text{crit}},0)$, and $(0,0)$ missing, respectively. Although robust designs with a missing factorial or center run have the same $G$-efficiency, their precisions for predictions are different and depend on a location of the point for prediction. The maximum SPV of the designs with a missing $(-1,-1)$, $(-\alpha_{\text{crit}},0)$, and $(0,0)$ are $23.6, 18$, and $23.5$, respectively.

## 6.2. Three-Factor Min-$G$ CCD

Figure 3.26 shows the behaviors of $G$-efficiencies for three-factor CCDs with a single missing point over different values of $\alpha$. When $\alpha < 1.3$, the corresponding CCD is rather sensitive to a missing axial run, and for $1.3 < \alpha < 1.449$, a factorial point is more important than the others because it causes the greatest reduction in $G$-efficiencies. For $\alpha > 1.449$, the $G$-efficiency drops rapidly to zero if the response at the center run is missing. For this case, $\alpha_{\text{crit}} = 1.449$, and the corresponding CCD will be referred to as the robust CCD.

The $G$-efficiency and Min $G$ of three-factor CCDs with different values of $\alpha$ are plotted in Figure 3.27. Unlike the $D$-efficiency, the $G$-efficiency is not an increasing function of $\alpha$. The highest Min $G$ of 27.849% occurs at $\alpha_{\text{crit}}$. The $G$-efficiency of the robust design will drop considerably from 65.072 to 27.849% if a factorial or center run is missing. The spherical CCD has a $G$-efficiency of 66.684, slightly higher than that of the robust CCD.

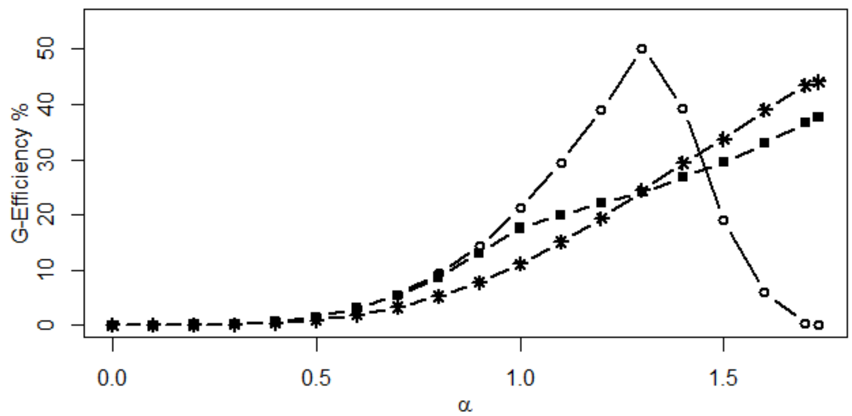



Figure 3.26: $G$-efficiencies for three-factor CCDs having a missing response: solid squares for a missing factorial, stars for a missing axial, and open circles for a missing center run.

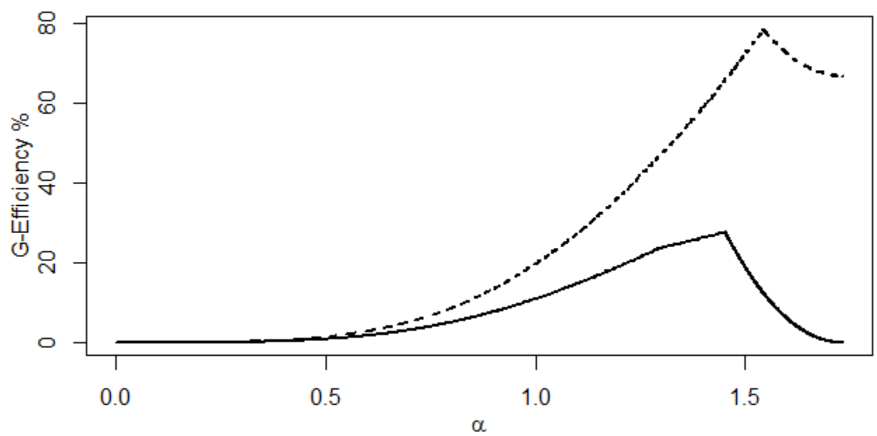
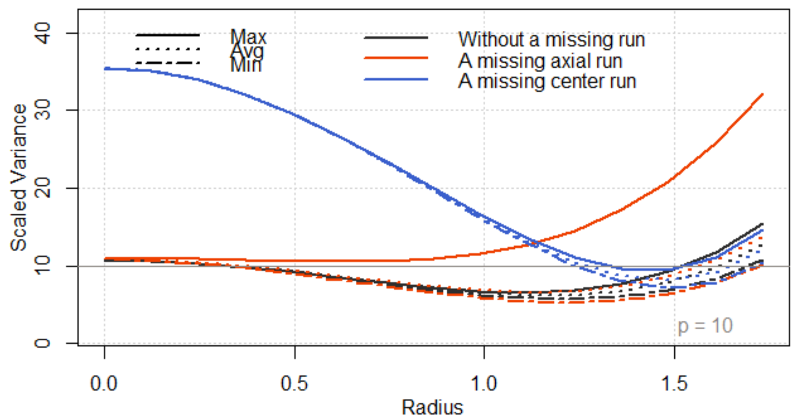


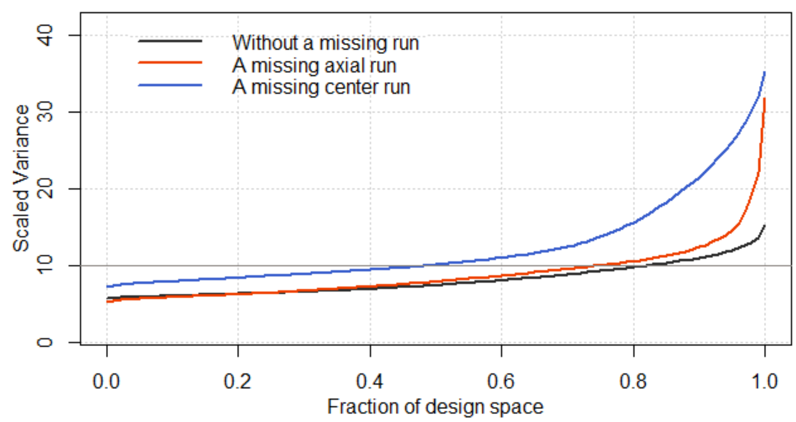

Figure 3.27: The $G$-efficiency and Min $G$ of three-factor CCDs: solid line for Min $G$'s and dashed line for $G$-efficiencies.

Figure 3.28 (a) show a comparison of VDGs of robust designs without a missing run, with a missing axial run, and with a missing center run which, hereafter, are referred to as $\xi$, $\xi_a$, and $\xi_c$, respectively. The SPV of $\xi_c$ can be as high as 35.418 at the center of the design. For all radii, $\xi$ and $\xi_a$ have about the same ASPV, as well as the MinSPV. Thus, although the MaxSPVs of $\xi_a$ are much larger than those of

$\xi$, this should be only concerned when the prediction at a factorial point missing is made. The FDS plots of $\xi$, $\xi_a$, and $\xi_c$ are shown in Figure 3.28(b). Both $\xi$ and $\xi_a$ have approximately 80% of the design space with SPVs < 10 while $\xi_c$ has only 48%.



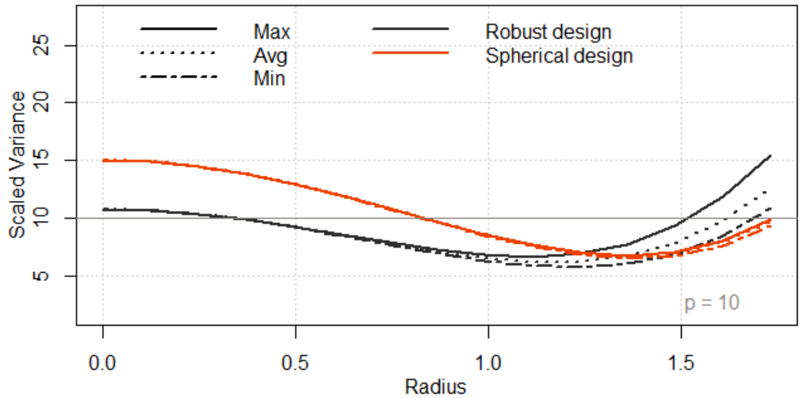

(a)



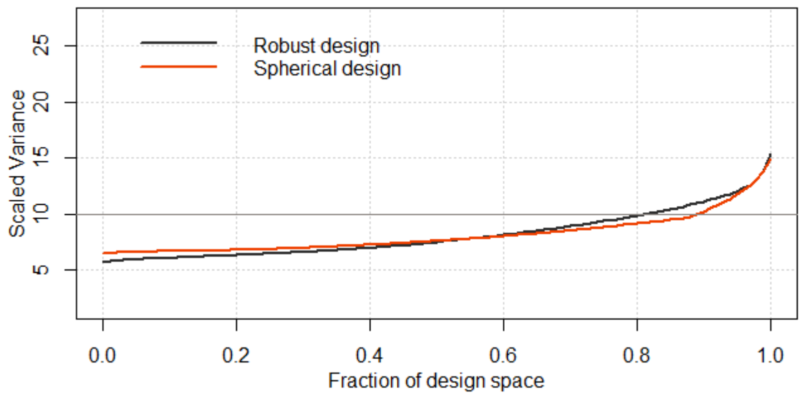

(b)

Figure 3.28: The VDGs (a) and FDS plots (b) of three-factor robust CCDs based on the Min $G$ without a missing run (black line), with a missing factorial run (red line), and with a missing center run (blue line).

Figure 3.29 (a) illustrates the VDGs for robust and spherical designs. Because axial points of the robust design are closer to the center of the design than those of the spherical design, when $r \lessapprox 1.24$, the VDG is lower for the robust design while




(a)




(b)

Figure 3.29: The VDGs (a) and FDS plots (b) of the three-factor spherical CCD and robust CCD based on the Min $G$.

for $r \gtrapprox 1.24$, the MaxSPVs are larger in the robust design. Also, the ASPVs of the robust design are slightly larger compared to those of the spherical design. The FDS plots are presented in Figure 3.29 (b). Approximately 81% of the design region of the robust design has SPVs $< 10$, the $G$-optimal value, and it is about 88% for the spherical design. Thus, in this case, the robust design is preferable because it is more robust to a missing point while its $G$-efficiency, as well as the percentage of a design space with SPVs $< 10$, is just slightly different from that of the spherical design.

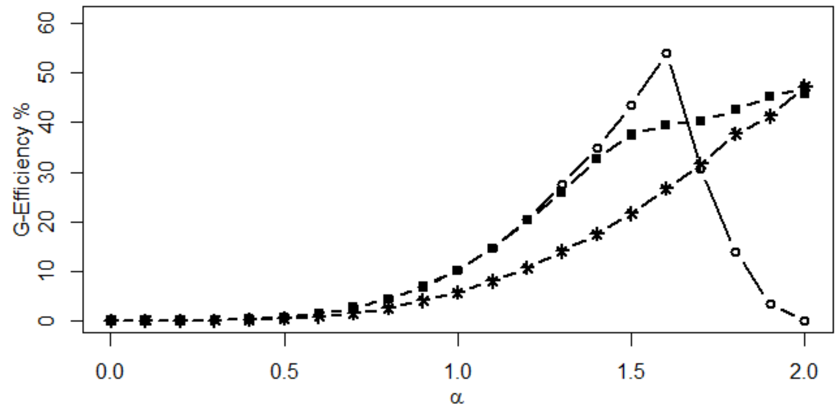



Figure 3.30: $G$-efficiencies for four-factor CCDs having a missing response: solid squares for a missing factorial, stars for a missing axial, and open circles for a missing center run.

## 6.3. Four-Factor Min-$G$ CCD

The $G$-efficiencies for four-factor CCDs with a single missing point over different values of $\alpha$ are plotted in Figure 3.30. For $\alpha < 1.7$, the axial point is more important than the others as it causes the greatest reduction in the $G$-efficiency, and when $\alpha > 1.7$ the center point is the most important because if it is lost, the $G$-efficiency will decrease quickly to zero. For this case, $\alpha_{\text{crit}} = 1.7$, and the corresponding CCD will be referred to as the robust CCD.

In Figure 3.31, both Min $G$ and $G$-efficiency are not increasing functions of $\alpha$. The highest Min $G$ is 30.39% for the robust design with $\alpha = \alpha_{\text{crit}}$. The $G$-efficiency of the robust design will considerably drop from 63.266 to 30.39% (Min $G$) if an axial or center run is missing while the spherical CCD has a $G$-efficiency of 60.064, slightly lower than that of the robust design.

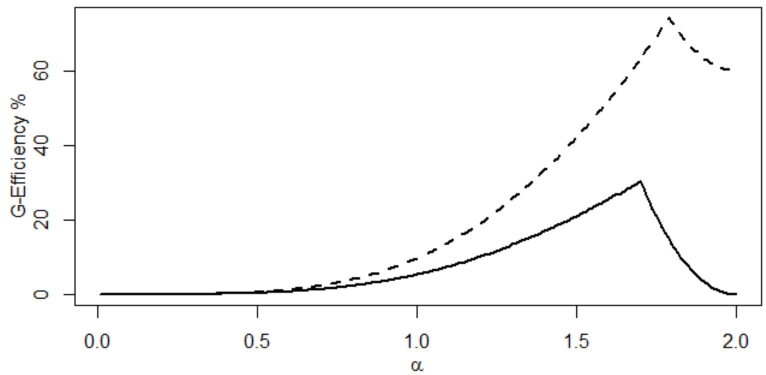
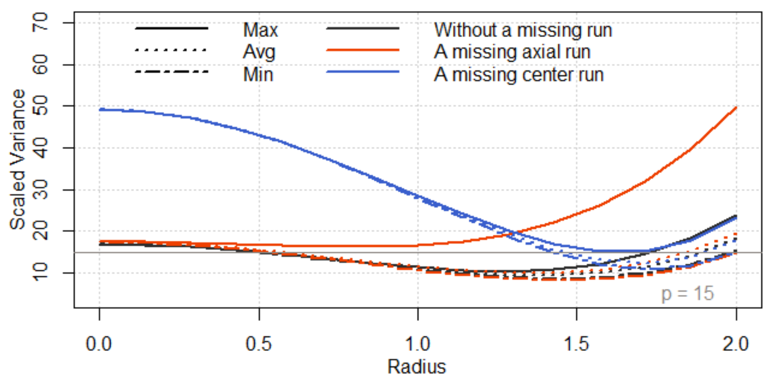
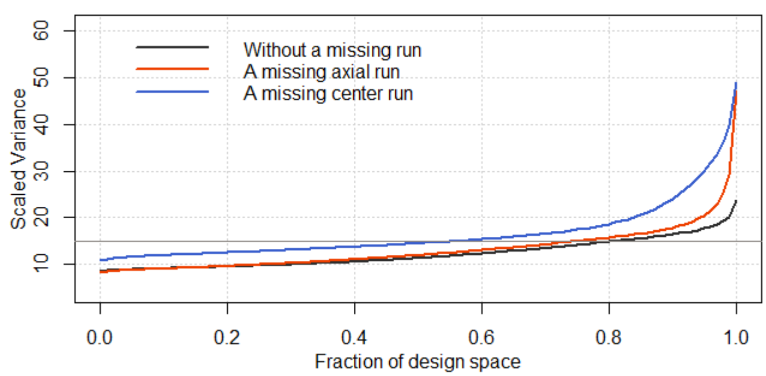



Figure 3.31: The $G$-efficiency and Min $G$ of four-factor CCDs: solid line for Min $G$'s and dashed line for $G$-efficiencies.

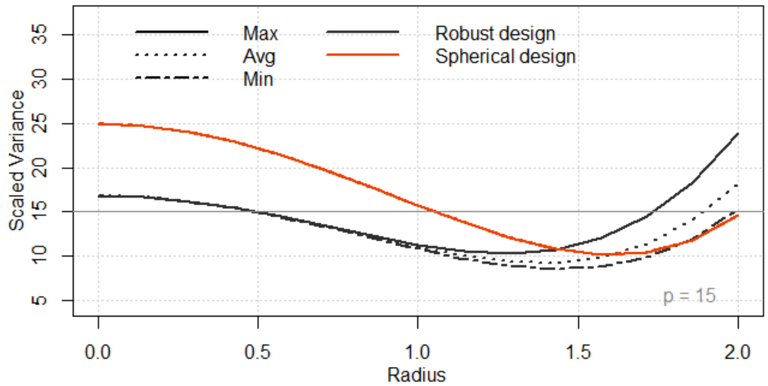



(a)

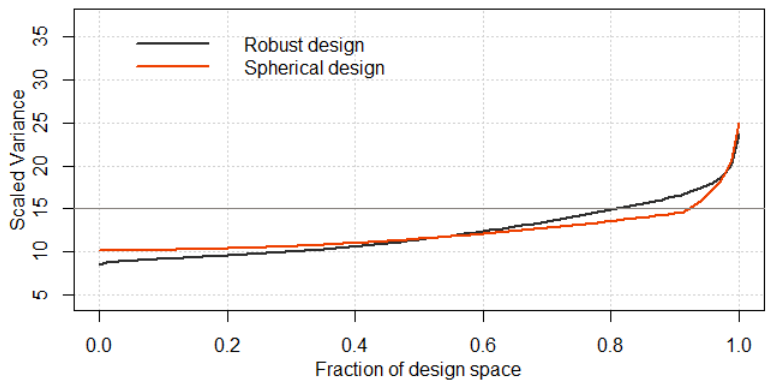



(b)

Figure 3.32: The VDGs (a) and FDS plots (b) of four-factor robust CCDs based on the Min $G$ without a missing run (black line), with a missing factorial run (red line), and with a missing center run (blue line).




(a)




(b)

Figure 3.33: The VDGs (a) and FDS plots (b) of the four-factor spherical CCD and robust CCD based on the Min $G$.

A comparison of VDGs of robust CCDs with different types of a missing value is illustrated in Figure 3.32 (a). The patterns for $\xi$, $\xi_a$, and $\xi_c$ are similar to those of the three-factor Min-$G$ CCD except the change in inflection occurs at $r = 1.7$, and the maximum SPV $\approx 50$. Also, the ASPVs, as well as MinSPVs, are very close between $\xi_a$ and $\xi$ for all radii. Notice that design $\xi$ is close to being rotatable with a maximum SPV $\approx 21$ occurring at $(\pm r, 0, 0, 0)$, $(0, \pm r, 0, 0)$, $(0, 0, \pm r, 0)$, and $(0, 0, 0, \pm r)$, $r = 2$. This is analogous to the three-factor case in Section 6.2. Figure 3.32 (b) shows the FDS plots of $\xi$, $\xi_a$, and $\xi_c$, respectively, having 55%, 75%, and 80% of the design space with SPVs $< 15$.

The VDGs of the robust and spherical designs are similar to those of the three-factor VDG in Figure 3.29 (a) except with the inflection point being $\approx 1.4$. The VDGs are lower in the robust design for $\alpha \lessapprox 1.4$ while for $\alpha \gtrapprox 1.4$, the ASPVs are slightly higher in the robust design compared to those of the spherical design. The FDS plots in Figure 3.33 (b) show that for the robust design, approximately 81% of the design region has SPVs $< 15$ (the $G$-optimal value), while it is about 92% for the spherical design.

## 7. Min-$IV$ Robust Composite Designs

In this section, the $\alpha$ that maximizes the Min $IV$ will be searched numerically. Because of the structure of CCDs, a missing observation can only occur as a factorial, axial, or center point. The integral part of the $IV$-efficiency is approximated by the Monte-Carlo integration as shown in equation (3.1).

### 7.1. Two-Factor Min-$IV$ CCD

The behaviors of $IV$-efficiencies for two-factor CCDs with a single missing point over different values of $\alpha$ are illustrated in Figure 3.34. Like other two-factor CCDs, a factorial point causes the greatest reduction in a design efficiency. For $.5 < \alpha < 1.03$, the CCD with a missing factorial run have the lowest $IV$-efficiency, and for $\alpha > 1.03$, the $IV$-efficiency of the design with a missing center run decreases quickly to zero. The critical value $\alpha = 1.03$ will be referred to as $\alpha_{\text{crit}}$.

The $IV$-efficiencies and Min $IV$'s are illustrated in Figure 3.35. Unlike the $D$-efficiency, the $IV$-efficiency is not an increasing function of $\alpha$. The highest Min $IV$ of 15.096% occurs at $\alpha = \alpha_{\text{crit}}$. The CCD with $\alpha_{\text{crit}}$ will subsequently be called the robust design. The $IV$-efficiency of the robust design will decrease from 19 to

15.096 (Min $IV$) if a factorial or center run is missing. The spherical CCD has the $IV$-efficiency of 19.04, close to that of the robust design.

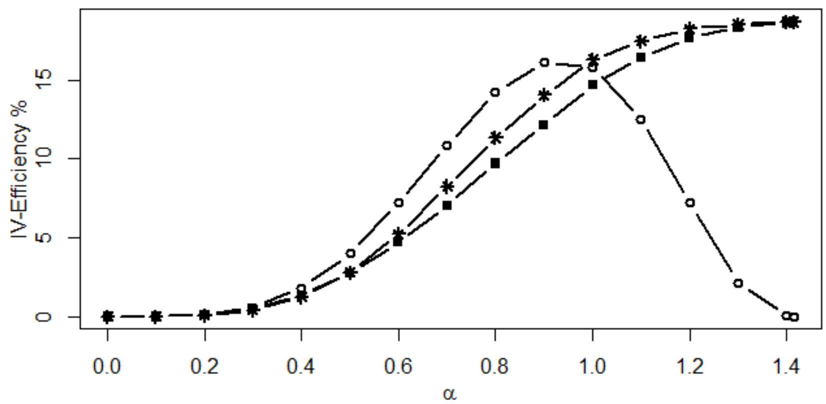



Figure 3.34: $IV$-efficiencies of two-factor CCDs having a missing response: solid squares for a missing factorial, stars for a missing axial, and open circles for a missing center run.

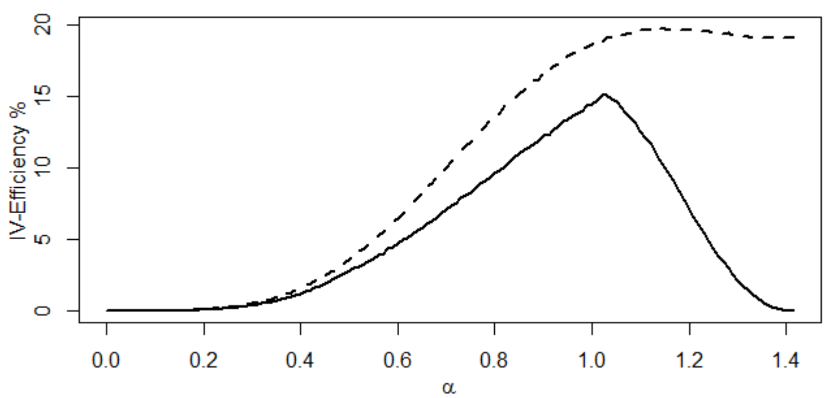



Figure 3.35: The $IV$-efficiency and Min $IV$ of two-factor CCDs: solid line for Min $IV$'s and dashed line for $IV$-efficiencies.

Figure 3.36 presents contours of SPVs of the robust design with different types of a missing run. Figures (a), (b), (c), and (d) correspond to the robust design without any missing runs, and design with $(-1, -1)$, $(-\alpha_{\text{crit}}, 0)$, $(0, 0)$ missing, respectively. Notice

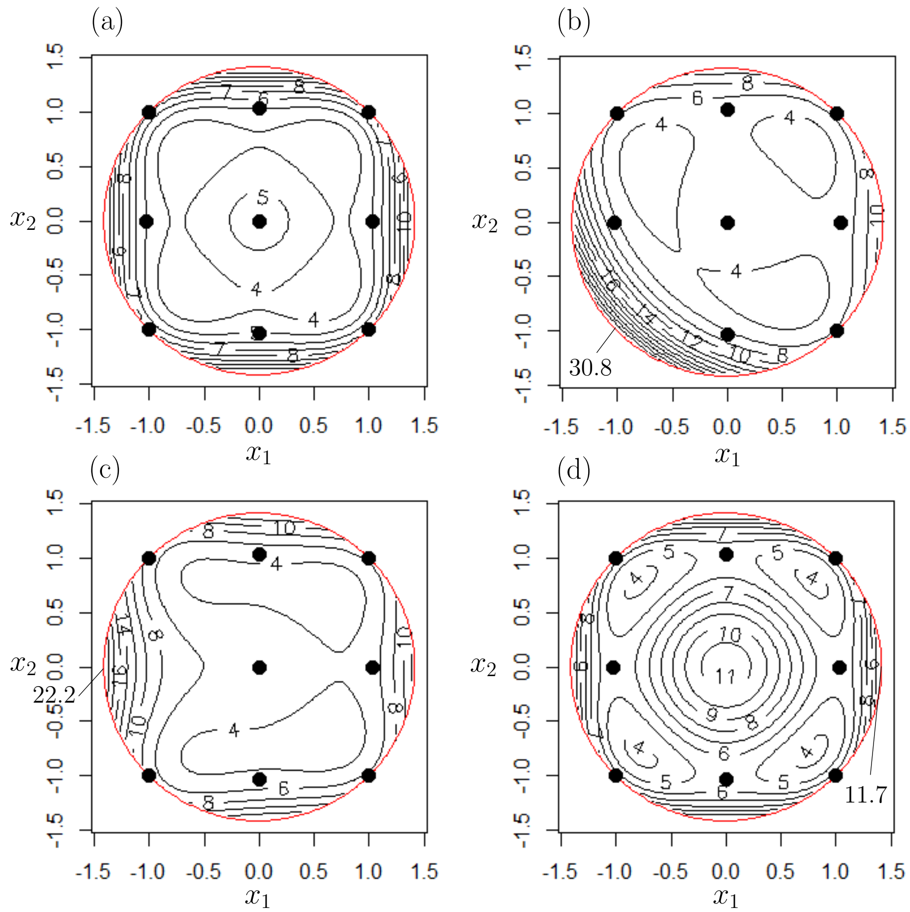



Figure 3.36: Contours of SPVs of the two-factor robust CCD based on the Min $IV$: (a) without a missing response; (b) a missing factorial point; (c) a missing axial point; and (d) a missing center point. Solid circles represent the design points.

that the robust design based the Min $IV$ is similar to the FCD because they have about the same axial point distance. Designs with a missing factorial or center run have the about same $IV$-efficiency, but their precisions for predictions are different and depend on a location of the point for prediction. The maximum SPV of the designs with a missing $(-1,-1)$, $(-\alpha_{\text{crit}}, 0)$, and $(0,0)$ are $30.8, 22.2$, and $11.7$, respectively.

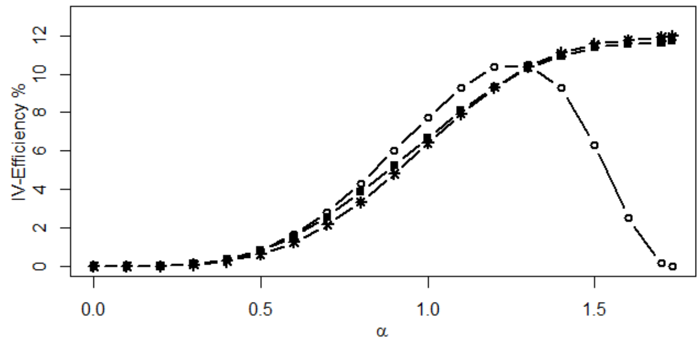



Figure 3.37: $IV$-efficiencies for three-factor CCDs having a missing response: solid squares for a missing factorial, stars for a missing axial, and open circles for a missing center run.

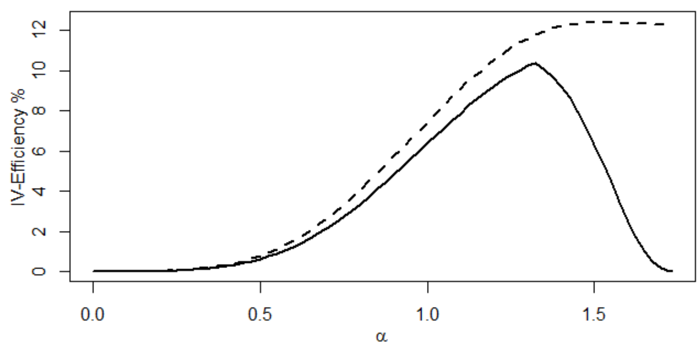
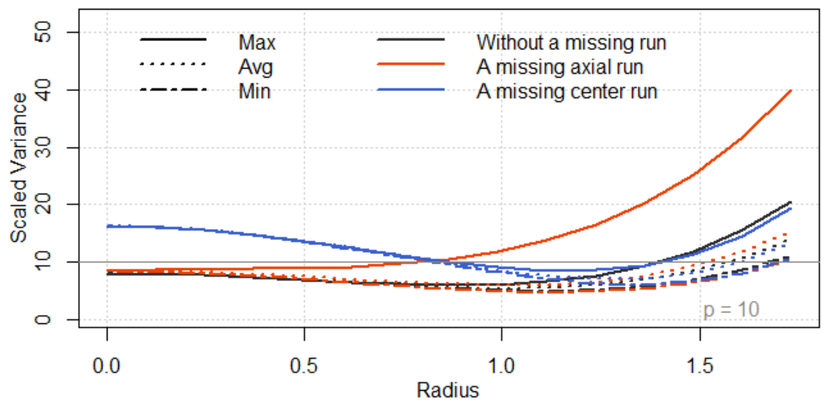



Figure 3.38: The $IV$-efficiency and Min $IV$ of three-factor CCDs: solid line for Min $IV$'s and dashed line for $IV$-efficiencies.

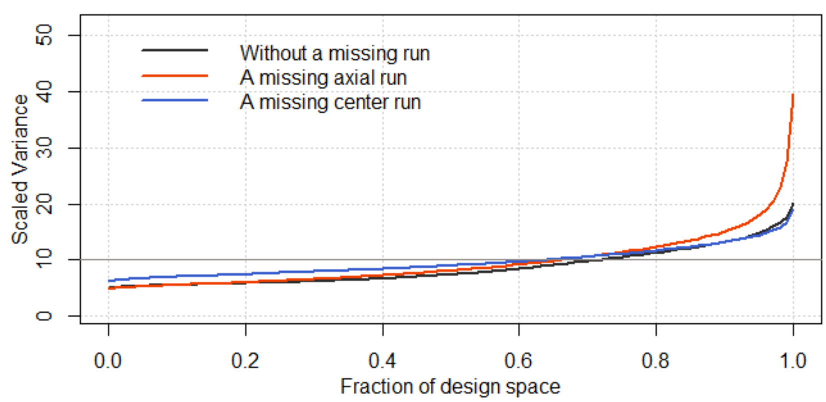
## 7.2. Three-Factor Min-$IV$ CCD

The behaviors of the $IV$-efficiencies for three-factor CCDs with a single missing point over different values of $\alpha$ are illustrated in Figure 3.37. For $\alpha < 1.315$, the missing factorial and axial points have about the same effect on $IV$-efficiencies. For $\alpha > 1.315$, the $IV$-efficiency of the design with a missing center run decreases quickly to zero. The critical value $\alpha = 1.315$ will be referred to as $\alpha_{\text{crit}}$, and the corresponding CCD will be called the robust design.

In Figure 3.38, the $IV$-efficiencies and Min $IV$'s of three-factor CCDs are plotted over different values of $\alpha$. The highest Min $IV$ of 10.4% occurs at $\alpha_{\text{crit}}$. The $IV$-efficiency of the robust design will decrease only slightly from 11.71 to 10.4% (Min $IV$) if a factorial, axial, or center run is lost. The spherical CCD has an $IV$-efficiency of 12.323, only slightly greater than that of the robust CCD.



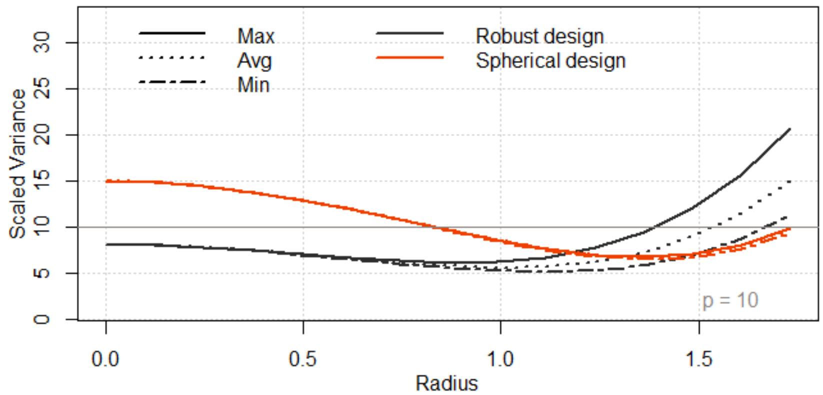

(a)



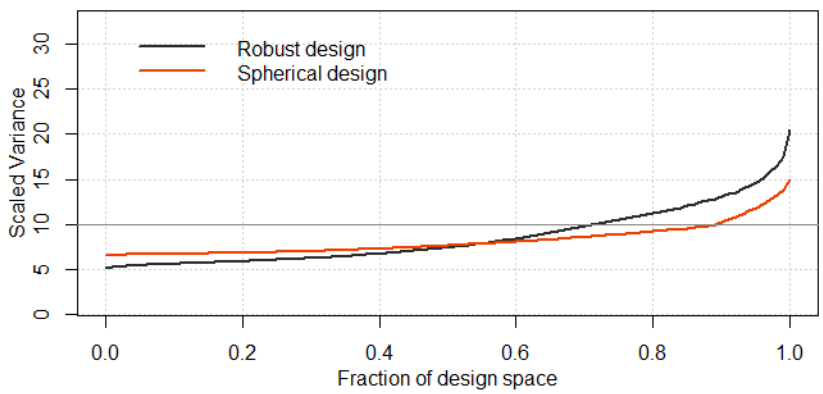

(b)

Figure 3.39: The VDGs (a) and FDS plots (b) of three-factor robust CCDs based on the Min $IV$ without a missing run (black line), with a missing factorial run (red line), and with a missing center run (blue line).

Figure 3.39 (a) shows a comparison of VDGs of robust designs without a missing run, with a missing axial run, and with a missing center run which, hereafter, are




(a)




(b)

Figure 3.40: The VDGs (a) and FDS plots (b) of the three-factor spherical CCD and robust CCD based on the Min $IV$.

referred to $\xi$, $\xi_a$, and $\xi_c$, respectively. All designs $\xi$, $\xi_a$, and $\xi_c$ have about the same ASPV for $r > 1.2$. Although the MaxSPV of $\xi_a$ can be as high as 40.99, this happens when the prediction at the spherical axial point being lost is made. Figure 3.39 (b) shows that percentages of the design space of $\xi, \xi_a$, and $\xi_c$ with SPVs $< 10$ ( the $G$-optimal value) are about the same.

The VDGs of the robust and spherical exact designs are shown in Figure 3.40 (a). Because axial points of the robust design are closer to the center of the design in the robust design, when $r \lessapprox 1.17$, the VDG is lower for the robust design. Its MaxSPV can be as high as 20.648 at $r = \sqrt{3}$. However, the ASPVs of the robust design are

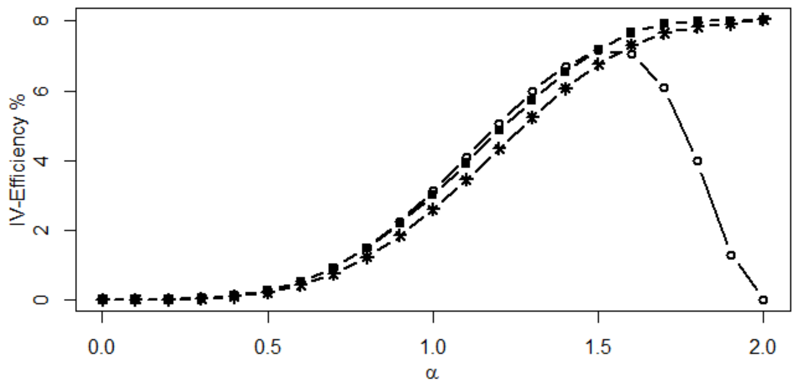



Figure 3.41: $IV$-efficiencies for four-factor CCDs having a missing response: solid squares for a missing factorial, stars for a missing axial, and open circles for a missing center run.

at most 5 larger than those of the spherical design. Figure 3.40 (b) shows the FDS plots. Approximately 72% of the design region of the robust design has SPVs $< 10$ (the $G$-optimal value) while it is 89% for the spherical design.

## 7.3. Four-Factor Min-$IV$ CCD

The behaviors of $IV$-efficiencies for four-factor CCDs with a single missing point over different values of $\alpha$ are rather different from the three-factor Min-$IV$ CCDs. The axial points are more important than the others. For $\alpha < 1.567$, an axial missing point causes the greatest reduction in the $IV$-efficiency, and for $\alpha > 1.567$, if a center run is missing, the $IV$-efficiency will decrease quickly to zero. For this case, $\alpha_{\text{crit}} = 1.567$, and the corresponding CCD will be referred to as the robust design.

In Figure 3.42, the highest Min $IV$ is 7.188% for the robust design with $\alpha = \alpha_{\text{crit}}$. The $IV$-efficiency of the robust design will decrease slightly from 7.784 to 7.188% if an axial or center run is missing while the spherical CCD has the $IV$-efficiency of 8.232. Thus, using $\alpha = \alpha_{\text{crit}}$ slightly changes the $IV$-efficiency, but the resulting design will be more robust to a missing point.

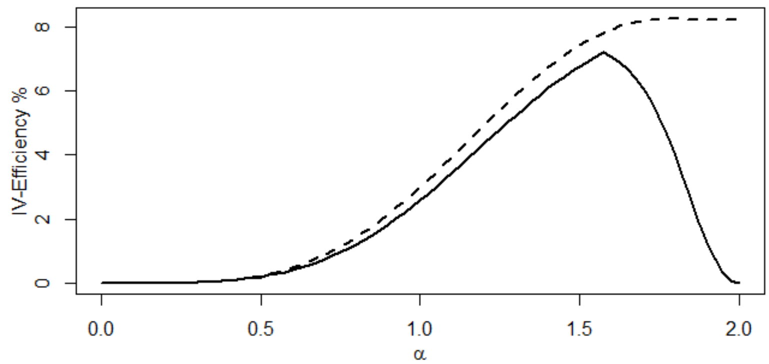



Figure 3.42: The $IV$-efficiency and Min $IV$ of four-factor CCDs: solid line for Min $IV$'s and dashed line for $IV$-efficiencies.

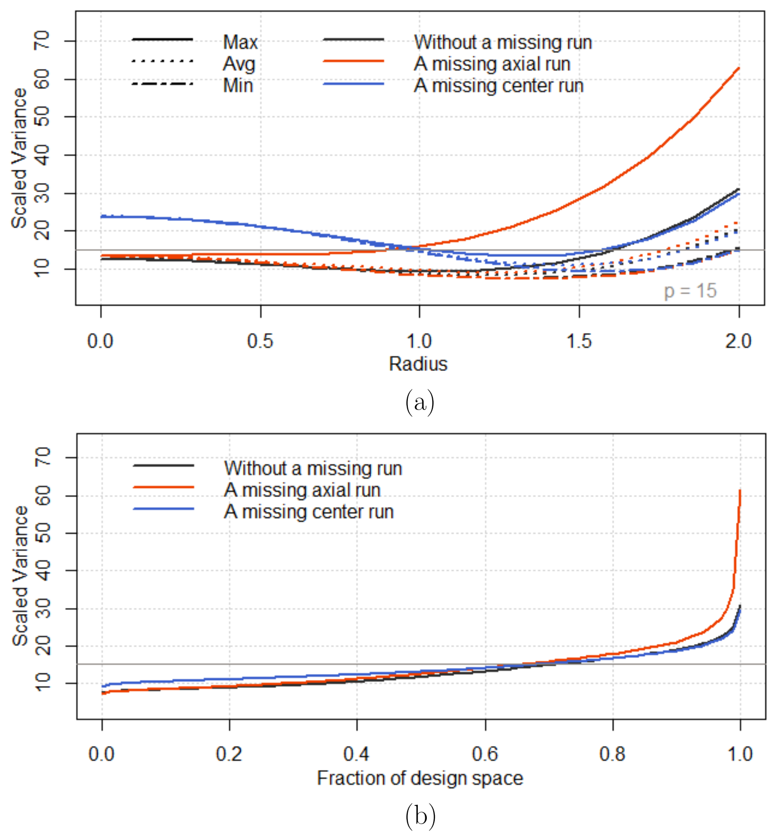



Figure 3.43: The VDGs (a) and FDS plots (b) of four-factor robust CCDs based on the Min $IV$ without a missing run (black line), with a missing factorial run (red line), and with a missing center run (blue line).

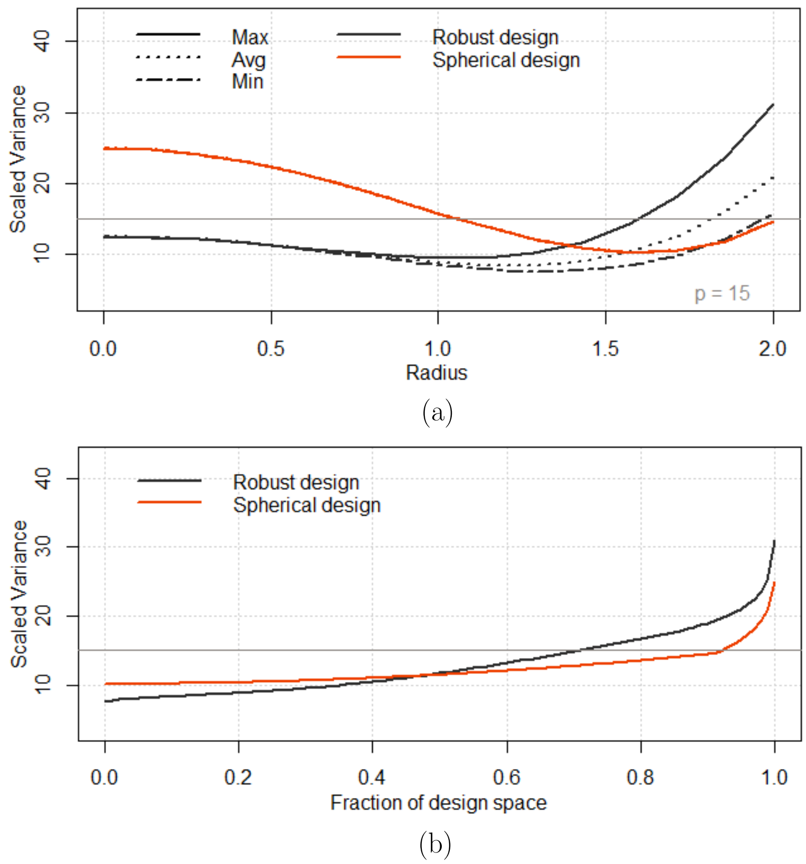



Figure 3.44: The VDGs (a) and FDS plots (b) of the four-factor spherical CCD and robust CCD based on the Min $IV$.

Figure 3.43 (a) shows a comparison of VDGs of robust designs without a missing run, with a missing axial run, and with a missing center run which, hereafter, are referred to as $\xi$, $\xi_a$, and $\xi_c$, respectively. All designs $\xi$, $\xi_a$, and $\xi_c$ have about the same ASPV for $r \gtrapprox 1.5$. The MaxSPV of $\xi_a$ can be as high as 63.017; this happens when the prediction of points near or at a missing axial design point is made. Figure 3.43 (b) shows FDS plots. Both $\xi_a$ and $\xi_c$ have approximately 65% of the design space with SPVs $< 15$ (the $G$-optimal value), and it is 71% for the robust design.

The VDGs of the robust and spherical designs are illustrated in Figure 3.44 (a). It is seen that when $r \lessapprox 1.38$, the VDG is lower in the robust design while for $r \gtrapprox 1.55$,

Table 3.1: A comparison of $\alpha$ values.

| Criteria | Number of Factors ($k$) | | |
|---|---|---|---|
| | 2 | 3 | 4 |
| Spherical | 1.414 | 1.732 | 2.000 |
| Rotatable | 1.414 | 1.682 | 2.000 |
| Min $D$ | 1.143 | 1.466 | 1.767 |
| Min $A$ | 0.974 | 1.176 | 1.360 |
| Min $G$ | 1.142 | 1.449 | 1.700 |
| Min $IV$ | 1.030 | 1.315 | 1.567 |

the ASPVs become larger than those of the spherical deign. The maximum MaxSPV of the robust design is 31.1, but the maximum ASPV is only 20.77. The FDS plots indicate that for the robust design, approximately 7% of the design space has SPVs $> 20$, and 52% of design space has SPVs greater than those of the spherical design.

## 8. Summary and Discussion

When experimenters use a spherical CCD with $n_c = 1$, one or more center runs are necessary. If a center run is missing, the information matrix will be singular, and then $D$-, $A$-, $G$-, and $IV$-efficiencies will be zero. In Section 3.4 to 3.7, the $\alpha$'s that maximize Min $D$, Min $A$, Min $G$, and Min $IV$ have been search numerically, and they are summarized Table 3.1.

In each $k$, the values of $\alpha$ based on the Min $D$ and Min $G$ are close to each other, and the $\alpha$ obtained from the Min $A$ criterion is always the lowest. Moreover, in each $k$ the $\alpha$ values can be ordered as $\sqrt{k} > \alpha^{\text{Min } D} > \alpha^{\text{Min } G} > \alpha^{\text{Min } IV} > \alpha^{\text{Min } A}$. Thus, both Min $D$ and Min $G$ criteria seem to place the axial points farther but not on the hypersphere surface to avoid singularity if a center run is missing. Notice that most values of robust $\alpha$ are greater than one, cuboidal $\alpha$, and are less extreme than the spherical value $\alpha$. This is the same idea as "practical $\alpha$ values" where when $k$ is

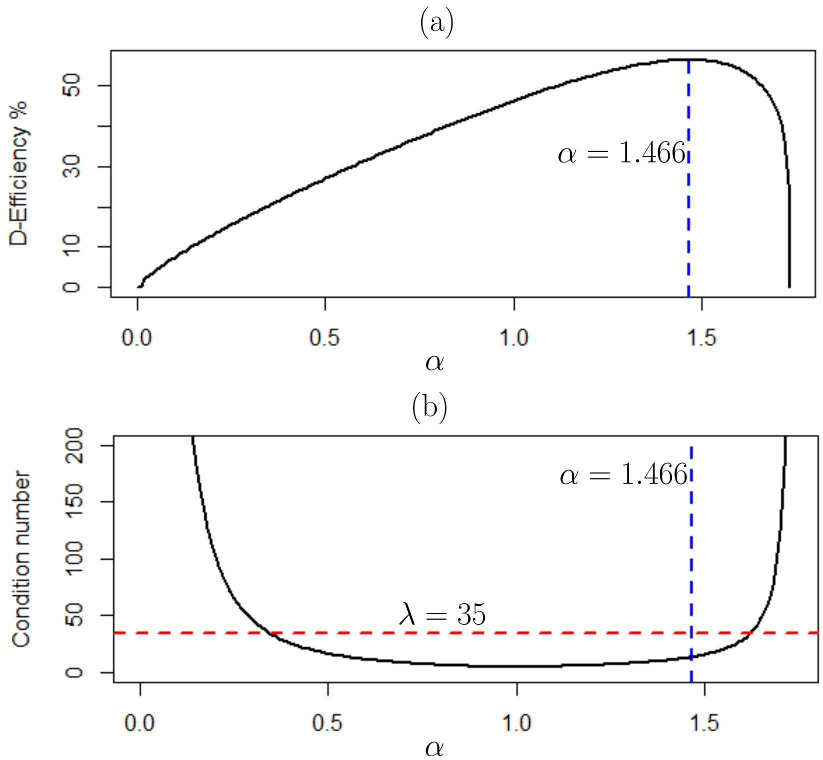



Figure 3.45: The $D$-efficiencies (a) and condition numbers (b) of three-factor CCD having a missing center run.

large, the spherical $\alpha$ becomes large, but this may not be a practical level for factors of interest compared to factor levels in factorial points (Li et al., 2009). Thus, this could be a benefit of using $\alpha$ less than $\sqrt{k}$.

In the plots of the $D$-, $A$-, $G$-, and $IV$-efficiencies versus the axial point distance $\alpha$ (e.g. Figures 3.4, 3.8), as $\alpha$ increases, the design efficiency of designs with a missing center run increases until a certain $\alpha$, and then the curve drops dramatically to zero. Thus, as the $\alpha$ approaches $\sqrt{k}$, the information matrix becomes nearly singular and is singular at $\alpha = \sqrt{k}$. We can explicitly demonstrate a relationship between $D$-efficiency and singularity of matrix $\mathbf{X}^{\mathrm{T}}\mathbf{X}$ by plotting the condition number $\lambda$ versus axial distance $\alpha$. For example, Figure 3.45 (a) shows a plot of $D$-efficiencies of CCDs with a missing center run versus $\alpha$'s, and Figure 3.45 (b) shows a plot of condition numbers $\lambda$ versus the corresponding $\alpha$. It can be seen that a considerable decrease in $D$-efficiency corresponds to a dramatic increase in the condition number. Usually, if the $\lambda$ is large ($> 35$), the precision of parameter estimates is very low and the instability in the estimates is very high. Note that the condition number, $\lambda$, is the positive square root of the ratio of the largest to the smallest eigenvalue of $\mathbf{X}^{\mathrm{T}}\mathbf{X}$.

# CHAPTER 4

## ALPHABETIC OPTIMAL ROBUST EXACT DESIGNS

In this chapter, our goal is to construct alphabetic optimal robust exact designs. The distinction between approximate and exact designs was discussed in Chapter 1, Section 3.6. The useful matrix properties will be described in Section 1, and in Section 2, the proposed modified point-exchange algorithm to generate robust exact designs will be proposed. In Sections 3 to 6, the $D$-, $A$-, $G$-, $IV$-optimal robust exact designs are, respectively, provided for particular sample sizes. Each robust exact design will be compared to the corresponding optimal exact design generated by a genetic algorithm in Borkowski (2003b). The resulting robust exact designs and existing exact designs will be evaluated using all criteria previously discussed in Chapter 3, Section 3.

### 1. Useful Matrix Properties

The following properties are used in the modified point-exchange algorithm.

1. Rank-One Update

   If $\mathbf{A}_{p\times p}$ is nonsingular, and if $\mathbf{c}$ and $\mathbf{d}$ are $p \times 1$ column vectors, then

$$\det(\mathbf{A} + \mathbf{c}\mathbf{d}^{\mathrm{T}}) = \det(\mathbf{A})(1 + \mathbf{d}^{\mathrm{T}}\mathbf{A}^{-1}\mathbf{c}),$$

   (Meyer, 2001).

   *Proof* Consider the following matrix product:

$$\begin{bmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{d}^{\mathrm{T}} & 1 \end{bmatrix} \begin{bmatrix} \mathbf{I} + \mathbf{c}\mathbf{d}^{\mathrm{T}} & \mathbf{c} \\ \mathbf{0} & 1 \end{bmatrix} \begin{bmatrix} \mathbf{I} & \mathbf{0} \\ -\mathbf{d}^{\mathrm{T}} & 1 \end{bmatrix} = \begin{bmatrix} \mathbf{I} & \mathbf{c} \\ \mathbf{0} & 1 + \mathbf{d}^{\mathrm{T}}\mathbf{c} \end{bmatrix}.$$

Since determinants of the first and third matrices on the left-hand side equal one, from product rules,

$$\det\left(\mathbf{I}+\mathbf{c}\mathbf{d}^{\mathrm{T}}\right)=\det\left(1+\mathbf{d}^{\mathrm{T}}\mathbf{c}\right).$$

Because $\mathbf{A}+\mathbf{c}\mathbf{d}^{\mathrm{T}}=\mathbf{A}(\mathbf{I}+\mathbf{A}^{-1}\mathbf{c}\mathbf{d}^{\mathrm{T}})$, we will have:

$$\begin{aligned}\det\left(\mathbf{A}+\mathbf{c}\mathbf{d}^{\mathrm{T}}\right) &= \det\left(\mathbf{A}\right)\det\left(\mathbf{I}+\mathbf{A}^{-1}\mathbf{c}\mathbf{d}^{\mathrm{T}}\right)\\ &= \det\left(\mathbf{A}\right)\det\left(1+\mathbf{d}^{\mathrm{T}}\mathbf{A}^{-1}\mathbf{c}\right) \qquad \blacksquare\end{aligned}$$

In a context of constructing a design, if a single observation $\mathbf{a}_{p\times 1}$ from a set of candidate points, $\mathcal{X}$, is added to the design matrix, $\mathbf{X}_{n\times p}$, a new information matrix in terms of $\mathbf{X}_{(n+1)\times p}$ is

$$\mathbf{X}_{n+1}^{\mathrm{T}}\mathbf{X}_{n+1}=\mathbf{X}_{n}^{\mathrm{T}}\mathbf{X}_{n}+\mathbf{a}\mathbf{a}^{\mathrm{T}}.$$

In the point-exchange algorithm, the rank-one update is related to the $D$-optimality criterion as it is the determinant of the information matrix. Applying the rank-one update property, the updated determinant is

$$\begin{aligned}\det\left(\mathbf{X}_{n+1}^{\mathrm{T}}\mathbf{X}_{n+1}\right) &= \det\left(\mathbf{X}_{n}^{\mathrm{T}}\mathbf{X}_{n}+\mathbf{a}\mathbf{a}^{\mathrm{T}}\right),\\ &= \det\left(\mathbf{X}_{n}^{\mathrm{T}}\mathbf{X}_{n}\right)\times\left[1+\mathbf{a}^{\mathrm{T}}(\mathbf{X}_{n}^{\mathrm{T}}\mathbf{X}_{n})^{-1}\mathbf{a}\right],\\ &= \det\left(\mathbf{X}_{n}^{\mathrm{T}}\mathbf{X}_{n}\right)\times\left[1+\mathrm{Var}(\hat{y}(\mathbf{a}))\right].\end{aligned}$$

Thus, the new determinant increases proportional to the prediction variance of point $\mathbf{a}$, $\mathrm{Var}(\hat{y}(\mathbf{a}))$. Likewise, if point $\mathbf{a}^{*}$ in the design is removed from the design matrix, the relationship between two determinants can be expressed as:

$$\begin{aligned}\det(\mathbf{X}_{n-1}^{\mathrm{T}}\mathbf{X}_{n-1}) &= \det(\mathbf{X}_n^{\mathrm{T}}\mathbf{X}_n) \times [1 - \mathbf{a}^{*\mathrm{T}}(\mathbf{X}_n^{\mathrm{T}}\mathbf{X}_n)^{-1}\mathbf{a}^*], \\ &= \det(\mathbf{X}_n^{\mathrm{T}}\mathbf{X}_n) \times [1 - \mathrm{Var}(\hat{y}(\mathbf{a}^*))].\end{aligned}$$

2. Sherman−Morrison Rank-One Update

If $\mathbf{A}_{n\times n}$ is nonsingular, and $\mathbf{c}$ and $\mathbf{d}$ are $n \times 1$ columns such that $1+\mathbf{d}^{\mathrm{T}}\mathbf{A}^{-1}\mathbf{c} \neq 0$, then the sum $\mathbf{A} + \mathbf{c}\mathbf{d}^{\mathrm{T}}$ is not singular, and

$$(\mathbf{A} + \mathbf{c}\mathbf{d}^{\mathrm{T}})^{-1} = \mathbf{A}^{-1} - \frac{\mathbf{A}^{-1}\mathbf{c}\mathbf{d}^{\mathrm{T}}\mathbf{A}^{-1}}{1 + \mathbf{d}^{\mathrm{T}}\mathbf{A}^{-1}\mathbf{c}}.$$

If a single observation $\mathbf{a}_{p\times 1}^{\mathrm{T}}$ from a set of candidate points $\mathcal{X}$ is added to the design matrix, applying the Sherman−Morrison rank-one update formula then the updated inverse of the information matrix is

$$(\mathbf{X}_n^{\mathrm{T}}\mathbf{X}_n + \mathbf{a}\mathbf{a}^{\mathrm{T}})^{-1} = (\mathbf{X}_n^{\mathrm{T}}\mathbf{X}_n)^{-1} - \frac{(\mathbf{X}_n^{\mathrm{T}}\mathbf{X}_n)^{-1}\mathbf{a}\mathbf{a}^{\mathrm{T}}(\mathbf{X}_n^{\mathrm{T}}\mathbf{X}_n)^{-1}}{1 + \mathbf{a}^{\mathrm{T}}(\mathbf{X}_n^{\mathrm{T}}\mathbf{X}_n)^{-1}\mathbf{a}}$$

(Sherman and Morrison, 1950). Also, if design point $\mathbf{a}$ is removed from the design, the new inverse of the information matrix can be computed by the following formula:

$$(\mathbf{X}_n^{\mathrm{T}}\mathbf{X}_n - \mathbf{a}\mathbf{a}^{\mathrm{T}})^{-1} = (\mathbf{X}_n^{\mathrm{T}}\mathbf{X}_n)^{-1} + \frac{(\mathbf{X}_n^{\mathrm{T}}\mathbf{X}_n)^{-1}\mathbf{a}\mathbf{a}^{\mathrm{T}}(\mathbf{X}_n^{\mathrm{T}}\mathbf{X}_n)^{-1}}{1 - \mathbf{a}^{\mathrm{T}}(\mathbf{X}_n^{\mathrm{T}}\mathbf{X}_n)^{-1}\mathbf{a}}.$$

The latter relationship can help to compute the Min $G$ and Min $IV$ without recomputing an inverse of the information matrix when each point is removed one at a time (SAS Institute Inc., 2008).

## 2. A Modified Point-Exchange Algorithm

Suppose the goal is to generate an $n$-point design for $k$ independent variables from a set of $N$ candidate points, $S = \{\mathbf{y}_1, \mathbf{y}_2, \ldots, \mathbf{y}_N\}$ in $\mathbb{R}^k$ where $N \gg n$. Also, the $p$-parameter linear model form to be fitted is given such that we have a vector $f = (f_1, f_2, \ldots, f_p)$ of $p$ functions $f_1, f_2, \ldots, f_p : \mathbb{R}^k \longrightarrow \mathbb{R}$ where $p \leq n$. If the desired criterion is $D$-optimality and a constant variance assumption is satisfied, the goal is to find a set of $n$ points in $S$ that maximizes the determinant $|\mathbf{X}_{-i}^{\mathrm{T}}\mathbf{X}_{-i}|$. Even if the variance-covariance is not $\sigma^2\mathbf{I}$ but is a known matrix $\mathbf{V}$, we can maximize $|\mathbf{X}_{-i}^{\mathrm{T}}\mathbf{V}^{-1}\mathbf{X}_{-i}|$ instead of $|\mathbf{X}_{-i}^{\mathrm{T}}\mathbf{X}_{-i}|$. Whatever criterion is used, we want to find an $n$-point design from the set of all possible $N^n$ designs achieving a desirable value of the criterion. However, observing all possible $N^n$ designs is usually impossible. Therefore, we propose the modified point-exchange algorithm to construct $D$-, $A$-, $G$-, and $IV$-optimal robust exact designs. Two major steps in the algorithm are the following:

1. Generation of the Starting Design

Mitchell (1974) chose starting designs by starting from zero runs, i.e., an empty design, and sequentially adding one point with the highest prediction variance at a time. This approach is viewed as not as "good" as the randomized starting designs approach in terms of the efficiency of the design. However, it reduces the number of iterations of an algorithm (Triefenbach, 2008). Galil and Kiefer (1980) allowed the starting design to contain some random points in the beginning and then selected the "best" points from the support to add sequentially to the design. Miller and Nguyen (1994) suggested randomly choosing half of the total design points in the initial design and then adding points sequentially to maximize the rank and determinant of the subspace spanned by the current design.

The prior well-known property for the construction of $D$-optimal designs is that the final design points should span the design space to maximize the determinant $|\mathbf{X}^{\mathrm{T}}\mathbf{X}|$; thus, the design points should be scattered over the design space. To have scattered starting design points, we partition the design region and then randomly choose one point from each partition region. This approach ensures the starting design points are not clustered in one place which might happen in completely random selection of designs with a small sample size. Let $S$ denote a set of candidate points in $\mathbb{R}^k$ and $S = A_1 \cup A_2 \cup \ldots \cup A_m$ such that $A_1$, $A_2$, ..., $A_m$ form a mutually exclusive partition, i.e., $A_i \cap A_j = \varnothing$. In a hypercube, it is easy to partition set $S$; for example, for $k = 2$,

$$S = [-1, 1] \times [-1, 1] = A_1 \cup A_2 \cup A_3 \cup A_4,$$

where $A_1 = \{(x_1, x_2) : -1 \leq x_1 \leq 0, -1 \leq x_2 < 0\}$ , $A_2 = \{(x_1, x_2) : -1 \leq x_1 < 0, 0 \leq x_2 \leq 1\}$, $A_3 = \{(x_1, x_2) : 0 \leq x_1 \leq 1, 0 < x_2 \leq 1\}$, and $A_4 = \{(x_1, x_2) : 0 < x_1 \leq 1, -1 \leq x_2 \leq 0\}$. In the same manner, the number $m$ of sets in a partition for $k = 3$, 4, 5, 6, and 7 will be $m = 8$, 16, 32, 64, and 128, respectively. When $k \geq 4$, $m$ is greater than $p$, the number of parameters in a second-order model, so in this case only $p$ out of $m$ sets are randomly chosen, and one design point is randomly selected from each chosen partition set. Thus, for $k \leq 3$, at this stage there are $m$ points, $m \leq p$, in the design. Next, the $m$-point design is sequentially filled with $n-m$ points that have the highest prediction variance, which is equivalent to maximizing the determinant according to the rank-one updated formula. The initial design is then checked to see if it has rank $k$. If the rank is less than $k$, the process is repeated from the beginning until the rank equals $k$.

2. Point Exchanging

Each point $\mathbf{a}_i$, $i = 1, 2, \ldots, n$, in the design will be exchanged with point $\mathbf{y}_j$,

$j = 1, 2, \ldots, N$, of the candidate set $S$. For each exchange, the robust criterion, e.g. Min $D$ or Min $G$, is calculated. Note that algorithms based on the Fedorov delta function (Fedorov, 1972), Wynn-Mitchell (Wynn, 1972), Van Schalkwyk and Mitchell (Mitchell, 1974), can not be used because criteria Min $D$, Min $A$, Min $G$, and Min $IV$ are new. This is to say that, for example, the goal is to maximize the minimum of $D$-efficiency instead of a usual $D$-efficiency. Suppose the objective function is the Min $D$. In each iteration, there are $nN$ designs needed to calculate Min $D$, and two points are switched if the corresponding Min $D$ is the highest among $nN$ Min $D$'s. This stage is repeated until the improvement in the Min $D$ is less than the specified tolerance.

The amounts of time required for calculating the Min $D$, Min $A$, Min $G$, and Min $IV$ are substantially different. In order to calculate the Min $D = \min_{1 \le i \le N} \{D_{-i}\}$ and save computational time, the rank-one update can be applied to find the min $D$. For the Min $G$, and Min $IV$, we can use the Sherman-Morrison rank-one update to help to calculate them, but this is still very time consuming compared to the Min $D$ criterion. To calculate Min $A$, we have to actually recompute the $A$-efficiency when each design point is removed because there is no relationship between traces of moment matrices before and after removing a row in the design matrix.

As the algorithm might find a local optimum, it is common to generate several designs to have, hopefully, a global optimum. Mitchell (1974) mentioned that 10 tries will be usually enough, and if the best design has presented only once, 10 more designs will be generated. In this dissertation, we made 20 attempts at constructing each robust design, and if the best design appeared only once, 10 more tries were generated. In our experience, although the best design occurred only once, it could, however, be the global maximum if that design is symmetric because most exact designs catalogued in Borkowski (2003b) are symmetric.

The details of the point-exchange algorithm are explained in the following pseudocode. Let M denote the number of repetitions, N denote the size of a candidate set of points, n denote the size of a design to be constructed, Φ denote the value of a criterion Min $D$, Min $A$, Min $G$, or Min $IV$, and Δ denote the absolute value of difference between Φ's obtained from two consecutive iterations. The algorithm to generate a robust design is:

**FOR** 1 to $M$ **DO**
  generate a set of candidate points of size $N$, $\{\mathbf{y}_j\}, j = 1, 2, \ldots, N$;
  generate an initial design of size $n$, $\{\mathbf{x}_i\}, i = 1, 2, \ldots, n$;
  calculate the Φ for this design;
    **WHILE** $\Delta <$ tolerance
        **FOR** 1 to $n$
          **FOR** 1 to $N$
            exchange point $\mathbf{x}_i$ with point $\mathbf{y}_j$ in the set of candidate points;
            calculate the Φ for this new design;
            keep the Φ value for this exchange;
          **END**
        **END**
      find the maximum of Φ's;
      identify the points $\mathbf{x}_i^*$ and $\mathbf{y}_j^*$ yielding the highest Φ;
      replace point $\mathbf{x}_i^*$ in the design by $\mathbf{y}_j^*$;
      calculate the Φ for this updated design;
      calculate the Δ;
    **END**
  keep the latest design as the optimal robust exact design for the $i$th attempt.
**END**

After implementing the code above, we will have $M$ designs and the robust design will be the one having the highest value of the criterion. On many occasions, twenty tries are not enough, and more than ten repetitions are required to find the best design. The modified criteria have many local maxima points in a hypercube, thus it is very easy to get stuck at a local peak. For example, consider design matrices $\mathbf{D}_1$ and $\mathbf{D}_2$ with two factors:

$$\mathbf{D}_1 = \begin{pmatrix} \pm 1 & -1 \\ x_{31} & x_{32} \\ -1 & .7 \\ 0 & \pm 1 \\ 0 & 0 \end{pmatrix} \quad \text{and} \quad \mathbf{D}_2 = \begin{pmatrix} \pm 1 & \pm 1 \\ .5 & 1 \\ -.5 & -1 \\ 1 & -.5 \\ -1 & .5 \\ x_{91} & x_{92} \end{pmatrix}.$$

Suppose we want to find point $(x_{31}, x_{32})$ in matrix $\mathbf{D}_1$ that maximizes the Min $D$ and find $(x_{91}, x_{92})$ in matrix $\mathbf{D}_2$ that maximizes the Min $G$ for fitting a second-order model. As illustrated in Figure 4.1, the surface of Min $D$'s is complex, making it easy to get trapped. In this case, $(x_{31}, x_{32}) = (1, .7)$ will maximize the Min $D$. Figure 4.2 illustrates the plot of Min $G$'s and the highest Min $G$ corresponds to point $(0, 0)$. These examples have only one design point (2 coordinates) to be searched, but in reality, there are $n$ $k$-dimensional design points in a $k$-factor optimal design. Note that Figures 4.1 and 4.2 were produced by `trisurf` function in Matlab (MATLAB, 2014) which employs the a linear interpolation of vertices of the triangulation for criteria values to create the surface.

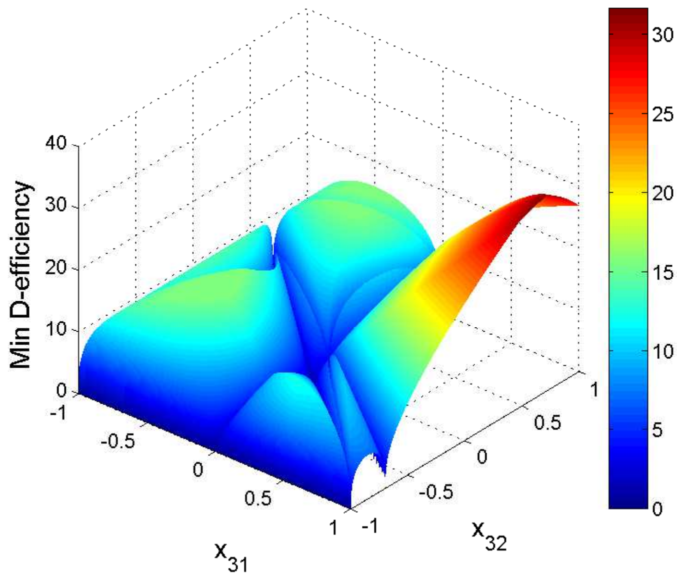



Figure 4.1: The Min $D$'s of design $\mathbf{D}_1$ containing point $(x_{31}, x_{32})$.

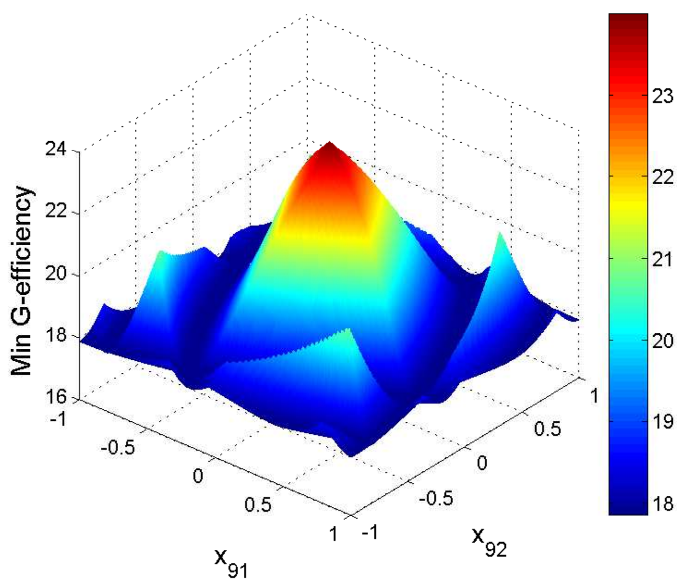



Figure 4.2: The Min $G$'s of design $\mathbf{D}_2$ containing point $(x_{91}, x_{92})$.

# 3. $D$-Optimal Robust Exact Designs

We will now formally introduce the $D$-optimal robust exact designs. Let $\Xi$ be the set of all possible exact designs on $\mathcal{X}$, $\Theta$ be the set of potential design points, and $\mathbf{x}_i$ be a design point in $\Theta$. The Min $D$ criterion seeks a design $\xi^*$ satisfying

$$\xi^* = \arg\max_{\xi \in \Xi} \min_{\mathbf{x}_i \in \Theta} |\mathbf{M}(\xi_{-\mathbf{x}_i})|, \tag{4.1}$$

where $\mathbf{M}(\xi_{-\mathbf{x}_i})$ is the moment matrix of the design with a missing point $\mathbf{x}_i$. For this criterion, the goal is to assure that the $D$-efficiency is still maximized even if a missing point resulting in a minimum $D$-efficiency or Min $D$ occurs in an experimentation. The resulting design will be called a $D$-optimal robust exact design and, in brief, called a robust design. Note that our robust exact designs are constructed to be robust to only one missing point, but we can assess the robustness to two and three missing points by using leave-2-out and leave-3-out $D$-efficiencies, respectively.

In this study, $D$-optimal robust exact designs will be generated for $n$-point two-factor experiments, $n = 7$ to 10 in a cuboidal region. For three-factor experiments, the sample sizes are 11, 12, and 13. As the sample size increases, the exact and robust exact $D$-optimal designs are not much different in terms of the $D$-efficiency. The candidate set of points is $\{-1, -.9, \ldots, .9, 1\}^k$, $k = 2$ and 3, thus there are 441 and $9,261$ candidate points for $k = 2$ and 3, respectively. In each case, twenty or more repetitions are generated to find the design having the highest Min $D$.

## 3.1. Two-Factor $D$-Optimal Designs

### 3.1.1. The 7-Point Design:

The 7-point $D$-optimal exact and robust exact designs are illustrated in Figure 4.3. The exact design was generated by a genetic

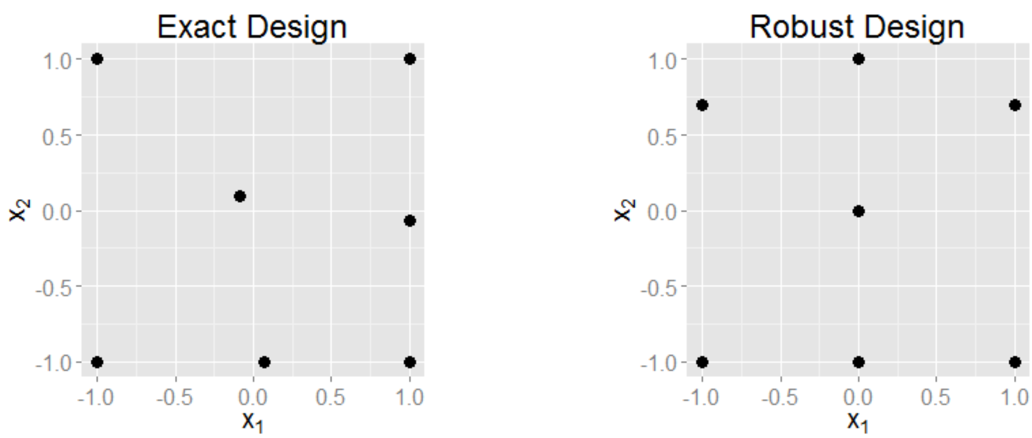



Figure 4.3: Seven-point $D$-optimal exact (left) and robust exact (right) designs for a second-order model in two factors.

algorithm and cataloged in Borkowski (2003b). The design points of the robust design are $(\pm 1, -1)$, $(\pm 1, .7)$, $(0, \pm 1)$, and $(0, 0)$. Compared to the exact design, the robust design has only two points at vertices, and like the exact design, one point is located near or at the origin $(0, 0)$. We observed that design points of the robust design are placed in such a way that if an arbitrary point is missing, there will be another point nearby. Suppose the response is missing at point $(-1, -1)$ in the exact design, there are no other points left in Quadrant III, so this missing point results in the lowest $D$-efficiency. This is the same for point $(1, 1)$ in Quadrant I. A commonality of exact and robust exact designs is that most design points tend to be on the boundary.

The comparisons of all criteria being evaluated for exact and robust exact designs are summarized in Table 4.1. It is seen that both designs have about the same precision of predictions because the $G$-efficiencies, as well as the $IV$-efficiencies, of both designs are about the same. The robust exact design increases the Min $D$ by 6.5, but the $D$-efficiency also drops by 4.4. However, on average both designs have the same robustness to a missing point because the leave-1-out efficiencies are not

Table 4.1: Properties of the 7-point 2-factor $D$-optimal designs.

| | 7-point $D$-optimal | |
|---|---|---|
| Criteria Evaluated | Exact Design | Robust Design |
| $D$-efficiency | 45.029 | 40.567 |
| Min $D$-efficiency | 25.144 | *31.576* |
| Leave-1-out $D$-efficiency | 34.789 | 33.239 |
| | (8.230) | (3.547) |
| $A$-efficiency | 26.598 | 23.534 |
| Min $A$-efficiency | 3.128 | 4.565 |
| Leave-1-out $A$-efficiency | 12.509 | 14.290 |
| | (7.635) | (5.771) |
| $G$-efficiency | 63.117 | 57.125 |
| Min $G$-efficiency | 1.217 | 8.125 |
| Leave-1-out $G$-efficiency | 18.728 | 17.776 |
| | (16.531) | (20.753) |
| $IV$-efficiency | 21.670 | 20.343 |
| Min $IV$-efficiency | 2.568 | 3.635 |
| Leave-1-out $IV$-efficiency | 10.470 | 12.609 |
| | (7.089) | (5.034) |

Numbers in parentheses represent standard deviations

much different, but the standard deviation is lower in the robust design than in the exact design.

3.1.2. The 8-Point Design: For the 8-point $D$-optimal design, the design points of the exact and robust exact designs are plotted in Figure 4.4. The exact design is generated by a genetic algorithm and the corresponding design points are cataloged in Borkowski (2003b). For the robust design, the resulting design points are $(\pm1,\pm1)$, $(\pm1,0)$, and $(0,\pm1)$. Both designs have points at four vertical points $(\pm1,\pm1)$ as a commonality. The only difference is that the robust exact design does not include an interior point. Losing point $(-1,-1)$ or $(1,-1)$ in the exact design will give the lowest $D$-efficiency while it is a missing vertex for the robust exact design.

Table 4.2: Properties of the 8-point 2-factor *D*-optimal designs.

| | 8-point *D*-optimal | |
|---|---|---|
| Criteria Evaluated | Exact Design | Robust Design |
| *D*-efficiency | 45.616 | 45.428 |
| Min *D*-efficiency | 33.648 | *38.515* |
| Leave-1-out *D*-efficiency | 40.380 | 40.873 |
| | (4.581) | (2.521) |
| Leave-2-out *D*-efficiency | 31.035 | 29.809 |
| | (9.063) | (12.761) |
| *A*-efficiency | 28.899 | 22.500 |
| Min *A*-efficiency | 15.192 | 16.590 |
| Leave-1-out *A*-efficiency | 21.134 | 17.012 |
| | (4.642) | (0.451) |
| Leave-2-out *A*-efficiency | 11.325 | 10.165 |
| | (6.394) | (5.205) |
| *G*-efficiency | 66.501 | 60.000 |
| Min *G*-efficiency | 6.680 | 17.143 |
| Leave-1-out *G*-efficiency | 31.912 | 29.531 |
| | (21.152) | (13.214) |
| Leave-2-out *G*-efficiency | 12.228 | 13.175 |
| | (12.475) | (10.911) |
| *IV*-efficiency | 22.641 | 16.698 |
| Min *IV*-efficiency | 11.350 | 11.681 |
| Leave-1-out *IV*-efficiency | 16.705 | 13.092 |
| | (4.483) | (1.099) |
| Leave-2-out *IV*-efficiency | 9.310 | 7.822 |
| | (5.462) | (4.043) |

Numbers in parentheses represent standard deviations

When comparing the criteria based on *D*-optimality for both designs as shown in Table 4.2, the Min *D* is higher by about 5 in the robust design, but *D*-efficiencies of both designs are about the same. The Min *A*, Min *G*, and Min *IV* are also higher in the robust design than in the exact design. This means that the *D*-optimal robust exact design is also robust in terms of other criteria not being used to construct it. Based on the *G*- or *IV*-criteria, the exact design has higher precision of predictions,

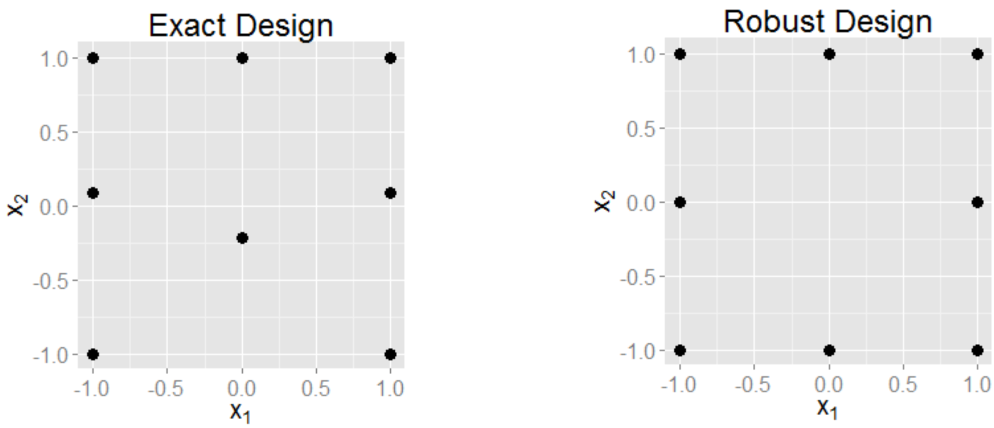



Figure 4.4: Eight-point $D$-optimal exact (left) and robust exact (right) designs for a second-order model in two factors.

but when there are one or two missing points, the precisions of predictions of both designs are about the same.

3.1.3. The 9-Point Design: Based on the set of candidate points we used, we have not found the design having a higher Min $D$-efficiency than that of the exact design. Thus, the exact $D$-optimal design generated by a genetic algorithm in Borkowski (2003b) is also a $D$-optimal robust exact design. The design points are $(\pm1, \pm1)$, $(0, \pm1)$, $(\pm1, 0)$, and $(0, 0)$ as depicted in Figure 4.5. This design is also called three-level two-factor full factorial design. Losing one of the vertices will give the lowest $D$-efficiency, which is 39.581 as shown in Table 4.3.

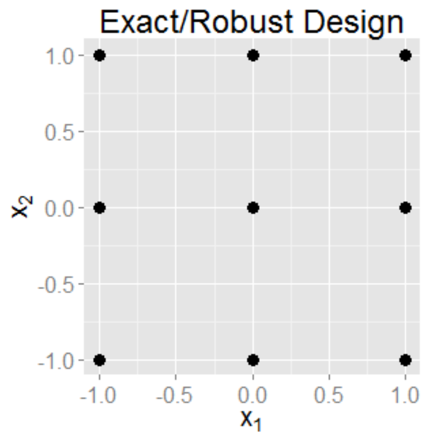



Figure 4.5: Nine-point $D$-optimal exact/robust exact design for a second-order model in two factors.

Table 4.3: Properties of the 9-point 2-factor $D$-optimal designs.

| | 9-point $D$-optimal |
|---|---|
| Criteria Evaluated | Exact Design & Robust Design |
| $D$-efficiency | 46.224 |
| Min $D$-efficiency | *39.581* |
| Leave-1-out $D$-efficiency | 42.829 |
| | (3.082) |
| Leave-2-out $D$-efficiency | 38.165 |
| | (4.238) |
| $A$-efficiency | 31.169 |
| Min $A$-efficiency | 22.500 |
| Leave-1-out $A$-efficiency | 25.968 |
| | (2.530) |
| Leave-2-out $A$-efficiency | 19.269 |
| | (3.651) |
| $G$-efficiency | 82.759 |
| Min $G$-efficiency | 18.104 |
| Leave-1-out $G$-efficiency | 41.379 |
| | (22.081) |
| Leave-2-out $G$-efficiency | 24.015 |
| | (17.499) |

Table 4.3 (continued)

| Criteria Evaluated | 9-point $D$-optimal Exact Design & Robust Design |
|---|---|
| $IV$-efficiency | 24.650 |
| Min $IV$-efficiency | 16.726 |
| Leave-1-out $IV$-efficiency | 20.921 |
| | (1.844) |
| Leave-2-out $IV$-efficiency | 15.727 |
| | (3.220) |

Numbers in parentheses represent standard deviations

Based on the Min $D$, leave-1-out and leave-2-out $D$-efficiencies in Table 4.3, the design is rather robust to one missing point. The leave-1-out $D$-efficiency is 42.829 with standard deviation of 3.08. However, if one of the vertices is lost and the prediction is made at that point, the precision of prediction will be very poor as the Min $G$ is only 18.104; however, the average precision is not too bad because the Min $IV$ is 16.726, dropped by 7 from the $IV$-efficiency.

3.1.4. The 10-Point Design: Figure 4.6 shows design points of $D$-optimal exact and robust exact designs. Both designs contain points at vertices $(\pm 1, \pm 1)$ as a commonality. Notice that the exact design is similar to the 9-point $D$-optimal design but has two replicates at point $(1, -1)$. With several attempts, the design consisting of points $(\pm 1, \pm 1), (-1, 1)$, $(-1, -.5)$, $(.3, -1)$, $(.5, 1)$, $(0, .1)$, and $(1, -.2)$ has the highest Min $D$. So, this is the robust exact design. Because the number of design points is four more than the number of parameters in a second-order model, both exact and robust designs are expected to be robust to a missing point. In our experience, the more points in a design, the less the impact of a missing point.

Table 4.4: Properties of the 10-point 2-factor $D$-optimal designs.

| | 10-point $D$-optimal | |
|---|---|---|
| Criteria Evaluated | Exact Design | Robust Design |
| $D$-efficiency | 45.989 | 44.517 |
| Min $D$-efficiency | 39.400 | *40.404* |
| Leave-1-out $D$-efficiency | 43.477 | 42.308 |
| | (2.834) | (1.678) |
| Leave-2-out $D$-efficiency | 40.083 | 38.948 |
| | (4.238) | (3.941) |
| $A$-efficiency | 29.338 | 25.223 |
| Min $A$-efficiency | 20.704 | 14.383 |
| Leave-1-out $A$-efficiency | 25.764 | 22.567 |
| | (3.434) | (3.621) |
| Leave-2-out $A$-efficiency | 21.101 | 18.440 |
| | (4.926) | (5.722) |
| $G$-efficiency | 75.964 | 85.360 |
| Min $G$-efficiency | 17.737 | 28.177 |
| Leave-1-out $G$-efficiency | 49.297 | 45.279 |
| | (23.648) | (17.439) |
| Leave-2-out $G$-efficiency | 31.486 | 31.029 |
| | (20.040) | (14.487) |
| $IV$-efficiency | 23.311 | 20.320 |
| Min $IV$-efficiency | 15.554 | 10.340 |
| Leave-1-out $IV$-efficiency | 20.482 | 18.261 |
| | (2.746) | (3.156) |
| Leave-2-out $IV$-efficiency | 17.011 | 15.397 |
| | (4.194) | (5.018) |

Numbers in parentheses represent standard deviations

The comparisons of criteria of exact and robust exact designs are summarized in Table 4.4. The $D$-efficiencies, as well as Min $D$'s, of both designs are slightly different. Overall, both designs are similarly robust to a missing point in terms of criteria related to $D$-optimality, e.g., leave-2-out $D$-efficiency. Observing the precision of predictions, the robust design has higher $G$-efficiency and Min $G$, but it is uniformly inferior to the exact design in terms of $A$- and $IV$-related criteria, e.g., leave-1-out A-efficiency.

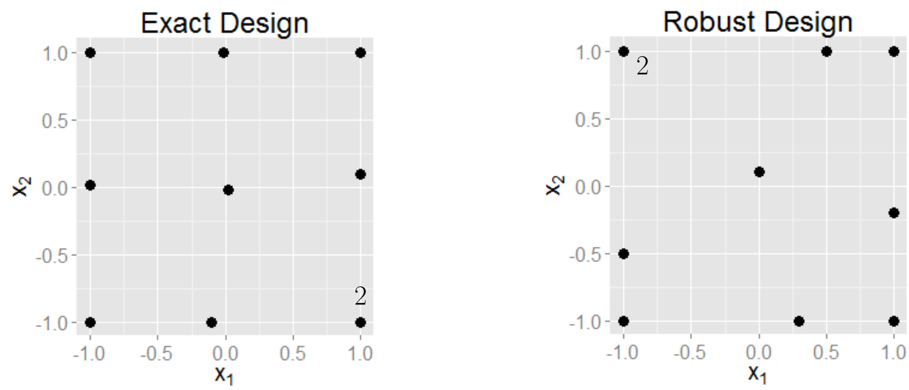



Figure 4.6: Ten-point $D$-optimal exact (left) and robust exact (right) designs for a second-order model in two factors. Numbers represent the number of replications.

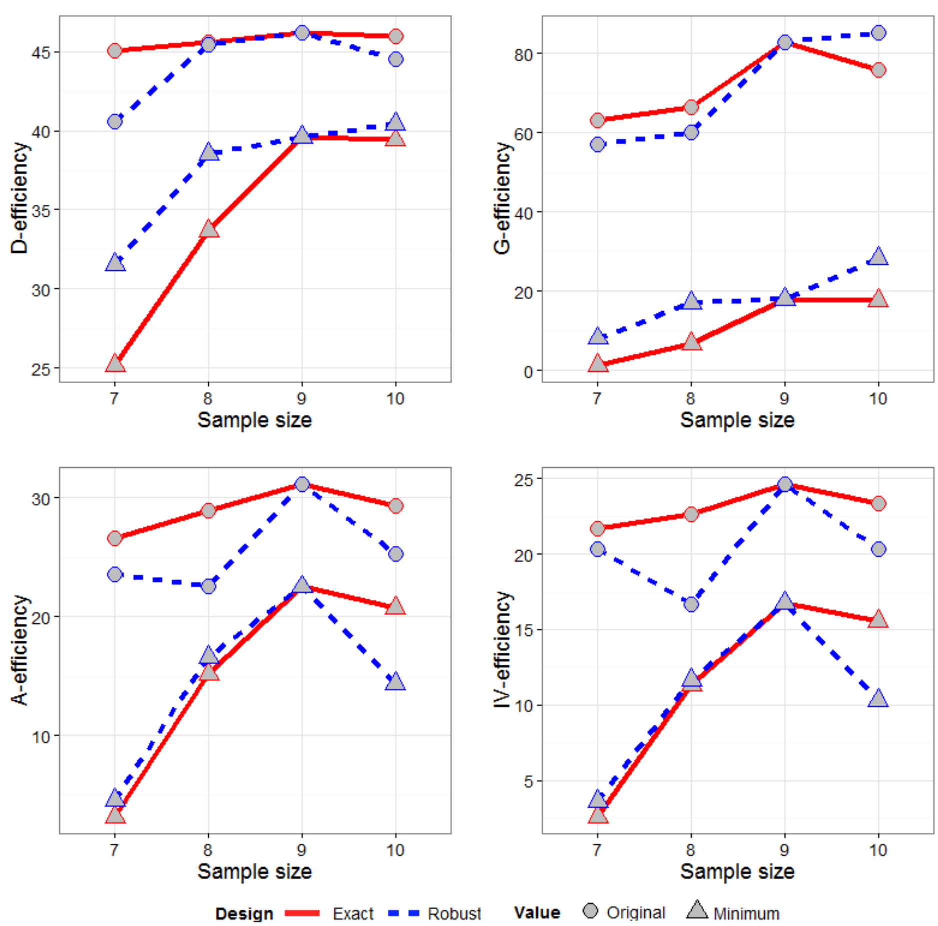



Figure 4.7: Summary of $D$-, $A$-, $G$-, $IV$-efficiencies and corresponding minimum efficiencies of two-factor $D$-optimal exact and robust exact designs.

All efficiencies and corresponding minimum efficiencies being evaluated for $D$-optimal exact and robust exact designs are plotted in Figure 4.7. It is seen that the Min $D$ of the robust design increases as the sample size increases, but this is not the case for the $D$-efficiency. The patterns of the Min $D$ and Min $G$ are rather similar. The Min $G$ of the robust design also increases as the sample size increases. The $A$- and $IV$-optimality criteria seems to have the same pattern. For example, the values of the $A$-efficiency and Min $A$ are very close in each $n$, $n = 7$, 8, and 9, and this is the same for the $IV$-efficiency and Min $IV$. When the sample size increases from 9 to 10, both $A$-efficiency and Min $A$ decrease in about the same magnitude as the change in the $IV$-efficiency and Min $IV$.

### 3.2. Three-Factor $D$-Optimal Designs

Instead of sequentially describing each design for $k = 3$, we will begin with a summary of results shown in Table 4.5. For $n = 11$, the Min $D$ largely increases from 0 to 34.82% while the $D$-efficiency decreases slightly from 44.769 to 41.889% when using the robust design instead of the exact design. The leave-1-out of the robust design is also higher with a lower standard deviation of 1.422. For $n = 12$, the robust and exact designs are similar as the $D$-efficiencies, as well as Min $D$'s, are very close. This is also true for the 13-point designs.

In Figure 4.8, all design efficiencies and corresponding minimum efficiencies are plotted. The Min $G$ of the robust design gradually increases as the sample size increases while the $G$-efficiency does not necessarily increase. For $n = 11$, 12, and 13, the Min $G$'s of the robust designs are 6.212, 10.140, and 12.868, respectively. For the exact designs, neither Min $G$ nor $G$-efficiency increases as $n$ increases.

For $A$- and $IV$-optimality criteria, like two-factor $D$-optimal designs, they have the same pattern. When the sample size increases, the Min $A$ and Min $IV$ of exact

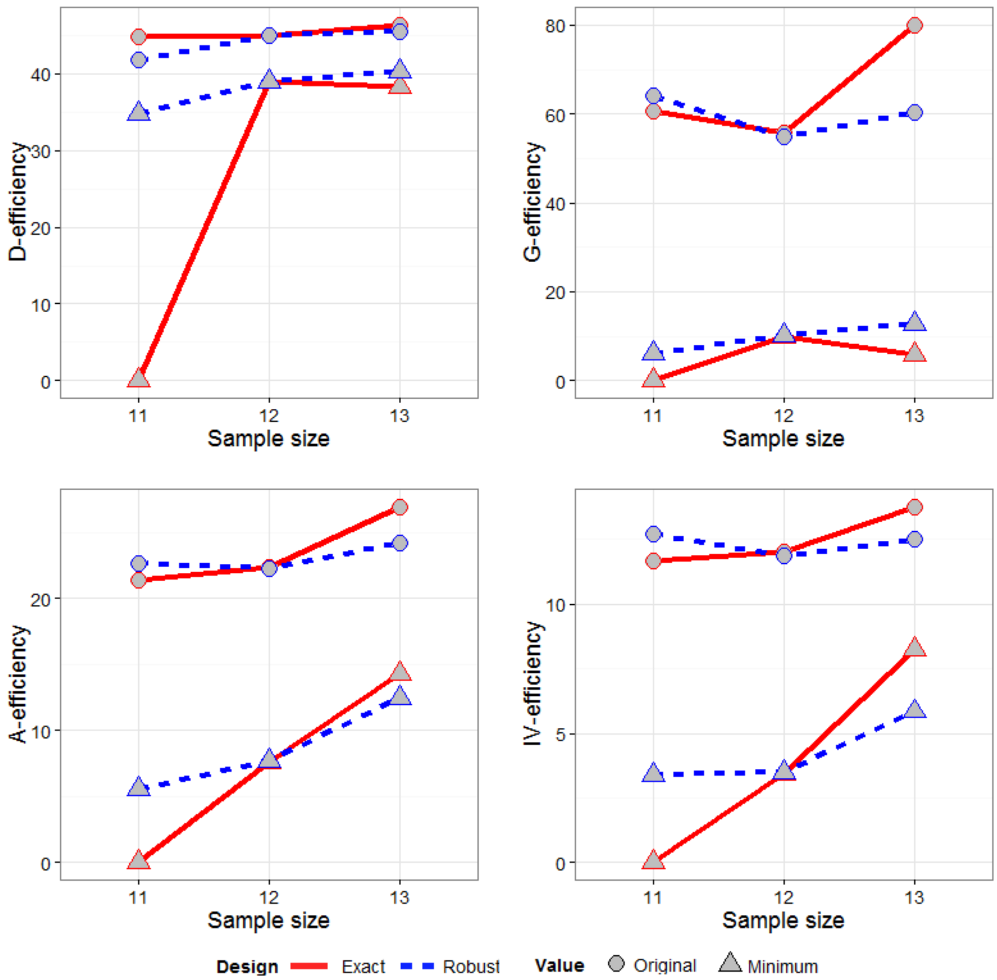



Figure 4.8: Summary of $D$-, $A$-, $G$-, $IV$-efficiencies and corresponding minimum efficiencies of three-factor $D$-optimal exact and robust exact designs.

and robust exact designs increases. In contrast, $A$- and $IV$-efficiencies of the robust exact design slightly decreases as the sample size increases from 11 to 12 and then increases as $n$ equals 13.

Table 4.5: Properties of the 3-factor $D$-optimal designs for $n = 11$, 12, and 13.

| | 11-point $D$-optimal | | 12-point $D$-optimal | | 13-point $D$-optimal | |
|---|---|---|---|---|---|---|
| Criteria Evaluated | Exact Design | Robust Design | Exact Design | Robust Design | Exact Design | Robust Design |
| $D$-efficiency | 44.769 | 41.889 | 44.986 | 44.921 | 46.391 | 45.443 |
| Min $D$-efficiency | 0.000 | *34.823* | 38.956 | *38.974* | 38.326 | *40.259* |
| Leave-1-out $D$-efficiency | 29.091 | 36.016 | 40.639 | 40.593 | 43.120 | 42.223 |
| | (18.684) | (1.422) | (1.844) | (1.809) | (1.866) | (1.720) |
| Leave-2-out $D$-efficiency | | | 29.831 | 30.441 | 38.555 | 37.582 |
| | | | (12.173) | (11.057) | (3.490) | (3.848) |
| $A$-efficiency | 21.390 | 22.592 | 22.364 | 22.273 | 26.948 | 24.149 |
| Min $A$-efficiency | 0.000 | 5.600 | 7.642 | 7.731 | 14.335 | 12.425 |
| Leave-1-out $A$-efficiency | 13.244 | 13.404 | 16.688 | 16.637 | 21.986 | 19.788 |
| | (8.530) | (5.301) | (5.606) | (5.529) | (3.816) | (3.984) |
| Leave-2-out $A$-efficiency | | | 8.155 | 8.165 | 15.204 | 13.676 |
| | | | (6.220) | (6.167) | (5.637) | (5.596) |
| $G$-efficiency | 60.606 | 64.090 | 55.633 | 54.860 | 80.106 | 60.258 |
| Min $G$-efficiency | 0.000 | 6.212 | 10.021 | 10.140 | 5.938 | 12.868 |
| Leave-1-out $G$-efficiency | 10.390 | 9.759 | 19.700 | 19.598 | 26.091 | 26.263 |
| | (6.673) | (4.701) | (15.023) | (14.646) | (10.088) | (14.036) |
| Leave-2-out $G$-efficiency | | | 7.033 | 7.096 | 15.219 | 13.828 |
| | | | (5.628) | (5.690) | (9.863) | (9.775) |
| $IV$-efficiency | 11.671 | 12.724 | 12.022 | 11.901 | 13.783 | 12.511 |
| Min $IV$-efficiency | 0.000 | 3.380 | 3.451 | 3.506 | 8.247 | 5.851 |
| Leave-1-out $IV$-efficiency | 7.122 | 7.645 | 9.009 | 8.927 | 11.415 | 10.356 |
| | (4.600) | (2.904) | (3.061) | (3.002) | (2.159) | (2.311) |
| Leave-2-out $IV$-efficiency | | | 4.449 | 4.449 | 8.001 | 7.244 |
| | | | (3.333) | (3.301) | (2.941) | (3.033) |

Numbers in parentheses represent standard deviations

# 4. $A$-Optimal Robust Exact Designs

Let $\Xi$ be the set of all possible exact designs on $\mathcal{X}$, $\Theta$ be the set of potential design points, and $\mathbf{x}_i$ be a design point in $\Theta$. The proposed $A$-optimal robust exact designs satisfy:

$$\xi^* = \arg \max_{\xi \in \Xi} \min_{\mathbf{x}_i \in \Theta} \text{trace } \mathbf{M}(\xi_{-\mathbf{x}_i}), \tag{4.2}$$

where $\mathbf{M}(\xi_{-\mathbf{x}_i})$ is the moment matrix of the design with a missing point $\mathbf{x}_i$. For this criterion, the goal is to maximize the $A$-efficiency when the worst case of a missing value happens, and the resulting design will be called an $A$-optimal robust exact design.

The algorithm described in Section 2 was applied to construct the $A$-optimal robust exact design in a cuboidal region. The point-exchange algorithm is used, and a set of candidate points is $\{-1, -.9, \ldots, .9, 1\}^k, k = 2$ and 3. For two-factor designs, sample sizes in the study are 7, 8, 9, and 10, and for three-factor designs, sample sizes are 11, 12, and 13. As readers will notice at the end of this section, as the number of design points increases, both exact and robust exact designs will not be much different.

## 4.1. Two-Factor $A$-Optimal Designs

4.1.1. The 7-Point Design: For the robust exact design, several repetitions were run until the best one was found twice. The design having the highest Min $A$ consists of $(-1, .2)$, $(1, -.2)$, $(-.1, 0)$, $(.7, .8)$, $(-.9, 1)$, $(-1, -1)$, and $(.4, -.8)$. As seen in Figure 4.9, the $A$-optimal exact design (Borkowski, 2003b) is symmetric with respect to the $y$-axis, but this is not the case for the robust exact design. For the exact design, if one of the points on the boundary is lost, the $A$-efficiency will be zero

Table 4.6: Properties of the 7-point 2-factor $A$-optimal designs.

| | 7-point $A$-optimal | |
|---|---|---|
| Criteria Evaluated | Exact Design | Robust Design |
| $D$-efficiency | 38.535 | 34.066 |
| Min $D$-efficiency | 0.000 | 23.627 |
| Leave-1-out $D$-efficiency | 11.444 | 27.976 |
| | (19.544) | (3.214) |
| $A$-efficiency | 27.797 | 21.259 |
| Min $A$-efficiency | 0.000 | *9.970* |
| Leave-1-out $A$-efficiency | 7.123 | 11.888 |
| | (12.166) | (3.025) |
| $G$-efficiency | 43.450 | 28.309 |
| Min $G$-efficiency | 0.000 | 4.573 |
| Leave-1-out $G$-efficiency | 13.054 | 11.764 |
| | (22.294) | (8.587) |
| $IV$-efficiency | 25.200 | 19.377 |
| Min $IV$-efficiency | 0.000 | 6.846 |
| Leave-1-out $IV$-efficiency | 6.231 | 11.634 |
| | (10.259) | (3.405) |

meaning that the model is not estimable. The greatest loss in the $A$-efficiency in the robust exact design occurs when point $(-.1, 0)$ is missing.

Table 4.6 summarizes all comparison criteria. The Min $A$ increases from 0 to 9.97, but the $A$-efficiency drops by 6.5 in exchange for being robust to a missing point. The robust design has a higher leave-1-out $A$-efficiency with a lower standard deviation of 3.03. Not only the Min $A$ increases, but also min $D$, min $G$, and min $IV$ increase. Without a missing point, the exact design seems to have higher precisions of predictions than the robust design.

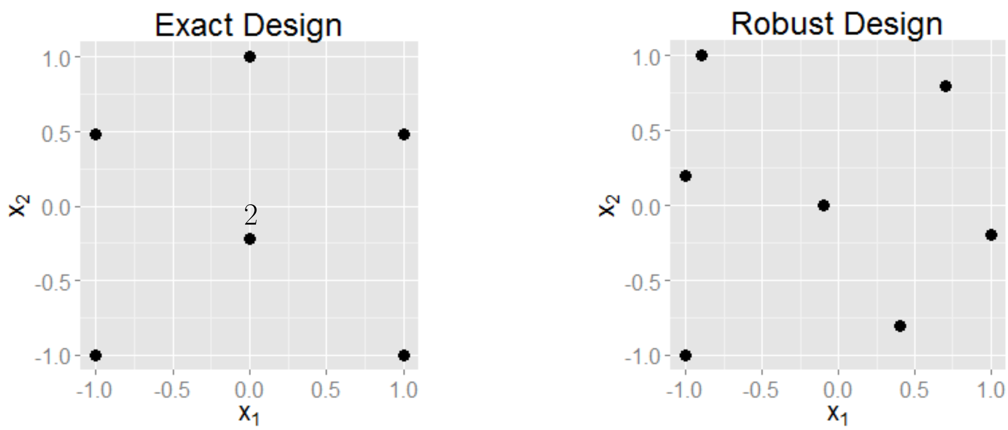



Figure 4.9: Seven-point $A$-optimal exact (left) and robust exact (right) designs for a second-order model in two factors. Numbers represent the number of replications.

4.1.2. The 8-Point Design: The design points of the exact (Borkowski, 2003b) and robust exact designs are plotted in Figure 4.10. The new robust exact design contains points $(\pm 1, \pm 1)$, $(\pm .7, 0)$, and $(0, \pm 1)$. They are vertically symmetric. Both designs have six design points on the boundary of the design space, but the exact design chooses places two points near the origin $(0, 0)$.

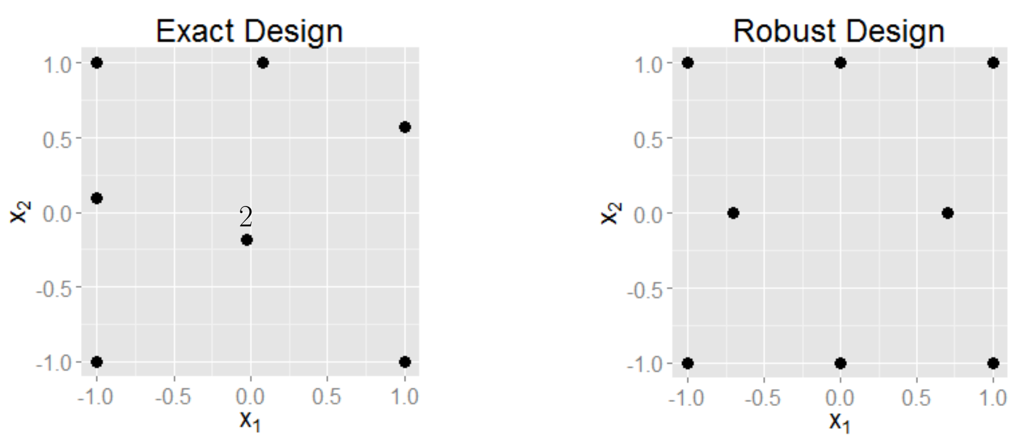



Figure 4.10: Eight-point $A$-optimal exact (left) and robust exact (right) designs for a second-order model in two factors. Numbers represent the number of replications.

Table 4.7: Properties of the 8-point 2-factor $A$-optimal designs.

| | 8-point $A$-optimal | |
|---|---|---|
| Criteria Evaluated | Exact Design | Robust Design |
| $D$-efficiency | 41.618 | 44.039 |
| Min $D$-efficiency | 23.972 | 35.938 |
| Leave-1-out $D$-efficiency | 34.885 | 39.254 |
| | (7.571) | (3.580) |
| Leave-2-out $D$-efficiency | 15.691 | 28.208 |
| | (17.695) | (12.437) |
| $A$-efficiency | 29.301 | 27.396 |
| Min $A$-efficiency | 4.216 | *19.388* |
| Leave-1-out $A$-efficiency | 17.945 | 20.439 |
| | (9.608) | (1.137) |
| Leave-2-out $A$-efficiency | 6.434 | 11.449 |
| | (8.649) | (5.916) |
| $G$-efficiency | 46.549 | 83.717 |
| Min $G$-efficiency | 1.429 | 13.095 |
| Leave-1-out $G$-efficiency | 25.487 | 28.437 |
| | (21.841) | (16.416) |
| Leave-2-out $G$-efficiency | 8.422 | 12.855 |
| | (14.810) | (14.917) |
| $IV$-efficiency | 25.219 | 22.598 |
| Min $IV$-efficiency | 4.720 | 15.858 |
| Leave-1-out $IV$-efficiency | 15.411 | 17.112 |
| | (8.315) | (1.237) |
| Leave-2-out $IV$-efficiency | 5.457 | 9.582 |
| | (7.274) | (4.745) |

Numbers in parentheses represent standard deviations

The criteria evaluated are summarized in Table 4.7. The Min $A$ is improved by approximately 15.2, and the $A$-efficiency slightly decreases. For the leave-1-out and leave-2-out $D$-, $A$-, $G$-, and $IV$-efficiencies, the robust exact design is uniformly superior to the exact design. The leave-1-out $A$-efficiency has a very small standard deviation indicating that when an arbitrary missing point occurs, the $A$-efficiency inappreciably changes from the leave-1-out $A$-efficiency. It is also surprising that the $G$-efficiency of the robust design is very high and almost as high as that of the $G$-optimal exact design shown in Table 4.12.

4.1.3. The 9-Point Design: That the 9-point $A$-optimal exact design is also $D$-optimal was already known in Borkowski (2003b), and we have found that the exact $D$-optimal design is also the robust exact design. However, based on a set of candidate points $\{-1, -.9, \ldots, .9, 1\}^2$, the Min $A$ can be improved a little by placing design points at $(\pm1, \pm1)$, $(-.9, 0)$, $(1, 0), (-.1, \pm1)$, and $(0, 0)$. Figure 4.11 shows design points of exact and robust exact designs which are only subtly different.

From Table 4.8, the Min $A$ increases slightly when using the robust exact design instead of the exact design. Both designs are similar in all aspects regarding to $D$-, $A$-, $G$-, and $IV$-related criteria. For example, they have the same robustness against two missing points as corresponding leave-2-out A-efficiencies are slightly different.

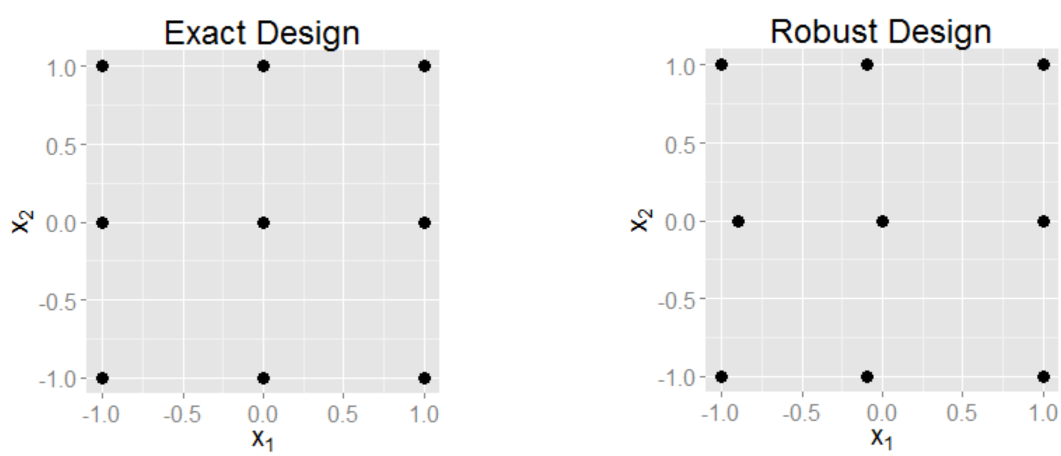



Figure 4.11: Nine-point $A$-optimal exact (left) and robust exact (right) designs for a second-order model in three factors.

Table 4.8: Properties of the 9-point 2-factor $A$-optimal designs.

| Criteria Evaluated | 9-point $A$-optimal Exact Design | 9-point $A$-optimal Robust Design |
|---|---|---|
| $D$-efficiency | 46.224 | 45.424 |
| Min $D$-efficiency | 39.581 | 38.327 |
| Leave-1-out $D$-efficiency | 42.829 | 42.012 |
| | (3.082) | (3.273) |
| Leave-2-out $D$-efficiency | 38.165 | 37.350 |
| | (4.238) | (4.456) |
| $A$-efficiency | 31.168 | 30.828 |
| Min $A$-efficiency | 22.500 | *23.476* |
| Leave-1-out $A$-efficiency | 25.968 | 25.528 |
| | (2.530) | (2.326) |
| Leave-2-out $A$-efficiency | 19.269 | 18.797 |
| | (3.651) | (3.503) |
| $G$-efficiency | 82.759 | 81.103 |
| Min $G$-efficiency | 18.104 | 16.241 |
| Leave-1-out $G$-efficiency | 41.379 | 40.620 |
| | (22.081) | (22.574) |
| Leave-2-out $G$-efficiency | 24.024 | 22.888 |
| | (17.488) | (16.951) |
| $IV$-efficiency | 24.705 | 24.742 |
| Min $IV$-efficiency | 16.859 | 16.706 |
| Leave-1-out $IV$-efficiency | 21.189 | 20.995 |
| | (1.825) | (1.704) |
| Leave-2-out $IV$-efficiency | 15.872 | 15.877 |
| | (3.169) | (3.008) |

Numbers in parentheses represent standard deviations

4.1.4. The 10-Point Design: The $A$-optimal robust exact design is found to be the same as the exact design provided by Borkowski (2003b). The design points are $(\pm1, \pm1), (0, \pm1)$, $(\pm1, 0)$, and two $(0, 0)$'s and are shown in Figure 4.12. The lowest $A$-efficiency is a result of losing one of the points at $(\pm1, \pm1)$. Table 4.9 shows all criteria evaluated for the design. Overall, this design is very robust to one missing point in terms of estimating parameters in a second-order model because the Min $A$, as well as the Min $D$, are close to the corresponding efficiency of the design without

Table 4.9: Properties of the 10-point 2-factor $A$-optimal designs.

| | 10-point $A$-optimal |
|---|---|
| Criteria Evaluated | Exact Design & Robust Design |
| $D$-efficiency | 44.781 |
| Min $D$-efficiency | 38.125 |
| Leave-1-out $D$-efficiency | 42.082 |
| | (3.515) |
| Leave-2-out $D$-efficiency | 38.514 |
| | (5.034) |
| $A$-efficiency | 33.378 |
| Min $A$-efficiency | *25.564* |
| Leave-1-out $A$-efficiency | 28.767 |
| | (2.761) |
| Leave-2-out $A$-efficiency | 22.972 |
| | (4.571) |
| $G$-efficiency | 75.224 |
| Min $G$-efficiency | 16.915 |
| Leave-1-out $G$-efficiency | 47.560 |
| | (27.719) |
| Leave-2-out $G$-efficiency | 28.814 |
| | (21.318) |
| $IV$-efficiency | 27.170 |
| Min $IV$-efficiency | 20.672 |
| Leave-1-out $IV$-efficiency | 23.809 |
| | (1.802) |
| Leave-2-out $IV$-efficiency | 19.072 |
| | (3.842) |

a missing point. The $A$-efficiency is most sensitive if one of the vertices is lost as the $A$-efficiency will decrease from 33.4 to 25.6%. The $G$-efficiency is also very sensitive to a missing vertical point with the $G$-efficiency dropping from 75.2 to only 16.9%.

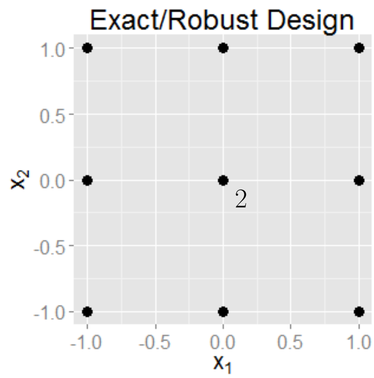



Figure 4.12: Ten-point $A$-optimal exact/robust robust design for a second-order model in two factors. Numbers represent the number of replications.

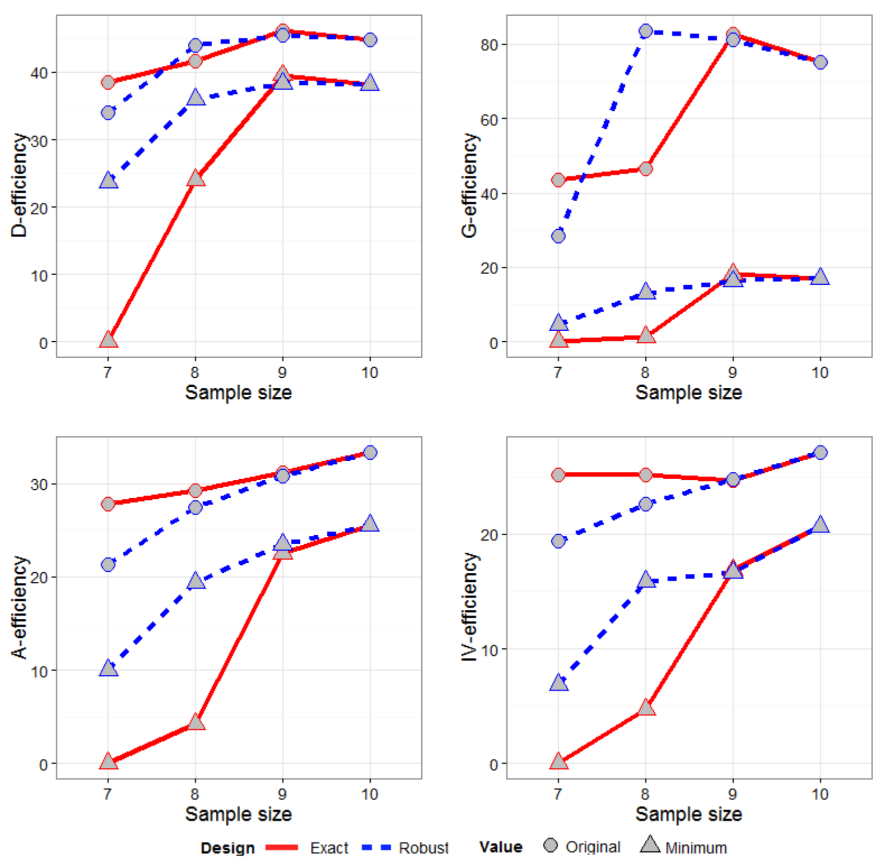



Figure 4.13: Summary of $D$-, $A$-, $G$-, $IV$-efficiencies and corresponding minimum efficiencies of two-factor $A$-optimal exact and robust exact designs.

All minimum and original efficiencies of the $A$-optimal exact and robust exact are plotted in Figure 4.13. For the $A$-optimal criteria, when sample sizes are 7 and 8, the improvement of the Min $A$ is noticeable. For $n = 9$, the Min $A$'s (also $A$-efficiencies) of the robust exact and exact designs are about the same, and for $n = 10$ as previously discussed both designs are the same. Like the $A$-efficiency and Min $A$, the $IV$-efficiency and Min $IV$ of the $A$-optimal robust exact design increase as the sample size increases. The is also the case for $D$- and $G$-efficiencies.

## 4.2. Three-Factor $A$-Optimal Designs

Instead of sequentially describing each design for $k = 3$, we will begin with a summary of results shown in Table 4.10. For $n = 11$, the $A$-, $G$-, and $IV$-efficiencies of the exact design are close to zero. Although the Min $A$ appreciably increases from 0.014 to 8.488%, the $A$-efficiency decreases by 10. For this case, the exact design seems to be preferable to the robust exact design. For $n = 12$, both designs are about the same robust to an arbitrary missing point as their leave-1-out $A$-efficiencies are about the same. This is also the case for two missing points and leave-2-out $A$-efficiencies. For $n = 13$, the robust exact design has a higher Min $A$, leave-1-out and leave-2-out $A$-efficiencies. The precision of predictions is just slightly lower than that of the exact design as the $G$-efficiencies of both designs are not too different. This is also true for the $IV$-efficiency. Overall, the $A$-optimal robust exact design seems preferable because the robustness against a missing point is appreciably increased.

Table 4.10: Properties of the 3-factor $A$-optimal designs for $n = 11$, 12, and 13.

| | 11-point $A$-optimal | | 12-point $A$-optimal | | 13-point $A$-optimal | |
|---|---|---|---|---|---|---|
| Criteria Evaluated | Exact Design | Robust Design | Exact Design | Robust Design | Exact Design | Robust Design |
| $D$-efficiency | 40.887 | 28.963 | 42.177 | 40.504 | 40.272 | 39.079 |
| Min $D$-efficiency | 16.020 | 22.511 | 30.313 | 33.023 | 19.314 | 33.747 |
| Leave-1-out $D$-efficiency | 28.041 | 24.643 | 36.464 | 36.412 | 34.726 | 36.225 |
| | (10.107) | (1.600) | (4.600) | (2.191) | (7.262) | (1.741) |
| Leave-2-out $D$-efficiency | | | 27.108 | 29.527 | 27.086 | 32.358 |
| | | | (8.861) | (5.142) | (10.789) | (2.868) |
| $A$-efficiency | 28.891 | 17.477 | 28.909 | 23.703 | 29.669 | 25.099 |
| Min $A$-efficiency | 0.014 | *8.488* | 4.737 | *14.962* | 0.124 | *18.794* |
| Leave-1-out $A$-efficiency | 8.905 | 9.413 | 16.971 | 17.118 | 19.684 | 20.283 |
| | (8.650) | (1.553) | (8.269) | (2.482) | (9.585) | (1.870) |
| Leave-2-out $A$-efficiency | | | 6.378 | 8.082 | 10.312 | 14.038 |
| | | | (6.160) | (4.779) | (9.063) | (4.029) |
| $G$-efficiency | 45.100 | 18.300 | 42.259 | 35.917 | 54.504 | 50.729 |
| Min $G$-efficiency | 0.003 | 2.585 | 1.470 | 5.226 | 0.020 | 8.716 |
| Leave-1-out $G$-efficiency | 9.234 | 6.224 | 17.815 | 15.736 | 23.969 | 23.304 |
| | (14.648) | (3.839) | (16.516) | (8.722) | (21.643) | (13.625) |
| Leave-2-out $G$-efficiency | | | 4.643 | 5.724 | 9.377 | 11.397 |
| | | | (7.728) | (5.202) | (12.956) | (8.222) |
| $IV$-efficiency | 16.505 | 11.132 | 16.357 | 13.382 | 17.097 | 14.683 |
| Min $IV$-efficiency | 0.008 | 4.330 | 2.653 | 7.500 | 0.066 | 10.010 |
| Leave-1-out $IV$-efficiency | 5.367 | 6.067 | 9.780 | 9.861 | 11.615 | 11.987 |
| | (4.782) | (1.176) | (4.451) | (1.411) | (5.387) | (1.128) |
| Leave-2-out $IV$-efficiency | | | 3.796 | 4.761 | 6.156 | 8.381 |
| | | | (3.531) | (2.756) | (5.327) | (2.385) |

Numbers in parentheses represent standard deviations

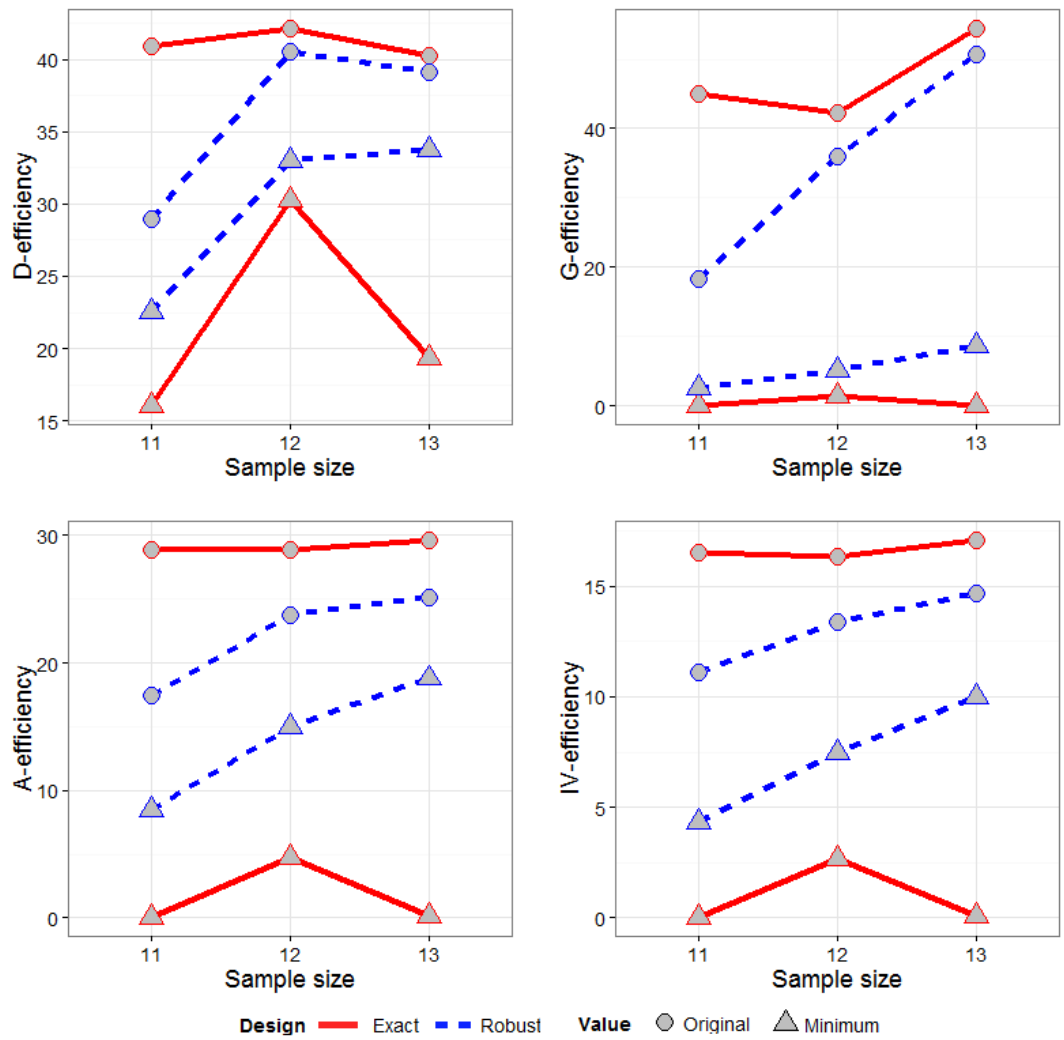



Figure 4.14: Summary of $D$-, $A$-, $G$-, $IV$-efficiencies and corresponding minimum efficiencies of three-factor $A$-optimal exact and robust exact designs.

In conclusion, the robustness against a missing point in terms of the $A$-efficiency is considerably improved. As illustrated in Figure 4.14, as the sample size increases the Min $A$, as well as the Min $IV$, increases. This is also the case for $A$- and $IV$-efficiencies. The exact design of $n = 13$ seems to not very robust to a missing point because its Min $A$, Min $G$, and Min $IV$ are very close to zero. It is seen that the difference between $A$-efficiencies of the exact and robust exact designs decreases when the sample size increases, and this is also the case for $D$-, $G$, and $IV$-efficiencies.

## 5. $G$-Optimal Robust Exact Designs

The $G$-optimal robust exact design will now be presented. Let $\Xi$ be the set of all possible exact designs on $\mathcal{X}$, $\Theta$ be the set of potential design points, $\mathcal{X}$ be the cuboidal region, and $\mathbf{x}_i$ is a point in $\Theta$. Our criterion seeks a design $\xi^*$ satisfying

$$\xi^* = \arg\min_{\xi \in \Xi} \max_{\mathbf{x}_i \in \Theta} \left[ \max_{\mathbf{a} \in \mathcal{X}} \mathbf{a}^{\mathrm{T}(m)} \mathbf{M}^{-1}(\xi_{-\mathbf{x}_i}) \mathbf{a}^{(m)} \right], \tag{4.3}$$

where $\mathbf{M}^{-1}(\xi_{-\mathbf{x}_i})$ is an inverse of the moment matrix with missing point $\mathbf{x}_i$ in design $\xi$. The goal of this criterion is to assure that no point has an extremely high prediction variance in the worst-case scenario of a missing point. The resulting design will be called a $G$-optimal robust exact design.

The algorithm described in Section 2 was applied to construct the $G$-optimal robust exact design in a cuboidal region by applying the point-exchange algorithm on a set of candidate points $\{-1, -.9, \ldots, .9, 1\}^k$, $k = 2$ and 3. The sample sizes are 7 to 10 for two-factor designs and 11 to 13 for three-factor designs. In each case, several repetitions were used until the best design appeared twice.

### 5.1. Two-Factor $G$-Optimal Designs

5.1.1. The 7-Point Design: The design points of the robust exact design are $(-1, \pm 1)$, $(1, -1)$, $(-.6, .2)$, $(.2, 1)$, $(-.3, -1)$ and $(1, .4)$ as shown in Figure 4.15. The exact design points are catalogued in Borkowski (2003b). If point $(1, 1)$ is lost in the exact design, the $G$-efficiency will be zero (Min $G$) implying the moment matrix becomes singular. To increase the Min $G$, the robust exact has two design points close

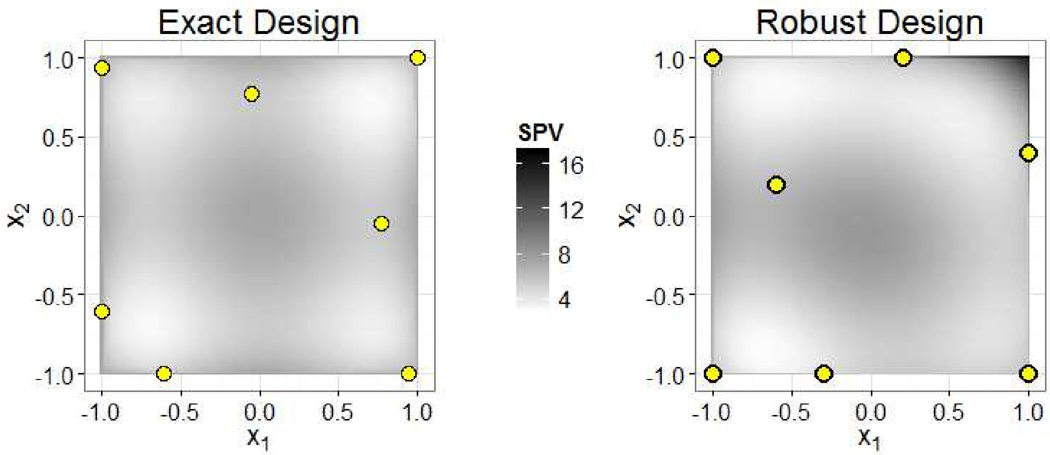



Figure 4.15: Seven-point $G$-optimal exact (left) and robust exact (right) designs for a second-order model in two factors.

to $(1, 1)$ but not at $(1, 1)$. The resulting design has now Min $G$ greater than zero, but has very large SPVs near vertex $(1, 1)$ as the shade of grey is darker near $(1, 1)$ in Figure 4.15. For the robust exact design, losing any point except for $(-.3, -1)$ will give the $G$-efficiency between 9.4 and 14.

When using the robust design instead of the exact design, the Min $G$ increases from 0 to 9.4%, but the $G$-efficiency drops by 42.8 as shown in Table 4.11. It appears that the $G$-efficiency is very sensitive to point changing while increasing in the Min $G$ does not necessarily seem to increase the $G$-efficiency. Although the robust exact design has a low $G$-efficiency, the model is always estimable. The $IV$-efficiencies of both designs indicate designs have about the same average precision of predictions. Actually, the approximated average SPVs of exact and robust exact designs are 5.37 and 5.51, respectively. According to $D$- and $A$-efficiencies, both designs also have about the same performance in precision of estimating parameters. In conclusion, attempting to improve the Min $G$ in this case results in a very poor design in terms of the $G$-efficiency.

Table 4.11: Properties of the 7-point 2-factor $G$-optimal designs.

| | 7-point $G$-optimal | |
|---|---|---|
| Criteria Evaluated | Exact Design | Robust Design |
| $D$-efficiency | 39.655 | 40.585 |
| Min $D$-efficiency | 0.000 | 31.435 |
| Leave-1-out $D$-efficiency | 29.068 | 33.542 |
| | (13.052) | (3.067) |
| $A$-efficiency | 21.271 | 21.629 |
| Min $A$-efficiency | 0.000 | 4.868 |
| Leave-1-out $A$-efficiency | 11.673 | 13.229 |
| | (5.715) | (4.566) |
| $G$-efficiency | 80.192 | 37.4278 |
| Min $G$-efficiency | 0.000 | *9.363* |
| Leave-1-out $G$-efficiency | 16.284 | 14.954 |
| | (10.966) | (10.875) |
| $IV$-efficiency | 18.653 | 18.233 |
| Min $IV$-efficiency | 0.000 | 3.643 |
| Leave-1-out $IV$-efficiency | 10.417 | 11.617 |
| | (5.460) | (3.764) |

Numbers in parentheses represent standard deviations

5.1.2. The 8-Point Design: The design points of the robust exact design are symmetric with respect to both $y$- and $x$-axes. As illustrated in Figure 4.16, design points are $(\pm1, \pm1)$, $(-.3, 1)$, $(-1, -.3)$, $(.3, -1)$, and $(1, .3)$. For the exact design, points are found in Borkowski (2003b). Both have design points at all vertices, and their Min $G$'s are the result of losing one of the vertices.

Multiple criteria values are summarized in Table 4.12. The Min $G$ is improved by 3.6, but like 7-point robust design, the $G$-efficiency drops considerably when using the robust design; however, the difference between $G$-efficiencies of both designs is smaller than that of the 7-point designs. In this case, the exact design is preferable to the robust one because only Min $G$ was improved, while criteria related to $A$- and $IV$-optimality are about the same or lower in the robust design. From Figure 4.16, prediction at the center of the robust exact design is rather poor. If researchers

Table 4.12: Properties of the 8-point 2-factor $G$-optimal designs.

| | 8-point $G$-optimal | |
|---|---|---|
| Criteria Evaluated | Exact Design | Robust Design |
| $D$-efficiency | 44.499 | 43.082 |
| Min $D$-efficiency | 36.953 | 36.872 |
| Leave-1-out $D$-efficiency | 39.847 | 38.834 |
| | (3.108) | (2.098) |
| Leave-2-out $D$-efficiency | 28.852 | 27.938 |
| | (12.530) | (12.224) |
| $A$-efficiency | 26.007 | 18.724 |
| Min $A$-efficiency | 18.777 | 14.056 |
| Leave-1-out $A$-efficiency | 19.549 | 14.219 |
| | (0.849) | (0.175) |
| Leave-2-out $A$-efficiency | 11.267 | 8.358 |
| | (5.744) | (4.752 |
| $G$-efficiency | 87.943 | 47.885 |
| Min $G$-efficiency | 14.792 | *18.355* |
| Leave-1-out $G$-efficiency | 29.208 | 26.011 |
| | (15.429) | (8.184) |
| Leave-2-out $G$-efficiency | 14.074 | 12.874 |
| | (15.581) | (9.902) |
| $IV$-efficiency | 20.987 | 14.082 |
| Min $IV$-efficiency | 14.849 | 9.753 |
| Leave-1-out $IV$-efficiency | 16.175 | 11.064 |
| | (1.205) | (1.058) |
| Leave-2-out $IV$-efficiency | 9.326 | 6.408 |
| | (4.659) | (3.789) |

Numbers in parentheses represent standard deviations

only make the prediction on the edge of the design region, the robust exact design is acceptable. The precision of the parameter estimation is about the same for both designs.

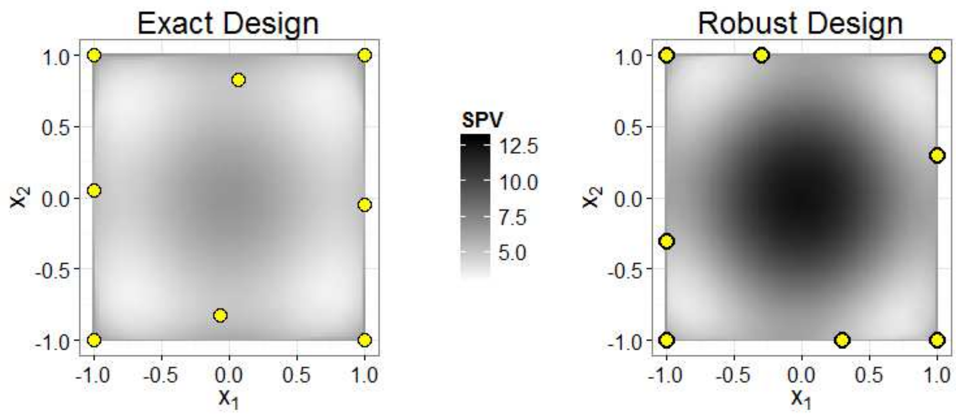



Figure 4.16: Eight-point $G$-optimal exact (left) and robust exact (right) designs for a second-order model in two factors.

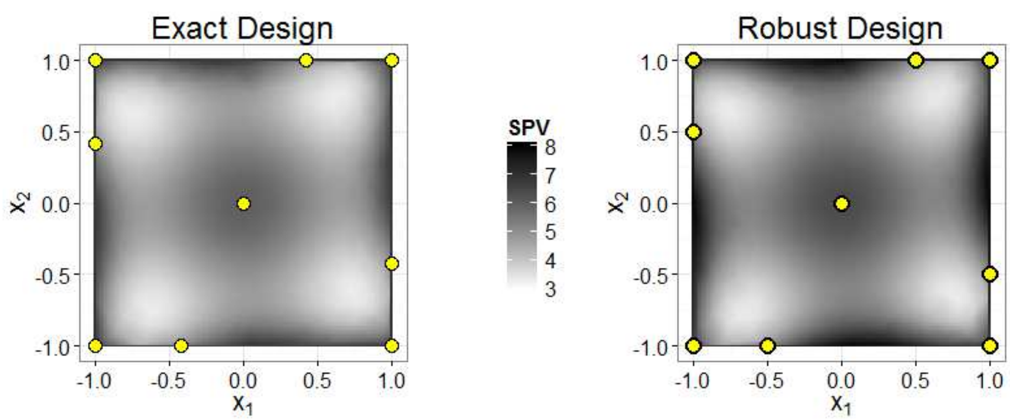



Figure 4.17: Nine-point $G$-optimal exact (left) and robust exact (right) designs for a second-order model in two factors.

5.1.3. The 9-Point Design: As illustrated in Figure 4.17, the 9-point robust exact design is similar to the exact design generated by a genetic algorithm (Borkowski, 2003b). The robust exact design contains points $(\pm 1, \pm 1), (.5, 1), (-.5, -1)$, $(1, -.5), (-1, .5)$, and $(0, 0)$. The Min $G$ of both designs is a result of losing one of the four vertices. It is seen that predictions at the edge of the design region in both design are less precise than those for interior points.

Table 4.13: Properties of the 9-point 2-factor $G$-optimal designs

| | 9-point $G$-optimal. | |
|---|---|---|
| Criteria Evaluated | Exact Design | Robust Design |
| $D$-efficiency | 43.387 | 42.128 |
| Min $D$-efficiency | 38.149 | 37.421 |
| Leave-1-out $D$-efficiency | 40.382 | 39.251 |
| | (2.199) | (1.942) |
| Leave-2-out $D$-efficiency | 35.827 | 34.727 |
| | (4.228) | (4.340) |
| $A$-efficiency | 25.126 | 22.547 |
| Min $A$-efficiency | 15.329 | 12.672 |
| Leave-1-out $A$-efficiency | 21.244 | 19.106 |
| | (2.460) | (2.521) |
| Leave-2-out $A$-efficiency | 15.559 | 13.865 |
| | (4.287) | (4.247) |
| $G$-efficiency | 86.350 | 75.075 |
| Min $G$-efficiency | 22.143 | *23.985* |
| Leave-1-out $G$-efficiency | 35.294 | 32.876 |
| | (12.875) | (9.258) |
| Leave-2-out $G$-efficiency | 22.428 | 22.039 |
| | (10.979) | (9.366) |
| $IV$-efficiency | 21.223 | 19.499 |
| Min $IV$-efficiency | 11.327 | 9.583 |
| Leave-1-out $IV$-efficiency | 18.066 | 17.176 |
| | (2.610) | (2.863) |
| Leave-2-out $IV$-efficiency | 13.681 | 12.964 |
| | (4.626) | (4.988) |

Numbers in parentheses represent standard deviations

The criteria values are summarized in Table 4.13. The Min $G$ is slightly improved, but because the design points of both designs are similar, the $D$-, $A$-, or $IV$-efficiencies of both designs are about the same. The $G$-efficiency, however, drops by 11 when using the robust design, but a big drop in the $G$-efficiency is typical because it is very sensitive to a missing point. In this case, the exact design is therefore preferable to the robust exact design.

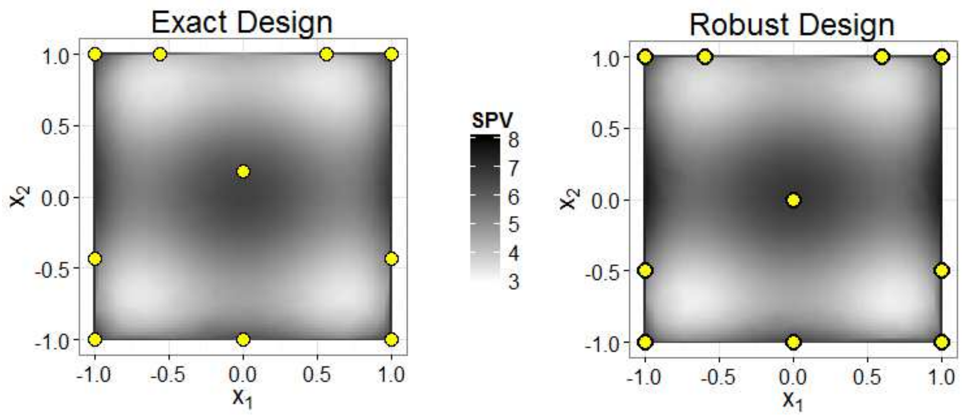



Figure 4.18: Ten-point $G$-optimal exact (left) and robust exact (right) designs for a second-order model in two factors.

5.1.4. The 10-Point Design: Design points of 10-point exact and robust exact designs are plotted in Figure 4.18 and are similar. The design points of the robust design are $(\pm 1, \pm 1)$, $(0, -1), (\pm .6, 1)$, $(\pm 1, -.5)$, and $(0, 0)$. The exact design points are listed in Borkowski (2003b). The Min $G$ of the exact design results from losing one of the vertices, and for the robust exact design, if one of points $(\pm 1, \pm 1)$ and $(0, 0)$ is lost, the $G$-efficiency will drop to around 31 to 33. It is also seen that predictions at the edge and center of the design region are rather poor compared to those at the middle.

Table 4.14: Properties of the 10-point 2-factor $G$-optimal designs.

| | 10-point $G$-optimal | |
|---|---|---|
| Criteria Evaluated | Exact Design | Robust Design |
| $D$-efficiency | 43.373 | 43.053 |
| Min $D$-efficiency | 39.574 | 39.551 |
| Leave-1-out $D$-efficiency | 41.184 | 40.902 |
| | (1.803) | (1.681) |
| Leave-2-out $D$-efficiency | 38.015 | 37.707 |
| | (3.548) | (3.645) |

Table 4.14 (continued)

| Criteria Evaluated | 10-point $G$-optimal Exact Design | 10-point $G$-optimal Robust Design |
|---|---|---|
| $A$-efficiency | 25.284 | 24.338 |
| Min $A$-efficiency | 15.166 | 13.395 |
| Leave-1-out $A$-efficiency | 22.572 | 21.785 |
| | (3.143) | (3.443) |
| Leave-2-out $A$-efficiency | 18.601 | 17.903 |
| | (4.922) | (5.300) |
| $G$-efficiency | 86.533 | 79.335 |
| Min $G$-efficiency | 29.481 | *31.287* |
| Leave-1-out $G$-efficiency | 42.399 | 42.105 |
| | (15.963) | (15.268) |
| Leave-2-out $G$-efficiency | 30.170 | 30.543 |
| | (12.264) | (11.932) |
| $IV$-efficiency | 20.855 | 20.523 |
| Min $IV$-efficiency | 10.758 | 10.117 |
| Leave-1-out $IV$-efficiency | 18.510 | 18.046 |
| | (2.884) | (3.161) |
| Leave-2-out $IV$-efficiency | 15.378 | 15.226 |
| | (4.608) | (4.855) |

Numbers in parentheses represent standard deviations

Table 4.14 shows that for each criterion, both designs have similar values. The Min $G$ slightly increases when using the robust design instead of the exact design. Although the $G$-efficiencies are somewhat different, the Min $G$ are about the same. Also, the Min $G$ is rather small compared to the $G$-efficiency. Overall, both designs are not very different. This is because the sample size is larger compared to the number of parameters in a second-order model.

All efficiencies of the exact and robust exact designs are plotted verses the sample sizes in Figure 4.19. As the sample size increase, the Min $G$ of the robust exact design gradually increases, and it is slightly greater than that of the exact design. The $G$-efficiency considerably improves when $n$ increases from 8 to 9. Like the Min $G$, the Min $D$ increases as the sample size increases. The patters of $A$- and $IV$-efficiencies are similar. For example, as $n$ increase from 7 to 8, both $A$- and $IV$-efficiencies escalate and decrease as $n$ increases from 8 to 9. The patterns of the Min $A$ and Min $IV$ are also similar.

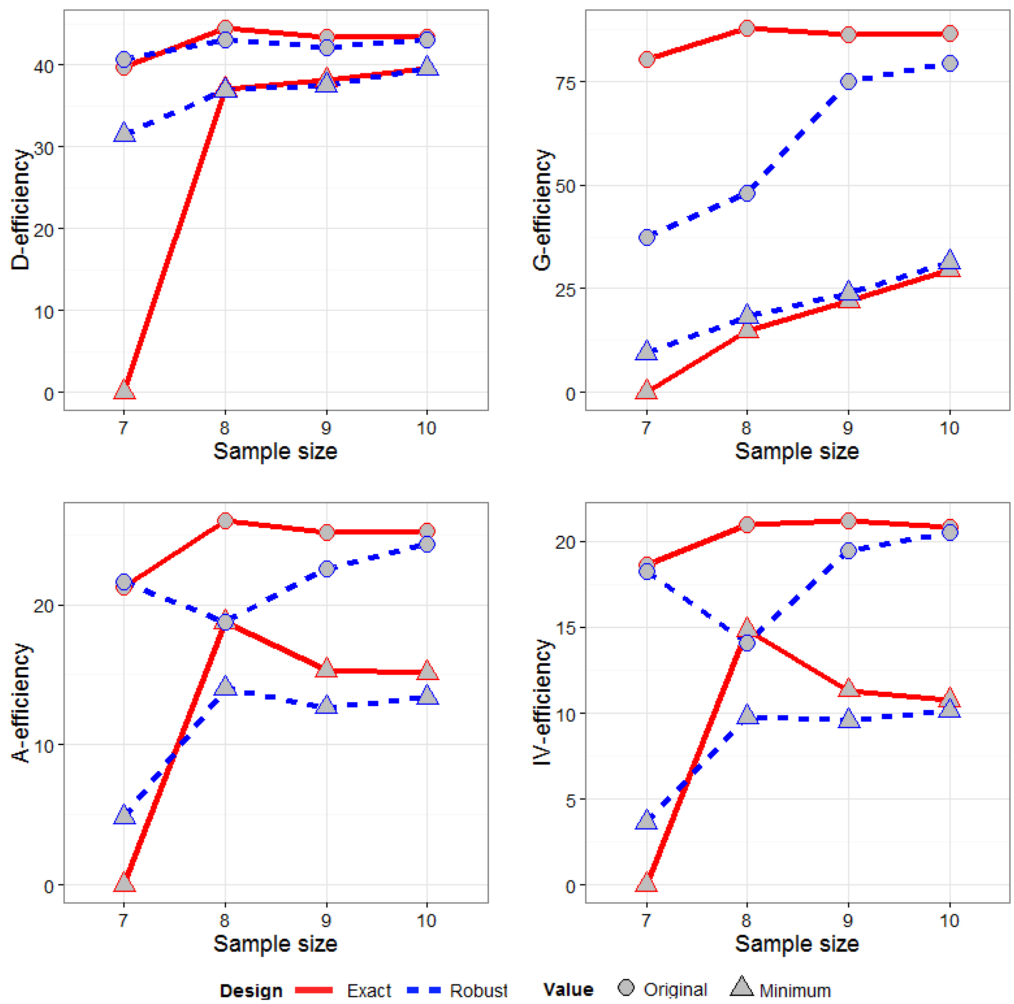



Figure 4.19: Summary of $D$-, $A$-, $G$-, $IV$-efficiencies and corresponding minimum efficiencies of two-factor $G$-optimal exact and robust exact designs.

## 5.2. Three-Factor $G$-Optimal Designs

Instead of sequentially describing each design for each design size for $k = 3$, we have summarized the results in Table 4.15. For $n = 11$, the Min $G$ increases by 5.5, but the $G$-efficiency drops by 37.9 when using the robust exact design instead of the exact design. Overall, the robust exact design has slightly lower precision. The criteria related to the $IV$-optimality are similar for both designs. For $n = 12$, both designs have similar $D$-, $A$-, and $IV$-efficiencies, while the $G$-efficiencies are rather different. This indicates that even though the maximum SPV is much higher in the robust design, but the average precision of predictions is about the same as that of the exact design. For $n = 13$, the Min $G$ increases from 7.462 to 15.856, and like other $G$-optimal robust exact designs, the $G$-efficiency is somewhat low compared to the exact designs. The leave-1-out, as well as leave-2-out, $G$-efficiencies of both designs are about the same. Furthermore, the precision of parameter estimations are, generally, not much different. Criteria related to $A$- and $IV$-optimality are slightly lower in the robust exact design than in the exact design.

All minimum and original design efficiencies of both designs are plotted in Figure 4.20. As the design size increases, the Min $G$ increases, but it is still low compared to that of the exact design. The patterns of the Min $A$ and Min $IV$ of the robust designs are similar. This is also true for the exact designs. In conclusion, the Min $G$ is not a very good criterion to be used for constructing robust designs because this criterion only improve the Min $G$ of the robust designs while other criteria are very poor.

Table 4.15: Properties of the 3-factor $G$-optimal designs for $n = 11$, 12, and 13.

| | 11-point $G$-optimal | | 12-point $G$-optimal | | 13-point $G$-optimal | |
|---|---|---|---|---|---|---|
| Criteria Evaluated | Exact Design | Robust Design | Exact Design | Robust Design | Exact Design | Robust Design |
| $D$-efficiency | 41.756 | 38.364 | 41.856 | 43.026 | 45.699 | 42.375 |
| Min $D$-efficiency | 30.817 | 32.313 | 27.875 | 38.227 | 38.561 | 38.226 |
| Leave-1-out $D$-efficiency | 35.169 | 33.085 | 37.301 | 38.987 | 42.481 | 39.437 |
| | (3.122) | (0.946) | (3.404) | (1.369) | (1.740) | (1.351) |
| Leave-2-out $D$-efficiency | | | 28.815 | 27.639 | 37.902 | 35.313 |
| | | | (7.060) | (12.593) | (3.541) | (2.836) |
| $A$-efficiency | 22.529 | 19.107 | 22.376 | 18.989 | 25.435 | 21.790 |
| Min $A$-efficiency | 3.282 | 4.801 | 0.714 | 8.416 | 14.379 | 8.185 |
| Leave-1-out $A$-efficiency | 12.876 | 11.701 | 16.253 | 14.412 | 20.853 | 18.089 |
| | (7.518) | (4.163) | (5.794) | (3.866) | (3.778) | (3.222) |
| Leave-2-out $A$-efficiency | | | 7.125 | 6.625 | 14.410 | 12.875 |
| | | | (6.779) | (5.017) | (5.650) | (4.812) |
| $G$-efficiency | 77.261 | 39.471 | 80.266 | 54.377 | 83.811 | 59.700 |
| Min $G$-efficiency | 1.880 | *7.442* | 0.654 | *13.390* | 7.462 | *15.856* |
| Leave-1-out $G$-efficiency | 9.802 | 9.589 | 18.327 | 18.478 | 25.357 | 24.578 |
| | (6.949) | (2.819) | (12.555) | (11.976) | (11.085) | (11.352) |
| Leave-2-out $G$-efficiency | | | 6.222 | 7.609 | 14.395 | 13.785 |
| | | | (6.897) | (6.359) | (9.000) | (7.194) |
| $IV$-efficiency | 12.417 | 12.344 | 11.807 | 10.682 | 13.032 | 11.608 |
| Min $IV$-efficiency | 1.427 | 1.411 | 0.353 | 3.077 | 7.576 | 3.273 |
| Leave-1-out $IV$-efficiency | 7.400 | 7.394 | 8.752 | 8.341 | 10.817 | 9.945 |
| | (3.949) | (3.929) | (3.201) | (2.053) | (2.240) | (2.057) |
| Leave-2-out $IV$-efficiency | | | 3.941 | 4.005 | 7.527 | 7.320 |
| | | | (3.759) | (3.070) | (3.026) | (2.850) |

Numbers in parentheses represent standard deviations

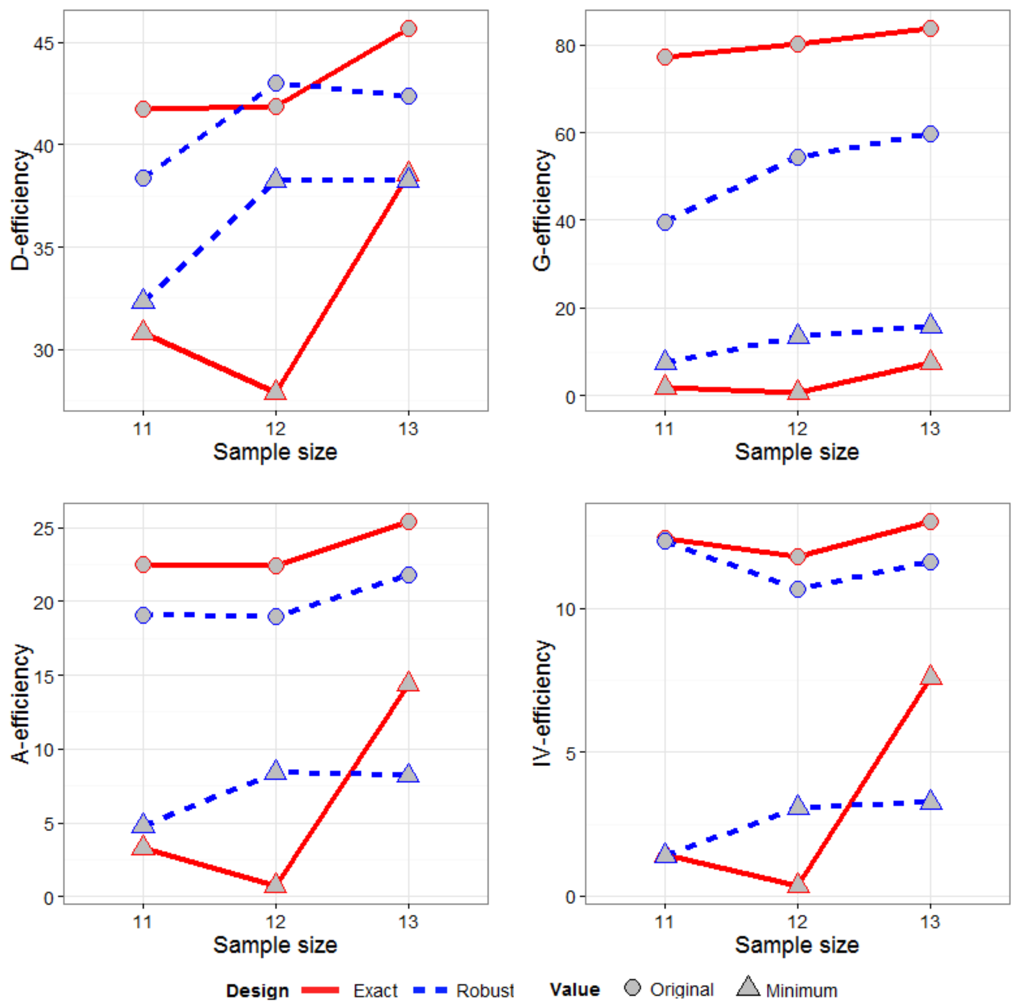



Figure 4.20: Summary of $D$-, $A$-, $G$-, $IV$-efficiencies and corresponding minimum efficiencies of three-factor $G$-optimal exact and robust exact designs.

## 6. $IV$-Optimal Robust Exact Designs

The $IV$-optimal robust exact designs will now be presented. Let $\Xi$ be the set of all possible exact designs on $\mathcal{X}$, $\Theta$ be the set of potential design points, $\mathcal{X}$ be the cuboidal region, and $\mathbf{x}_i$ be a point in $\Theta$. Our criterion seeks a design $\xi^*$ satisfying

$$\xi^* = \arg \min_{\xi \in \Xi} \max_{\mathbf{x}_i \in \Theta} \left[ \frac{1}{A} \int_{\mathcal{X}} \mathbf{a}^{\mathrm{T}(m)} \mathbf{M}^{-1}(\xi_{-\mathbf{x}_i}) \mathbf{a}^{(m)} \, d\mathbf{a} \right], \tag{4.4}$$

where $A$ is the volume of space $\mathcal{X}$ and $\mathbf{M}^{-1}(\xi_{-\mathbf{x}_i})$ is an inverse of the moment matrix $\mathbf{M}$ with design point $\mathbf{x}_i$ missing. The goal of this criterion is to minimize the maximum of the average scaled prediction variance when the worst case scenario of a missing point occurs. This means a missing point results to the maximum average SPV. The resulting design will be called an $IV$-optimal robust exact design.

The algorithm described in Section 2 was applied to construct $IV$-optimal robust exact designs in a cuboidal region with a set of candidate points $\{-1, -.9, \ldots, .9, 1\}^k$, $k = 2$ and 3. The sample sizes in the two-factor study are 7, 8, 9, and 10, and for three-factor designs, sample sizes are 11, 12, and 13. In each case, several repetitions were used until the best design appeared twice.

## 6.1. Two-Factor $IV$-Optimal Designs

6.1.1. The 7-Point Design: The robust exact design points are $(\pm 1, -1)$, $(-.9, .3)$, $(-.3, 1)$, $(.9, .8), (.3, 0)$, and $(.1, -1)$. Three of those are interior points as shown in Figure 4.21. Unlike the robust exact design, the exact design, generated by a genetic algorithm (Borkowski, 2003b), has five points on the boundary and two replicates near the origin $(0, 0)$. The exact design is not very robust to a missing point. If one of the points on the boundary is missing, the $IV$-efficiency will be zero, and thus the model will not be estimable. Both designs have high SPVs for points near or at $(-1, 1)$.

Table 4.16 summarizes criteria being evaluated for exact and robust exact designs. The Min $IV$ is considerably improved as it increases from 0 to 9.2%, and the $IV$-efficiency decreases by only 3 when using the robust design instead of the exact design. Considering $D$- and $A$-efficiencies, both designs have about the same performance in estimating parameters in a second-order model, but the robust exact design has much higher Min $D$- and $A$-efficiencies, as well as leave-1-out efficiencies, than those of the

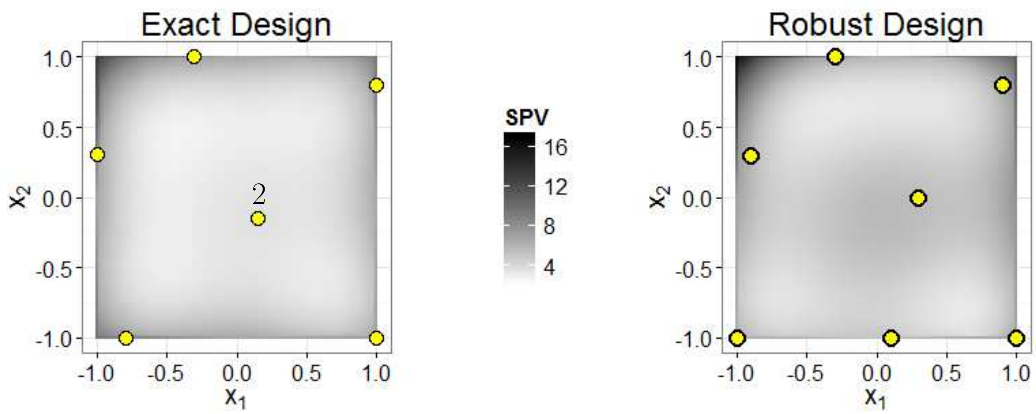



Figure 4.21: Seven-point $IV$-optimal exact (left) and robust exact (right) designs for a second-order model in two factors. Numbers represent the number of replications.

exact design. In conclusion, the robust design is preferable to the exact design because it is just slightly less $IV$-optimal but much more robust to a missing point.

Table 4.16: Properties of the 7-point 2-factor $IV$-optimal designs.

| | 7-point $IV$-optimal | |
|---|---|---|
| Criteria Evaluated | Exact Design | Robust Design |
| $D$-efficiency | 38.326 | 37.942 |
| Min $D$-efficiency | 0.000 | 25.409 |
| Leave-1-out $D$-efficiency | 11.382 | 31.043 |
| | (19.438) | (3.817) |
| $A$-efficiency | 27.427 | 23.619 |
| Min $A$-efficiency | 0.000 | 7.221 |
| Leave-1-out $A$-efficiency | 7.046 | 13.194 |
| | (12.034) | (4.253) |
| $G$-efficiency | 45.187 | 35.619 |
| Min $G$-efficiency | 0.000 | 3.709 |
| Leave-1-out $G$-efficiency | 13.101 | 14.301 |
| | (22.374) | (11.069) |
| $IV$-efficiency | 24.713 | 21.158 |
| Min $IV$-efficiency | 0.000 | *9.216* |
| Leave-1-out $IV$-efficiency | 6.095 | 12.056 |
| | (10.442) | (3.486) |

Numbers in parentheses represent standard deviations

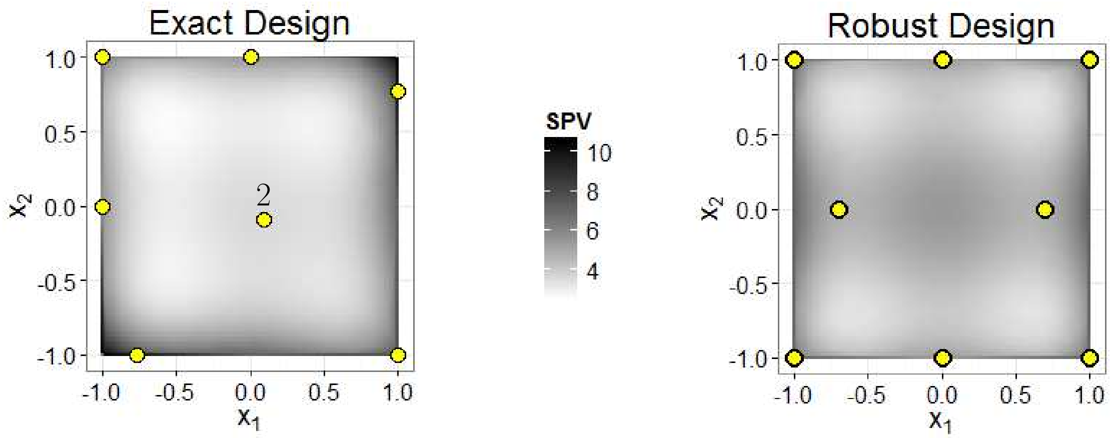



Figure 4.22: Eight-point $IV$-optimal exact (left) and robust exact (right) designs for a second-order model in two factors. Numbers represent the number of replications.

<u>6.1.2. The 8-Point Design:</u> The robust design points are $(\pm 1, \pm 1)$, $(0, \pm 1)$, and $(\pm .7, 0)$ and are illustrated in Figure 4.22. Those points are symmetric with respect to the $y$-axis. It turns out that this design is also $A$-optimal. The exact design points can be found in Borkowski (2003b). All design points of the robust design are near or on the boundary while the exact design contains two replicates near the origin.

Multiple criteria values are summarized in Table 4.17. For the exact design, if one of points $(1, .768)$ and $(-.768, -1)$ is missing, the $IV$-efficiency will decrease from 25.1 to 5.6%. However, both designs are not much different regarding to $D$-, $A$-, and $IV$-efficiencies. The Min $D$, Min $A$, Min $G$, and Min $IV$ are appreciably higher in the robust design than in the exact design. Also, the leave-1-out and leave-2-out $D$-, $A$-, $G$-, and $IV$-efficiencies are higher in the exact design.

Table 4.17: Properties of the 8-point 2-factor $IV$-optimal designs.

| | 8-point $IV$-optimal | |
|---|---|---|
| Criteria Evaluated | Exact Design | Robust Design |
| $D$-efficiency | 40.919 | 44.039 |
| Min $D$-efficiency | 26.183 | 35.938 |
| Leave-1-out $D$-efficiency | 34.482 | 39.254 |
| | (7.122) | (3.580) |
| Leave-2-out $D$-efficiency | 15.538 | 28.208 |
| | (17.455) | (12.437) |
| $A$-efficiency | 28.999 | 27.396 |
| Min $A$-efficiency | 5.861 | 19.388 |
| Leave-1-out $A$-efficiency | 18.000 | 20.439 |
| | (9.202) | (1.137) |
| Leave-2-out $A$-efficiency | 6.489 | 11.449 |
| | (8.578) | (5.916) |
| $G$-efficiency | 57.110 | 83.717 |
| Min $G$-efficiency | 2.253 | 13.095 |
| Leave-1-out $G$-efficiency | 28.245 | 28.437 |
| | (25.392) | (16.416) |
| Leave-2-out $G$-efficiency | 8.198 | 12.855 |
| | (13.637) | (14.917) |
| $IV$-efficiency | 25.133 | 22.598 |
| Min $IV$-efficiency | 5.580 | *15.858* |
| Leave-1-out $IV$-efficiency | 15.938 | 17.112 |
| | (8.205) | (1.237) |
| Leave-2-out $IV$-efficiency | 5.632 | 9.582 |
| | (7.496) | (4.745) |

Numbers in parentheses represent standard deviations

6.1.3. The 9-Point Design: The robust design points are $(\pm1, \pm1)$, $(0, \pm1)$, $(\pm.9, 0)$, and $(0, 0)$ and are illustrated in Figure 4.23. The design points are similar to those of the $D$- and $A$-optimal robust exact designs as shown in Figures 4.5 and 4.11, respectively. Comparing both designs, the exact design Borkowski (2003b) has only two design point at vertices and two points near the origin. Both designs are symmetric with respect to the $x$-axis. Generally, the SPVs of both designs are higher on the boundary of the design region.

Table 4.18: Properties of the 9-point 2-factor $IV$-optimal designs.

| Criteria Evaluated | 9-point $IV$-optimal Exact Design | 9-point $IV$-optimal Robust Design |
|---|---|---|
| $D$-efficiency | 41.930 | 44.804 |
| Min $D$-efficiency | 33.144 | 37.733 |
| Leave-1-out $D$-efficiency | 38.330 | 41.355 |
| | (4.175) | (3.468) |
| Leave-2-out $D$-efficiency | 32.548 | 36.669 |
| | (7.982) | (4.696) |
| $A$-efficiency | 30.584 | 30.773 |
| Min $A$-efficiency | 18.029 | 23.182 |
| Leave-1-out $A$-efficiency | 24.284 | 25.322 |
| | (4.107) | (2.254) |
| Leave-2-out $A$-efficiency | 16.196 | 18.493 |
| | (7.008) | (3.541) |
| $G$-efficiency | 60.810 | 80.904 |
| Min $G$-efficiency | 8.664 | 16.017 |
| Leave-1-out $G$-efficiency | 37.495 | 40.288 |
| | (25.067) | (23.926) |
| Leave-2-out $G$-efficiency | 18.932 | 22.037 |
| | (18.287) | (16.769) |
| $IV$-efficiency | 26.333 | 25.361 |
| Min $IV$-efficiency | 14.701 | *19.285* |
| Leave-1-out $IV$-efficiency | 21.028 | 21.119 |
| | (3.639) | (1.332) |
| Leave-2-out $IV$-efficiency | 14.104 | 15.755 |
| | (6.208) | (2.995) |

Numbers in parentheses represent standard deviations

Multiple criteria values are summarized in Table 4.18. The $IV$-efficiency is slightly greater in the exact design, but the Min $IV$ of the robust exact design is 4.6 more than that of the exact design. All robust criteria, e.g., leave-1-out $G$-efficiency, Min $A$, indicate that the robust design is much more robust to one and two missing points than the exact design. The Min $IV$ of the exact design is a result of losing one of points $(1, .836)$ and $(1, -.836)$.

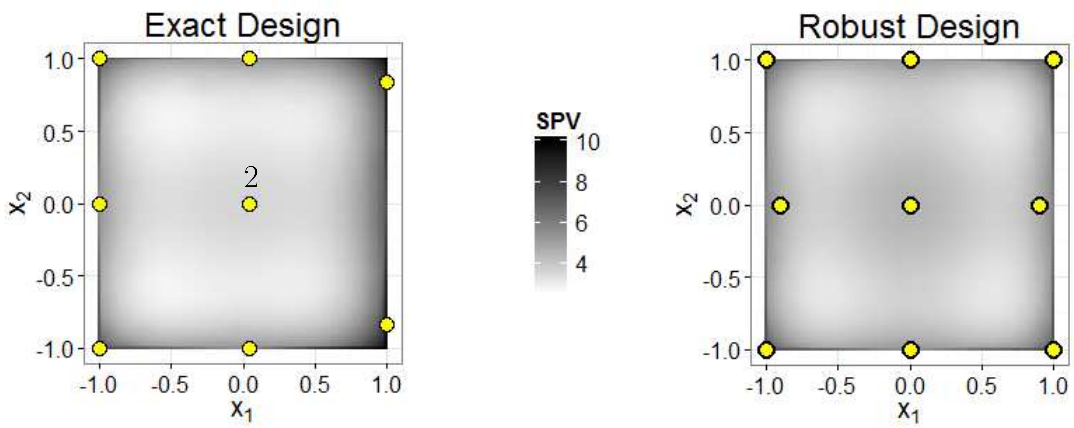



Figure 4.23: Nine-point $IV$-optimal exact (left) and robust exact (right) designs for a second-order model in two factors. Numbers represent the number of replications.

6.1.4. The 10-Point Design: For ten design points, the $IV$-optimal robust design is the same as the exact design generated by a genetic algorithm in Borkowski (2003b). This design is also a central composite design with a unit axial distance, $A$-optimal exact and robust exact designs. The properties of the design have been summarized in Table 4.9.

It can be seen from Figure 4.24 that the Min $IV$ and $IV$-efficiency of the $IV$-optimal robust exact design increase as the sample size increases. When $n = 9$, the exact and robust exact designs have about the same $IV$-efficiency. This pattern is also true for the Min $A$ and $A$-efficiency. For $n = 8$ and 9, the $D$-efficiency and Min $D$ are higher in the robust exact design than in the exact design. This is also the same for the Min $G$ and $G$-efficiency. Overall, the robust exact designs constructed based on the Min $IV$ are not only robust to a missing point, but when there is no missing value, their $IV$-efficiencies are just slightly lower than those of the exact designs.

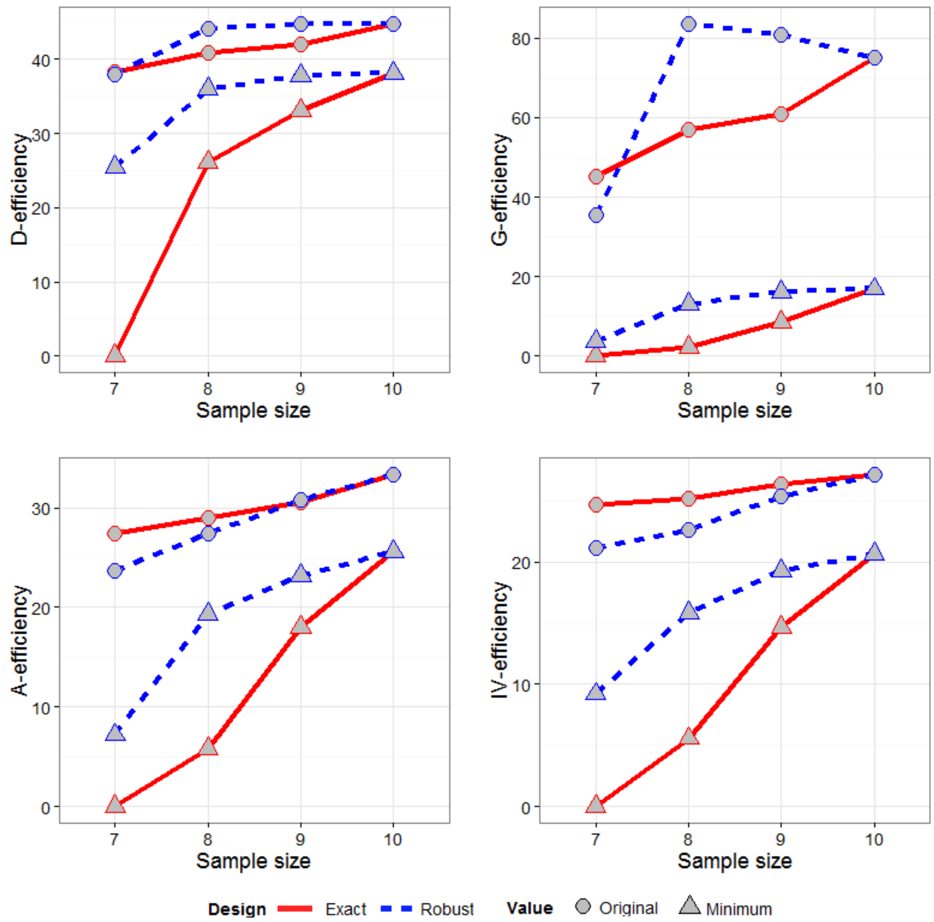



Figure 4.24: Summary of $D$-, $A$-, $G$-, $IV$-efficiencies and corresponding minimum efficiencies of two-factor $IV$-optimal exact and robust exact designs.

## 6.2. Three-Factor $IV$-Optimal Designs

Instead of sequentially describing each design size for $k = 3$, we will summarize results for $k = 3$ in Table 4.19. For $n = 11$, the Min $IV$ is improved by 4.8 while the Min $D$, Min $A$, and Min $G$ are also improved although they are not the criteria used to construct the design. However, when there is no missing point, $D$-, $A$-, and $G$-efficiencies are rather low in the robust exact design relative to the exact design. For $n = 12$, the Min $IV$ is considerably improved from 0.046% to 9.718%, and also the leave-1-out $IV$-efficiency, as well as the leave-2-out $IV$-efficiency, is greater in the robust design than in the exact design. For $n = 13$, although the number of design points is 3 more than the number of parameters in a second-order model, the Min $A$, Min $G$, and Min $IV$ are still close to zero. For this case, the robust exact design is preferable as it is much more robust to a missing point.

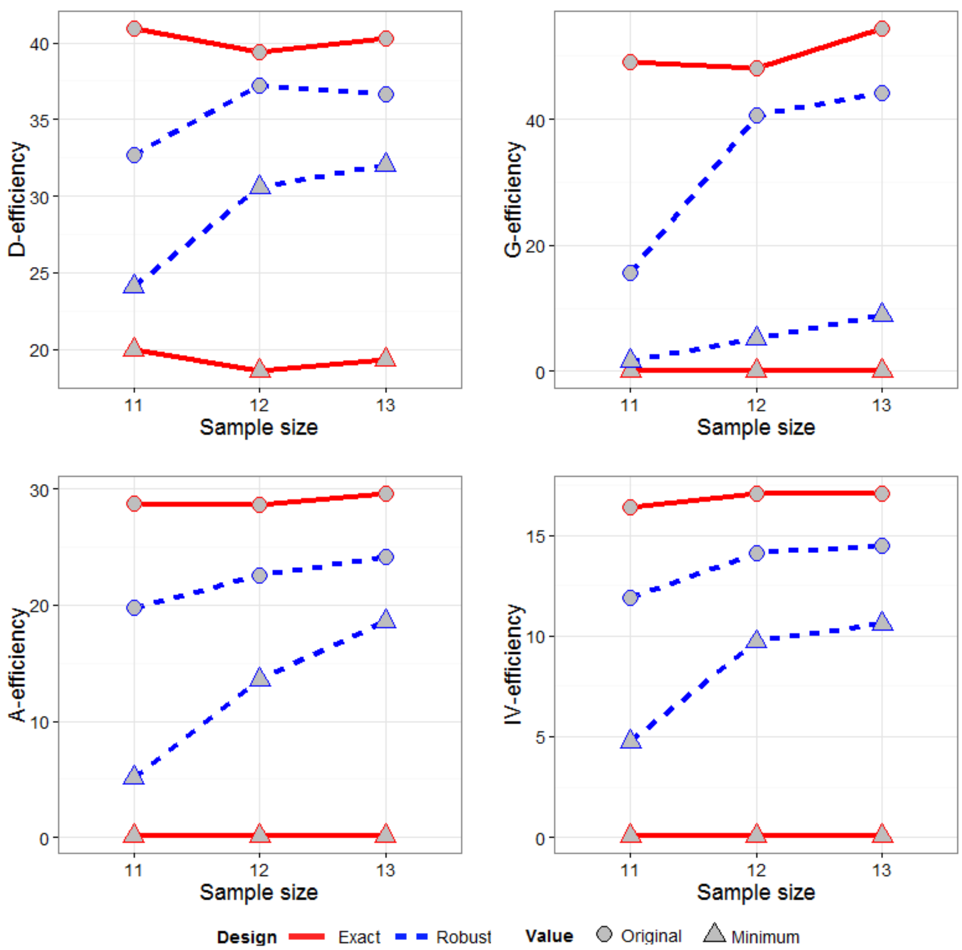



Figure 4.25: Summary of $D$-, $A$-, $G$-, $IV$-efficiencies and corresponding minimum efficiencies of three-factor $IV$-optimal exact and robust exact designs.

Table 4.19: Properties of the 3-factor $IV$-optimal designs for $n = 11$, 12, and 13.

| | 11-point $IV$-optimal | | 12-point $IV$-optimal | | 13-point $IV$-optimal | |
|---|---|---|---|---|---|---|
| Criteria Evaluated | Exact Design | Robust Design | Exact Design | Robust Design | Exact Design | Robust Design |
| $D$-efficiency | 40.969 | 32.716 | 39.435 | 37.196 | 40.272 | 36.643 |
| Min $D$-efficiency | 19.951 | 24.082 | 18.571 | 30.581 | 19.314 | 32.030 |
| Leave-1-out $D$-efficiency | 29.470 | 27.225 | 30.386 | 33.486 | 34.726 | 34.082 |
| | (8.302) | (2.617) | (8.518) | (1.885) | (7.262) | (1.275) |
| Leave-2-out $D$-efficiency | | | 9.413 | 26.477 | 27.086 | 30.521 |
| | | | (14.561) | (5.663) | (10.789) | (2.482) |
| $A$-efficiency | 28.734 | 19.796 | 28.623 | 22.613 | 29.669 | 24.123 |
| Min $A$-efficiency | 0.131 | 5.120 | 0.078 | 13.601 | 0.124 | 18.622 |
| Leave-1-out $A$-efficiency | 8.720 | 9.308 | 12.660 | 16.272 | 19.684 | 19.601 |
| | (8.506) | (3.083) | (10.403) | (2.518) | (9.585) | (1.127) |
| Leave-2-out $A$-efficiency | | | 2.842 | 7.461 | 10.312 | 13.633 |
| | | | (5.930) | (4.901) | (9.063) | (3.958) |
| $G$-efficiency | 49.196 | 15.609 | 48.033 | 40.589 | 54.504 | 44.206 |
| Min $G$-efficiency | 0.029 | 1.729 | 0.021 | 5.171 | 0.020 | 8.986 |
| Leave-1-out $G$-efficiency | 9.590 | 5.412 | 14.555 | 15.633 | 23.969 | 21.603 |
| | (15.858) | (3.696) | (19.228) | (9.431) | (21.643) | (10.421) |
| Leave-2-out $G$-efficiency | | | 2.686 | 5.582 | 9.367 | 11.591 |
| | | | (8.172) | (5.913) | (12.940) | (6.599) |
| $IV$-efficiency | 16.410 | 11.883 | 17.106 | 14.105 | 17.078 | 14.498 |
| Min $IV$-efficiency | 0.067 | 4.772 | 0.046 | 9.718 | 0.068 | 10.610 |
| Leave-1-out $IV$-efficiency | 5.294 | 5.901 | 7.764 | 10.254 | 11.596 | 11.905 |
| | (4.765) | (1.730) | (6.147) | (1.274) | (5.394) | (0.794) |
| Leave-2-out $IV$-efficiency | | | 1.723 | 4.806 | 6.155 | 8.353 |
| | | | (3.521) | (3.080) | (5.299) | (2.404) |

Numbers in parentheses represent standard deviations

As shown in Figure 4.25, the Min $IV$ is considerably improved when using the robust exact design instead of the exact design for all sample sizes. Without a missing points, the $IV$-efficiency of the robust exact design is at most 4.5 less than that of the robust design. The patters of the Min $A$ and $A$-efficiency are similar to those of the Min $IV$ and $IV$-efficiency. When $n = 11$ corresponding to the smallest design in the study, most criteria of the robust exact design are very low compared to the exact design, and when $n$ increases from 11 to 12, the minimum of $D$-, $A$-, and $IV$-efficiencies noticeably increases.

## 7. Conclusions and Comments

The Min $D$, Min $A$, Min $G$, and Min $IV$-efficiencies of two-factor and three-factor optimal robust exact designs are summarized in Table 4.20 and 4.21, respectively. Each optimal robust exact design will have 100% relative efficiency for its corresponding criterion, but it can be evaluated by other criteria to see how the design far by the other criteria. Inspection of Tables 4.20 and 4.21 reveals that Min $D$ and Min $G$ criteria, as well as Min $A$ and Min $IV$ criteria, are highly correlated. This means that if one criterion is high (low) in the $D$-optimal robust exact design, the same criterion will be high (low) in the $G$-optimal robust exact design, and this is similar for $A$- and $IV$-optimal robust exact designs.

The $G$-optimal robust exact designs are the most time-consuming because the Min $G$ criterion itself seems to be too “rough” to optimize. Probably, using a grid search with the point-exchanging algorithm is not a very good method to find the best Min $G$ design. We had run $G$-optimal robust designs for several times, but different runs did not agree on Min $G$’s while other optimal robust designs are.

Table 4.20: Summary of two-factor robust exact designs.

| | | Efficiencies | | | | Relative Efficiencies | | | |
|---|---|---|---|---|---|---|---|---|---|
| $N$ | Criteria | Min $D$ | Min $A$ | Min $G$ | Min $IV$ | Min $D$ | Min $A$ | Min $G$ | Min $IV$ |
| 7 | Min $D$ | 31.576 | 4.565 | 8.125 | 3.635 | 100 | 45.787 | 86.778 | 39.442 |
| | Min $A$ | 23.627 | 9.970 | 4.573 | 6.846 | 74.826 | 100 | 48.841 | 74.284 |
| | Min $G$ | 31.435 | 4.868 | 9.363 | 3.643 | 99.553 | 48.826 | 100 | 39.529 |
| | Min $IV$ | 25.409 | 7.221 | 3.709 | 9.216 | 80.469 | 72.427 | 39.613 | 100 |
| 8 | Min $D$ | 38.515 | 16.590 | 17.143 | 11.681 | 100 | 85.568 | 93.397 | 73.660 |
| | Min $A$, $IV$ | 35.938 | 19.388 | 13.095 | 15.858 | 93.309 | 100 | 71.343 | 100 |
| | Min $G$ | 36.872 | 14.056 | 18.355 | 9.753 | 95.934 | 72.498 | 100 | 61.502 |
| 9 | Min $D$ | 39.581 | 22.500 | 18.104 | 16.726 | 100 | 95.843 | 75.481 | 86.731 |
| | Min $A$ | 38.327 | 23.476 | 16.241 | 16.706 | 96.832 | 100 | 67.713 | 86.627 |
| | Min $G$ | 37.421 | 12.672 | 23.985 | 9.583 | 94.543 | 53.979 | 100 | 49.691 |
| | Min $IV$ | 37.733 | 23.182 | 16.017 | 19.285 | 95.331 | 98.748 | 66.779 | 100 |
| 10 | Min $D$ | 40.404 | 14.383 | 28.177 | 10.340 | 100 | 56.263 | 90.060 | 50.019 |
| | Min $A$, $IV$ | 38.125 | 25.564 | 16.915 | 20.672 | 94.359 | 100 | 54.064 | 100 |
| | Min $G$ | 39.551 | 13.395 | 31.287 | 10.117 | 97.889 | 52.398 | 100 | 48.941 |

Table 4.21: Summary of three-factor robust exact designs.

| | | Efficiencies | | | | Relative Efficiencies | | | |
|---|---|---|---|---|---|---|---|---|---|
| $N$ | Criteria | Min $D$ | Min $A$ | Min $G$ | Min $IV$ | Min $D$ | Min $A$ | Min $G$ | Min $IV$ |
| 11 | Min $D$ | 34.823 | 5.600 | 6.212 | 3.380 | 100 | 65.975 | 83.472 | 70.830 |
| | Min $A$ | 22.511 | 8.488 | 2.585 | 4.330 | 64.644 | 100 | 34.735 | 90.738 |
| | Min $G$ | 32.313 | 4.801 | 7.442 | 1.411 | 92.792 | 56.562 | 100 | 29.568 |
| | Min $IV$ | 24.082 | 5.120 | 1.729 | 4.772 | 69.155 | 60.320 | 23.233 | 100 |
| 12 | Min $D$ | 38.974 | 7.731 | 10.140 | 3.506 | 100 | 51.671 | 77.334 | 36.077 |
| | Min $A$ | 33.023 | 14.962 | 5.226 | 7.500 | 84.731 | 100 | 39.857 | 77.176 |
| | Min $G$ | 38.227 | 8.416 | 13.390 | 3.077 | 97.452 | 61.068 | 100 | 68.780 |
| | Min $IV$ | 30.581 | 13.601 | 5.171 | 9.718 | 78.465 | 90.904 | 39.437 | 100 |
| 13 | Min $D$ | 40.259 | 12.425 | 12.868 | 5.851 | 100 | 66.112 | 84.259 | 55.146 |
| | Min $A$ | 33.747 | 18.794 | 8.716 | 10.010 | 83.825 | 100 | 57.072 | 93.350 |
| | Min $G$ | 38.226 | 8.125 | 15.856 | 3.273 | 85.355 | 39.151 | 100 | 30.848 |
| | Min $IV$ | 32.030 | 18.622 | 8.986 | 10.610 | 79.560 | 99.622 | 56.673 | 100 |

# CHAPTER 5

# OPTIMAL ROBUST EXACT MIXTURE DESIGNS

## 1. Impacts of a Missing Point on Standard Mixture Designs

The simple lattice designs and simplex centroid designs are commonly used in a mixture experiment. In this section, their robustness against a missing trial will be investigated.

### 1.1. Examples of Simplex Lattice Designs

The smallest simplex lattice design which can be used to fit the second-order mixture model is the SLD$\{3, 2\}$ having six distinct design points. Because the number of design points equals the number of parameters, a missing point cannot happen in the design. For $m = 3$, the SLD$\{3, 3\}$ contains design points $(1, 0, 0)$, $(0, 1, 0)$, $(0, 0, 1)$, $(\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$, $(\frac{2}{3}, \frac{1}{3}, 0)$, $(\frac{1}{3}, \frac{2}{3}, 0)$, $(\frac{2}{3}, 0, \frac{1}{3})$, $(\frac{1}{3}, 0, \frac{2}{3})$, $(0, \frac{2}{3}, \frac{1}{3})$, and $(0, \frac{1}{3}, \frac{2}{3})$. Suppose we use this design to fit the second-order model having six parameters. The $D$-efficiency is 22.370, and if one of the vertices is missing, the $D$-efficiency will drop to 17.315. If a non-vertex point is missing, the $D$-efficiency will be greater than 17.315. Thus, this design is rather robust to a missing point in terms of the precision of parameter estimation. The SLD$\{3, 3\}$ has $G$-efficiency of 67.742, but its $G$-efficiency will drop to only 8.602 if one of the vertices is lost. Its leave-1-out $G$-efficiency is 45.767 with a standard deviation of 26. Generally, the prediction made at a missing point will be very poor.

The number of design points in the SLD$\{q, m\}$ is $n = (q + m - 1)1/[m!(q - 1)1]$; thus, as $m$ increases $n$ increases quickly. For example, the SLD$\{3, m\}$, $m = 3, 4, 5, 6$, and 7 have $n$ of 10, 15, 21, 28, and 36, respectively. For four-component mixture designs, the smallest design able to fit the second-order model is the SLD$\{4, 2\}$ having 10 design points which equals the number of parameters in the model. The numbers of design points for the SLD$\{4, m\}$, $m = 3, 4, 5, 6$, and 7 are $20, 35, 56, 84$, and 120, respectively. It is seen that the number of design points of the SLDs is usually much larger than the number of parameters, thus SLDs seem be more robust to one or more missing values.

## 1.2. Examples of Simplex Centroid Designs

Simplex centroid designs were discussed in Chapter 1, Section 3.7. The number of distinct design points for 3-, 4-, 5-, and 6-component mixture designs are 7, 15, 31, and 63, respectively. The robustness of these designs against a missing value in terms of $D$- and $G$-efficiencies is respectively summarized in Tables 5.1 and 5.2 where $p$ is the number of parameters to be fitted in a second-order model and $q$ is the number of components. As $q$ increases, the number of design points, $n$, increases rapidly compared to $p$, so the effect of a missing point on the precision of parameter estimations will lessen when $q$ increases. The differences between the $D$-efficiencies and Min $D$'s and $D$-efficiencies and leave-1-out $D$ get smaller as $q$ increases. This is also the case for the $G$-efficiency.

Table 5.1: $D$-efficiencies of simplex centroid designs.

| $q$ | $n$ | $p$ | Efficiencies | | |
|---|---|---|---|---|---|
| | | | $D$ | Leave-1-out $D$ (s.d.) | Minimum $D$ |
| 3 | 7 | 6 | 24.600 | 17.884 (5.315) | 12.719 |
| 4 | 15 | 10 | 14.224 | 12.960 (1.708) | 10.444 |
| 5 | 31 | 15 | 7.692 | 7.462 (0.480) | 6.472 |
| 6 | 63 | 21 | 4.262 | 4.218 (0.138) | 3.831 |

Table 5.2: $G$-efficiencies of simplex centroid designs.

| $q$ | $n$ | $p$ | Efficiencies | | |
|---|---|---|---|---|---|
| | | | $G$ | Leave-1-out $G$ (s.d.) | Minimum $G$ |
| 3 | 7 | 6 | 86.369 | 20.524 (35.646) | 0.763 |
| 4 | 15 | 10 | 68.226 | 33.532 (29.981) | 1.671 |
| 5 | 31 | 15 | 50.709 | 35.796 (19.054) | 2.400 |
| 6 | 63 | 21 | 36.083 | 31.069 (10.137) | 2.794 |

## 2. $D$-Optimal Robust Exact Mixture Designs

### 2.1. Three-Component $D$-Optimal Mixture Designs

To construct $D$-optimal robust exact mixture designs, we applied criterion (4.1) previously proposed in Chapter 4, Section 3. The SLD$\{3, 100\}$ and SLD$\{3, 20\}$ are respectively used as support sets to construct $D$-optimal exact and robust exact designs. The coarser grid was used to construct robust exact designs. Although it is not a very time-consuming task for the Min $D$ criterion with support SLD$\{3, 100\}$, it is for Min $G$ and Min $IV$ which could take a few hours for only one try. The resulting designs should be consistent, based on the same set of candidate points across all criteria. Accordingly, the SLD$\{3, 20\}$ will be used for constructing all three-component robust exact designs. A Matlab program (MATLAB, 2014) was written to generate robust exact designs while exact designs were generated by the OPTEX procedure in SAS software (SAS Institute Inc., 2013). The sample sizes in the study are 7, 8, 9, and 10.

2.1.1. The 7-Point Design: As shown in Figure 5.1, the exact design is the SLD$\{3, 2\}$. Two points are replicated at $(1, 0, 0)$. However, the exact design is not unique since designs with an additional replicate either at vertices or middles of the

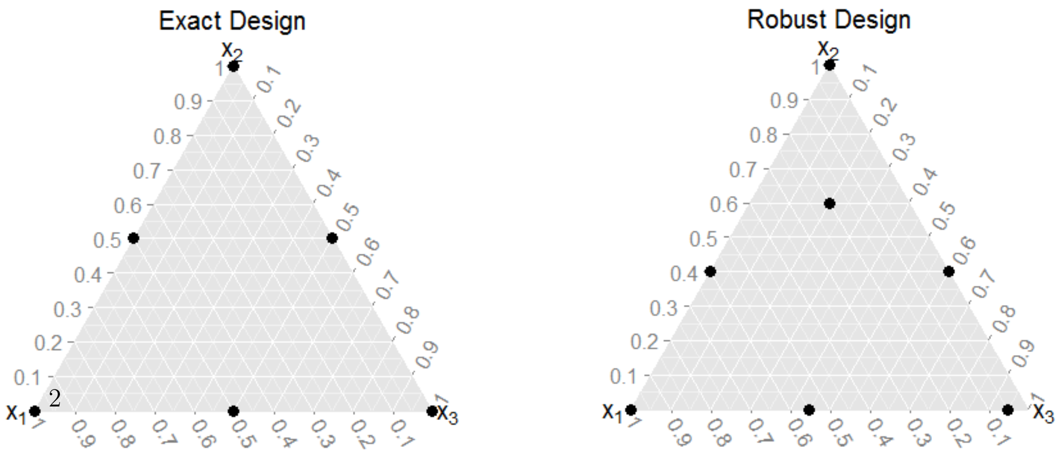



Figure 5.1: Seven-point three-component $D$-optimal exact (left) and robust exact (right) mixture designs for a second-order Scheffé polynomial. Numbers represent the number of replications.

edges have the same $D$-efficiency. The resulting robust design contains points $(1, 0, 0)$, $(0, 1, 0)$, $(.05, 0, .95)$, $(.6, .4, 0)$, $(0, .4, .6)$, $(.55, 0, .45)$, and interior point $(.2, .6, .2)$.

Other alphabetic optimality criteria are also evaluated for both designs as summarized in Table 5.3. The Min $D$, as well as the leave-1-out, is relatively higher in the robust exact design than in the exact design. Losing one of any unreplicated design points in the exact design leads to a $D$-efficiency of zero. The Min $D$ increases from 0 to 14.3, and the $D$-efficiency slightly decreases from 25.5 to 22.8 when using the robust exact mixture design instead of the exact mixture design. The leave-1-out $D$-, $A$- and $IV$-efficiencies are also improved even though they were not used to construct the design. Overall, the robust exact mixture design has higher values of many criteria compared to the exact design.

Table 5.3: Properties of the 7-point 3-component $D$-optimal mixture designs.

| Criteria Evaluated | 7-point $D$-optimal Exact Design on SLD$\{3, 100\}$ | 7-point $D$-optimal Robust Design on SLD$\{3, 20\}$ |
|---|---|---|
| $D$-efficiency | 25.454 | 22.792 |
| Min $D$-efficiency | 0.000 | *14.291* |
| Leave-1-out $D$-efficiency | 7.559 | 17.198 |
| | (12.910) | (3.997) |
| $A$-efficiency | 11.823 | 11.307 |
| Min $A$-efficiency | 0.000 | 1.062 |
| Leave-1-out $A$-efficiency | 3.810 | 4.767 |
| | (6.506) | (3.441) |
| $G$-efficiency | 85.714 | 63.777 |
| Min $G$-efficiency | 0.000 | 1.863 |
| Leave-1-out $G$-efficiency | 28.571 | 16.364 |
| | (48.795) | (25.347) |
| $IV$-efficiency | 23.007 | 25.609 |
| Min $IV$-efficiency | 0.000 | 2.396 |
| Leave-1-out $IV$-efficiency | 7.459 | 11.057 |
| | (12.738) | (6.764) |

Numbers in parentheses represent standard deviations

2.1.2. The 8-Point Design: The exact design contains the SLD$\{3, 2\}$ points and an additional replicate at two of these points. Figure 5.2 (left) illustrates an example of the exact mixture design having an additional replicate point at $(0, 1, 0)$ and $(0, 0, 1)$. Losing any unreplicated point will cause a decrease in the $D$-efficiency to zero. The robust exact design puts a single point at all vertices, $(.3, 0, .7)$, $(.7, 0, .3)$, $(.6, .4, 0)$, $(0, .4, .6)$, and interior point $(.15, .7, .15)$. It is seen that the robust mixture design does not replicate any points.

Table 5.4 shows comparisons of criteria evaluated for both exact and robust exact mixture designs. The $D$-efficiency is slightly lower in the robust design than in the exact design, but the Min $D$ is considerably higher in the robust design. With an arbitrary missing point, the robust exact design is uniformly superior to the exact

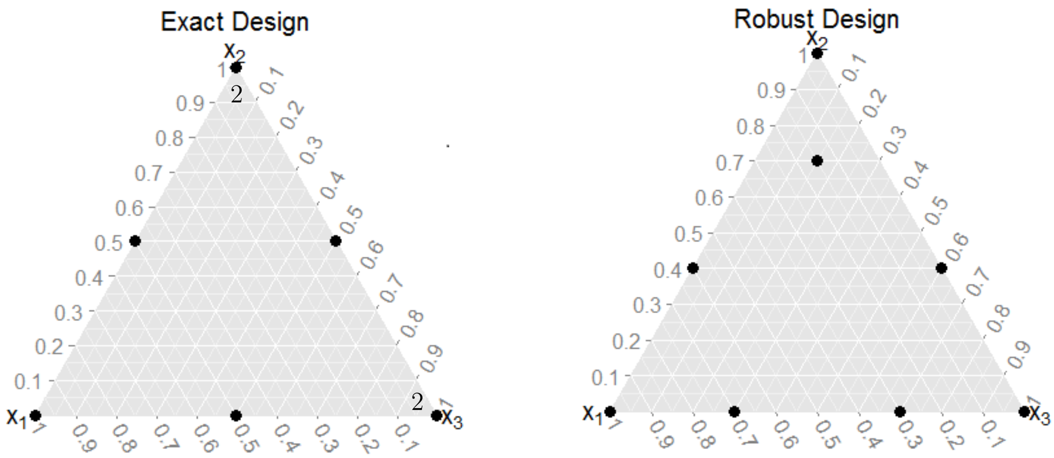



Figure 5.2: Eight-point three-component $D$-optimal exact (left) and robust exact (right) mixture designs for a second-order Scheffé polynomial. Numbers represent the number of replications.

design as it has higher Min $D$, leave-1-out, and leave-2-out values. Note that criteria related to the $IV$-optimality indicate the robust exact design has a higher average precision of predictions than the exact design.

Table 5.4: Properties of the 8-point 3-component $D$-optimal mixture designs.

| Criteria Evaluated | 8-point $D$-optimal | |
|---|---|---|
| | Exact Design on SLD$\{3,100\}$ | Robust Design on SLD$\{3,20\}$ |
| $D$-efficiency | 25.000 | 22.591 |
| Min $D$-efficiency | 0.000 | *16.884* |
| Leave-1-out $D$-efficiency | 12.727 | 19.559 |
| | (13.606) | (2.889) |
| Leave-2-out $D$-efficiency | 3.780 | 12.472 |
| | (9.428) | (7.373) |

Table 5.4 (continued)

| Criteria Evaluated | 8-point $D$-optimal Exact Design on SLD$\{3,100\}$ | 8-point $D$-optimal Robust Design on SLD$\{3,20\}$ |
|---|---|---|
| $A$-efficiency | 10.714 | 10.703 |
| Min $A$-efficiency | 0.000 | 4.085 |
| Leave-1-out $A$-efficiency | 5.911 | 7.191 |
| | (6.320) | (2.780) |
| Leave-2-out $A$-efficiency | 1.905 | 3.355 |
| | (4.751) | (2.911) |
| $G$-efficiency | 75.000 | 79.503 |
| Min $G$-efficiency | 0.000 | 7.273 |
| Leave-1-out $G$-efficiency | 42.857 | 29.214 |
| | (45.816) | (28.441) |
| Leave-2-out $G$-efficiency | 14.286 | 9.580 |
| | (35.635) | (15.931) |
| $IV$-efficiency | 20.716 | 23.959 |
| Min $IV$-efficiency | 0.000 | 9.436 |
| Leave-1-out $IV$-efficiency | 11.504 | 16.714 |
| | (12.298) | (5.208) |
| Leave-2-out $IV$-efficiency | 3.729 | 8.274 |
| | (9.303) | (6.303) |

Numbers in parentheses represent standard deviations

2.1.3. The 9-Point Design: It is seen from Figure 5.3, both exact and robust exact mixture designs have no interior points. The exact design contains the SLD$\{3,2\}$ points, and an additional replicated point can be added for any three SLD$\{3,2\}$ points. Thus, the $D$-optimal exact design is not unique. Figure 5.3 (left) gives an example of the exact design with an additional replicate at vertices. In Figure 5.3 (right), distinct design points of the robust exact design are "systematically" distributed over a boundary of the triangle. The lengths between points $(0,1,0)$ and $(0,.8,.2)$, $(0,.8,.2)$ and $(0,.4,.6)$, and $(0,.4,.6)$ and $(0,0,1)$ are .2, 4, and .4, respectively. This is the same for the other sides of the triangle.

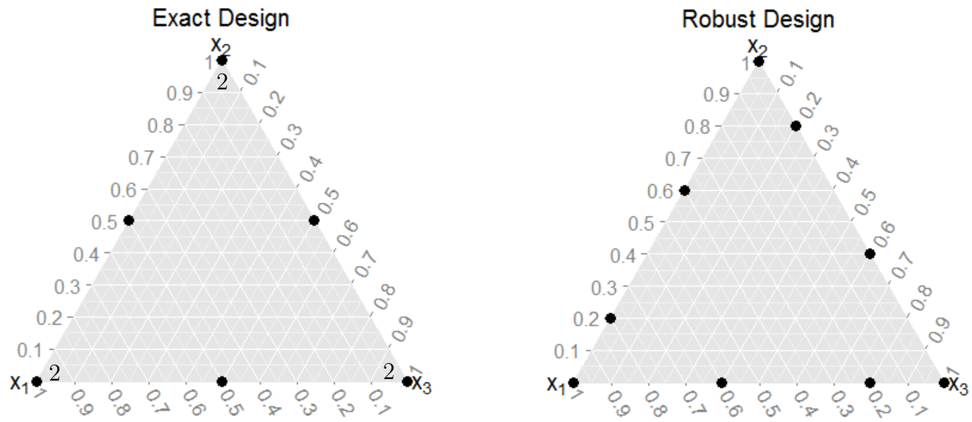



Figure 5.3: Nine-point three-component $D$-optimal exact (left) and robust exact (right) mixture designs for a second-order Scheffé polynomial. Numbers represent the number of replications.

Like 7- and 8-point $D$-optimal designs, losing one of the unreplicated points in the exact design causes a $D$-efficiency of zero. Table 5.5 shows that the robust exact mixture design is much more robust to a missing point than the exact design as the Min $D$ increases from 0 to 18.9%. The leave-1-out and leave-2-out $D$-efficiencies are also improved. Other criteria not being used to construct the designs are evaluated and show that the $D$-optimal robust exact design is superior to the exact design in terms of all criteria related to $A$- and $IV$-optimality.

Table 5.5: Properties of the 9-point 3-component $D$-optimal mixture designs.

| Criteria Evaluated | 9-point $D$-optimal | |
|---|---|---|
| | Exact Design on SLD$\{3, 100\}$ | Robust Design on SLD$\{3, 20\}$ |
| $D$-efficiency | 24.944 | 22.477 |
| Min $D$-efficiency | 0.000 | *18.949* |
| Leave-1-out $D$-efficiency | 16.667 | 20.695 |
| | (12.500) | (1.818) |
| Leave-2-out $D$-efficiency | 8.485 | 16.630 |
| | (12.170) | (5.956) |

Table 5.5 (continued)

| Criteria Evaluated | 9-point $D$-optimal Exact Design on SLD$\{3, 100\}$ | 9-point $D$-optimal Robust Design on SLD$\{3, 20\}$ |
|---|---|---|
| $A$-efficiency | 9.877 | 10.246 |
| Min $A$-efficiency | 0.000 | 6.542 |
| Leave-1-out $A$-efficiency | 7.143 | 8.258 |
| | (5.357) | (1.814) |
| Leave-2-out $A$-efficiency | 3.941 | 5.643 |
| | (5.652) | (3.055) |
| $G$-efficiency | 66.667 | 81.009 |
| Min $G$-efficiency | 0.000 | 16.135 |
| Leave-1-out $G$-efficiency | 50.000 | 36.104 |
| | (37.500) | (23.898) |
| Leave-2-out $G$-efficiency | 28.571 | 20.931 |
| | (40.979) | (19.678) |
| $IV$-efficiency | 18.964 | 22.093 |
| Min $IV$-efficiency | 0.000 | 13.791 |
| Leave-1-out $IV$-efficiency | 13.810 | 18.211 |
| | (10.358) | (3.591) |
| Leave-2-out $IV$-efficiency | 7.669 | 12.731 |
| | (11.000) | (6.618) |

Numbers in parentheses represent standard deviations

2.1.4. The 10-Point Design: Similar to previous $D$-optimal exact mixture designs, the 10-point exact design contains the SLD$\{3, 2\}$ points and two replicates at any four different SLD$\{3, 2\}$ points. Figure 5.4 (left) shows an example of the $D$-optimal design where an additional point is added to each vertex and point $(0, .5, .5)$. Design points of the robust exact design are $(1, 0, 0)$, two $(0, 1, 0)$'s, $(0, 0, 1)$, $(.45, .55, 0)$, $(0, .55, .45)$, $(0, .15, .85)$, $(.85, .15, 0)$, $(.5, 0, .5)$, and $(.4, .2, .4)$. It is also seen that design points of both designs are vertically symmetric. For the exact design, losing either unreplicated point $(.5, 0, .5)$ or $(.5, .5, 0)$ results in a $D$-efficiency of zero (or Min $D$).

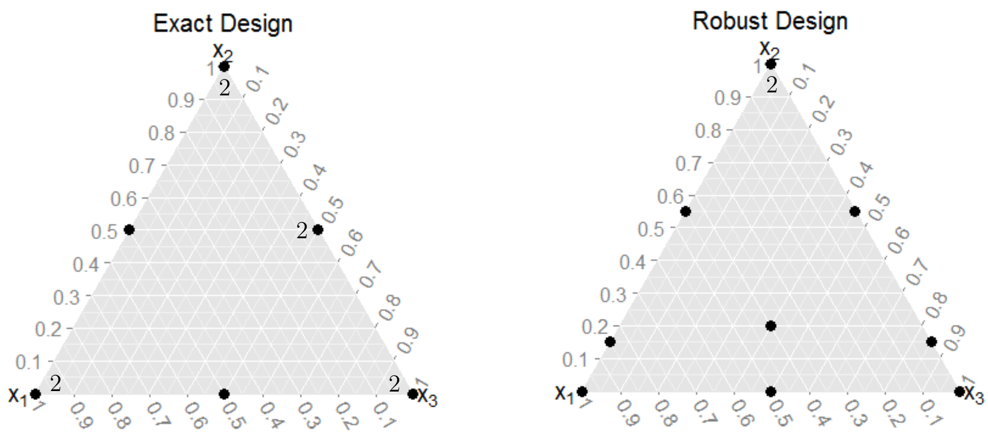



Figure 5.4: Ten-point three-component $D$-optimal exact (left) and robust exact (right) mixture designs for a second-order Scheffé polynomial. Numbers represent the number of replications.

The properties of the exact and robust exact designs are summarized in Table 5.6. Although the $D$-efficiency is slightly lower in the resulting robust exact design, its Min $D$ is much higher. The leave-1-out and leave-2-out $D$-efficiencies of the robust exact design are improved, and this indicates that the robust design is not only more robust to a missing point, but also robust to any two missing points.

Table 5.6: Properties of the 10-point 3-component $D$-optimal mixture designs.

| Criteria Evaluated | 10-point $D$-optimal | |
|---|---|---|
| | Exact Design on SLD$\{3, 100\}$ | Robust Design on SLD$\{3, 20\}$ |
| $D$-efficiency | 25.198 | 22.687 |
| Min $D$-efficiency | 0.000 | *19.420* |
| Leave-1-out $D$-efficiency | 19.955 | 21.332 |
| | (10.517) | (1.727) |
| Leave-2-out $D$-efficiency | 13.333 | 18.800 |
| | (12.613) | (4.381) |

Table 5.6 (continued)

| Criteria Evaluated | 10-point $D$-optimal | |
|---|---|---|
| | Exact Design on SLD$\{3, 100\}$ | Robust Design on SLD$\{3, 20\}$ |
| $A$-efficiency | 10.435 | 10.247 |
| Min $A$-efficiency | 0.000 | 5.346 |
| Leave-1-out $A$-efficiency | 8.642 | 8.822 |
| | (4.583) | (2.306) |
| Leave-2-out $A$-efficiency | 6.057 | 6.724 |
| | (5.750) | (3.404) |
| $G$-efficiency | 60.000 | 75.545 |
| Min $G$-efficiency | 0.000 | 17.557 |
| Leave-1-out $G$-efficiency | 53.333 | 43.770 |
| | (28.109) | (25.193) |
| Leave-2-out $G$-efficiency | 40.000 | 28.593 |
| | (37.839) | (24.428) |
| $IV$-efficiency | 20.121 | 23.048 |
| Min $IV$-efficiency | 0.000 | 12.671 |
| Leave-1-out $IV$-efficiency | 16.750 | 19.988 |
| | (8.893) | (4.787) |
| Leave-2-out $IV$-efficiency | 11.789 | 15.429 |
| | (11.200) | (7.340) |

Numbers in parentheses represent standard deviations

Figure 5.5 shows summary plots of all criteria comparing $D$-optimal exact and robust exact mixture designs versus the sample sizes. It is seen that the Min $D$'s of the exact designs are zero, and they are considerably improved in the robust exact designs. The Min $D$ and Min $G$ of the robust exact design seem to increase as the sample size increases. Without a missing value, both designs have about the same $A$-efficiency.

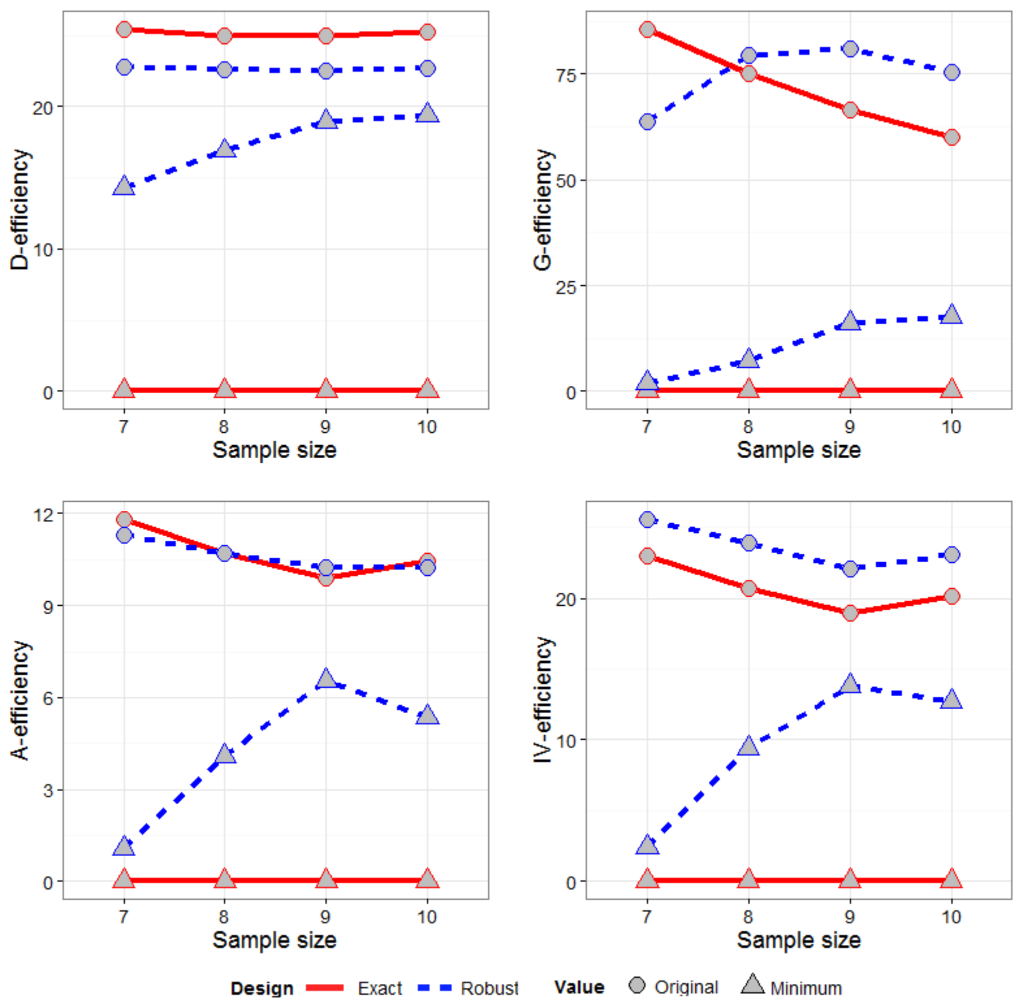



Figure 5.5: Summary of $D$-, $A$-, $G$-, $IV$-efficiencies and corresponding minimum efficiencies of three-component $D$-optimal exact and robust exact mixture designs.

## 2.2. Four-Component $D$-Optimal Mixture Designs

The $D$-optimal exact mixture designs were generated by the OPTEX procedure in SAS software (SAS Institute Inc., 2013). Because the SLD$\{4, 50\}$ was used as a support, the $i$th component has values $x_i = 0, \frac{1}{50}, \frac{2}{50}, \ldots, \frac{49}{50}, 1$, for $i = 1, 2, 3, 4$. With the constraint $\sum_{i=1}^{4} x_i = 1$, the number of points in the support is $(4+50-1)!/[4!(50-1)!] = 23,426$. The robust exact mixture designs use a coarser grid, SLD$\{4, 20\}$, for constructing designs. This support itself does not contain too many distinct points, but optimizing criterion (4.1) is a computationally expensive task, so the coarser grid was used for robust exact designs. Matlab programs (MATLAB, 2014) were written to generate robust exact designs, and the sample sizes in the study are 11, 12, 13, and 14.

2.2.1. The 11-Point Design: The resulting robust exact mixture design points are tabulated in Table 5.8. The exact and robust exact designs contain the ten SLD$\{4,2\}$ points. The exact design, however, puts one more replicate at $(1,0,0,0)$ while the robust exact design puts the last point at the centroid of the design. However, the exact design is not unique because the replicated point can be placed on any of the SLD$\{4,2\}$ points.

Table 5.7: Properties of the 11-point 4-component $D$-optimal mixture designs.

| Criteria Evaluated | 11-point $D$-optimal | |
|---|---|---|
| | Exact Design on SLD$\{4,50\}$ | Robust Design on SLD$\{4,20\}$ |
| $D$-efficiency | 16.964 | 16.413 |
| Min $D$-efficiency | 0.000 | *11.487* |
| Leave-1-out $D$-efficiency | 3.166 | 12.957 |
| | (7.043) | (1.698) |
| $A$-efficiency | 5.865 | 5.902 |
| Min $A$-efficiency | 0.000 | 1.015 |
| Leave-1-out $A$-efficiency | 1.136 | 1.862 |
| | (2.528) | (1.493) |
| $G$-efficiency | 90.909 | 91.908 |
| Min $G$-efficiency | 0.000 | 1.099 |
| Leave-1-out $G$-efficiency | 18.182 | 11.970 |
| | (40.452) | (29.245) |

Table 5.7 (continued)

| Criteria Evaluated | 11-point $D$-optimal Exact Design on SLD$\{4,50\}$ | 11-point $D$-optimal Robust Design on SLD$\{4,20\}$ |
|---|---|---|
| $IV$-efficiency | 17.441 | 20.007 |
| Min $IV$-efficiency | 0.000 | 5.572 |
| Leave-1-out $IV$-efficiency | 3.437 | 6.937 |
| | (7.646) | (3.974) |

Numbers in parentheses represent standard deviations

Table 5.7 summarizes criteria being evaluated for $D$-optimal exact and robust exact designs. The $D$-efficiency of the exact design will drop to zero if one of the unreplicated points is missing while the Min $D$ of the robust exact design is as high as 11.5. The leave-1-out $D$-efficiency is considerably improved from 3.17 to 12.96. Overall, the robust exact design is near $D$-optimal, but it is much more robust to a missing point in terms of precision of parameter estimation. Note that $A$-, $G$-, and $IV$-efficiencies are also higher in the robust design than in the exact design.

2.2.2. The 12-Point Design: The robust exact design contains the SLD$\{4,2\}$ points with any two different SLD$\{4,2\}$ points. In Table 5.8, for example, the design has two replicates at $(0,0,1,0)$ and $(0,0,0,1)$. For the robust exact design, the design points are tabulated in Table 5.8. The robust exact design consists of unreplicated vertices, distinct points on the edges of the design region, and one interior point; but, those edge points are not centered.

Table 5.8: Design points of 4-component $D$-optimal robust exact mixture designs for $n = 11$, 12, 13, and 14.

| Point Types | $n = 11$ | | | | $n = 12$ | | | | $n = 13$ | | | | $n = 14$ | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | $x_1$ | $x_2$ | $x_3$ | $x_4$ | $x_1$ | $x_2$ | $x_3$ | $x_4$ | $x_1$ | $x_2$ | $x_3$ | $x_4$ | $x_1$ | $x_2$ | $x_3$ | $x_4$ |
| Vertices | 1 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 1 | 0 | 0 | 0 |
| | 0 | 1 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 1 | 0 | 0 |
| | 0 | 0 | 1 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 1 | 0 |
| | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 1 |
| Edges | .5 | .5 | 0 | 0 | .55 | 0 | .45 | 0 | .5 | .5 | 0 | 0 | .5 | 0 | .5 | 0 |
| | .5 | 0 | .5 | 0 | .55 | 0 | 0 | .45 | .5 | 0 | 0 | .5 | .5 | 0 | 0 | .5 |
| | .5 | 0 | 0 | .5 | 0 | 0 | .45 | .55 | 0 | .5 | .5 | 0 | 0 | 0 | .5 | .5 |
| | 0 | .5 | .5 | 0 | 0 | .35 | .65 | 0 | 0 | 0 | .5 | .5 | .75 | .25 | 0 | 0 |
| | 0 | .5 | 0 | .5 | 0 | .35 | 0 | .65 | .65 | 0 | .35 | 0 | 0 | .25 | 0 | .75 |
| | 0 | 0 | .5 | .5 | .6 | .4 | 0 | 0 | .35 | 0 | .65 | 0 | 0 | .25 | .75 | 0 |
| | | | | | 0 | .6 | .4 | 0 | 0 | .35 | 0 | .65 | 0 | .6 | .4 | 0 |
| | | | | | | | | | 0 | .65 | 0 | .35 | .4 | .6 | 0 | 0 |
| | | | | | | | | | | | | | 0 | .7 | 0 | .3 |
| Interiors | .25 | .25 | .25 | .25 | .25 | .3 | .2 | .25 | .25 | .25 | .25 | .25 | | | | |
| Faces | | | | | | | | | | | | | .33 | 0 | .33 | .34 |

Table 5.9: Properties of the 12-point 4-component $D$-optimal mixture designs.

| Criteria Evaluated | 12-point $D$-optimal Exact Design on SLD$\{4, 50\}$ | 12-point $D$-optimal Robust Design on SLD$\{4, 20\}$ |
|---|---|---|
| $D$-efficiency | 16.667 | 15.527 |
| Min $D$-efficiency | 0.000 | *11.659* |
| Leave-1-out $D$-efficiency | 5.655 | 13.111 |
| | (8.353) | (1.764) |
| Leave-2-out $D$-efficiency | 1.055 | 6.457 |
| | (4.186) | (5.793) |
| $A$-efficiency | 5.556 | 5.330 |
| Min $A$-efficiency | 0.000 | 1.031 |
| Leave-1-out $A$-efficiency | 1.955 | 2.627 |
| | (2.888) | (1.762) |
| Leave-2-out $A$-efficiency | 0.379 | 0.863 |
| | (1.503) | (1.125) |
| $G$-efficiency | 83.333 | 71.110 |
| Min $G$-efficiency | 0.000 | 2.223 |
| Leave-1-out $G$-efficiency | 30.303 | 21.318 |
| | (44.761) | (32.104) |
| Leave-2-out $G$-efficiency | 6.061 | 3.960 |
| | (24.044) | (13.346) |
| $IV$-efficiency | 16.232 | 18.341 |
| Min $IV$-efficiency | 0.000 | 3.289 |
| Leave-1-out $IV$-efficiency | 5.814 | 9.820 |
| | (8.588) | (5.556) |
| Leave-2-out $IV$-efficiency | 1.146 | 3.496 |
| | (4.545) | (3.999) |

Numbers in parentheses represent standard deviations

Like other $D$-optimal exact mixture designs, losing any unreplicated points will lead to a $D$-efficiency of zero. Both robust exact and exact mixture designs are evaluated by other criteria and are summarized in Table 5.9. The Min $D$, leave-1-out and leave-2-out $D$-efficiencies are appreciably higher in the robust design than in the exact design, but their $D$-efficiencies are only slightly different. Thus, the robust design is preferable to the exact one.

2.2.3. The 13-Point Design: Like previous exact mixture designs, the 13-point exact design contains the SLD{4, 2} points and two replicates for any three different SLD{4, 2} points. The robust design points are also listed in Table 5.8. The design consists of all four vertices, eight points lying on the edges of the tetrahedron, and one point at the centroid.

Table 5.10: Properties of the 13-point 4-component *D*-optimal mixture designs.

| Criteria Evaluated | 13-point *D*-optimal | |
|---|---|---|
| | Exact Design on SLD{4, 50} | Robust Design on SLD{4, 20} |
| *D*-efficiency | 16.489 | 15.590 |
| Min *D*-efficiency | 0.000 | *12.375* |
| Leave-1-out *D*-efficiency | 7.692 | 13.771 |
| | (8.648) | (1.682) |
| Leave-2-out *D*-efficiency | 2.610 | 10.443 |
| | (6.160) | (4.432) |
| *A*-efficiency | 5.305 | 5.481 |
| Min *A*-efficiency | 0.000 | 1.479 |
| Leave-1-out *A*-efficiency | 2.564 | 3.403 |
| | (2.883) | (1.793) |
| Leave-2-out *A*-efficiency | 0.902 | 1.781 |
| | (2.130) | (1.498) |
| *G*-efficiency | 76.923 | 80.515 |
| Min *G*-efficiency | 0.000 | 3.891 |
| Leave-1-out *G*-efficiency | 38.462 | 30.386 |
| | (43.240) | (34.461) |
| Leave-2-out *G*-efficiency | 13.986 | 10.322 |
| | (33.012) | (21.468) |
| *IV*-efficiency | 15.216 | 18.929 |
| Min *IV*-efficiency | 0.000 | 4.804 |
| Leave-1-out *IV*-efficiency | 7.492 | 12.637 |
| | (8.422) | (5.911) |
| Leave-2-out *IV*-efficiency | 2.683 | 7.086 |
| | (6.334) | (5.335) |

Numbers in parentheses represent standard deviations

Table 5.10 summarizes criteria evaluated for exact and robust exact designs. It is seen that the robust exact design successfully improves the robustness against a missing observation. The $D$-efficiency slightly drops from 16.5 to 15.6, but Min $D$ increases from 0 to 12.4. The robust exact mixture design is also more robust to any two missing points than the exact design as the leave-2-out $D$-efficiency significantly increases. Also, the $A$-, $G$-, and $IV$-efficiencies are higher in the robust exact design than in the exact design.

2.2.4. The 14-Point Design: For the exact design, design points are similar to the 13-point $D$-optimal exact mixture designs. It is composed of the SLD$\{4, 2\}$ points with two replicates taken for any four different SLD$\{4, 2\}$ points. For the robust exact design, all points are on the boundary of the design region, and nine of those are lying on the edges as listed in Table 5.8.

Table 5.11: Properties of the 14-point 4-component $D$-optimal mixture designs.

| Criteria Evaluated | 14-point $D$-optimal | |
|---|---|---|
| | Exact Design on SLD$\{4, 50\}$ | Robust Design on SLD$\{4, 20\}$ |
| $D$-efficiency | 16.410 | 15.152 |
| Min $D$-efficiency | 0.000 | *13.077* |
| Leave-1-out $D$-efficiency | 9.422 | 14.097 |
| | (8.468) | (1.022) |
| Leave-2-out $D$-efficiency | 4.396 | 11.608 |
| | (7.385) | (4.133) |
| $A$-efficiency | 5.102 | 5.127 |
| Min $A$-efficiency | 0.000 | 2.864 |
| Leave-1-out $A$-efficiency | 3.032 | 4.013 |
| | (2.724) | (0.963) |
| Leave-2-out $A$-efficiency | 1.465 | 2.759 |
| | (2.462) | (1.451) |

Table 5.11 (continued)

| Criteria Evaluated | 14-point $D$-optimal Exact Design on SLD$\{4,50\}$ | 14-point $D$-optimal Robust Design on SLD$\{4,20\}$ |
|---|---|---|
| $G$-efficiency | 71.429 | 80.192 |
| Min $G$-efficiency | 0.000 | 9.438 |
| Leave-1-out $G$-efficiency | 43.956 | 31.848 |
| | (39.504) | (25.634) |
| Leave-2-out $G$-efficiency | 21.978 | 15.963 |
| | (36.925) | (17.474) |
| $IV$-efficiency | 14.351 | 17.506 |
| Min $IV$-efficiency | 0.000 | 9.738 |
| Leave-1-out $IV$-efficiency | 8.695 | 14.196 |
| | (7.814) | (2.661) |
| Leave-2-out $IV$-efficiency | 4.281 | 10.145 |
| | (7.192) | (4.751) |

Numbers in parentheses represent standard deviations

Similar to the 11-, 12-, and 13-point $D$-optimal exact designs, if one of the unreplicated points is missing, the $D$-efficiency will be zero. All four alphabetical optimality criteria are calculated for both exact and robust exact designs and are summarized in Table 5.11. The Min $D$ is much higher in the robust exact design than in the exact design. Most criteria related to $A$-, $G$-, and $IV$-opitmality also prefer the robust exact design over the exact mixture design. The robust exact design is just slightly less optimal in $D$-criterion compared to the exact design.

All criteria evaluated for both exact and robust mixture designs are summarized in Figure 5.6. All robust exact mixture designs have the Min $D$ of at least 10 while losing one of unreplicated points in the exact designs causes the model to be unestimable, i.e., $D$-, $A$-, $G$-, and $IV$-efficiencies are zero. The Min $D$ of the robust exact mixture design increases as the sample size increases, but this is not the case for $D$-, $A$-, $G$-, and $IV$-efficiencies. It is important to mention that all exact mixture designs are based on the SLD{4, 2} plus two replicates at any subset of $\binom{10}{n-10}$ points of SLD{4, 2}.

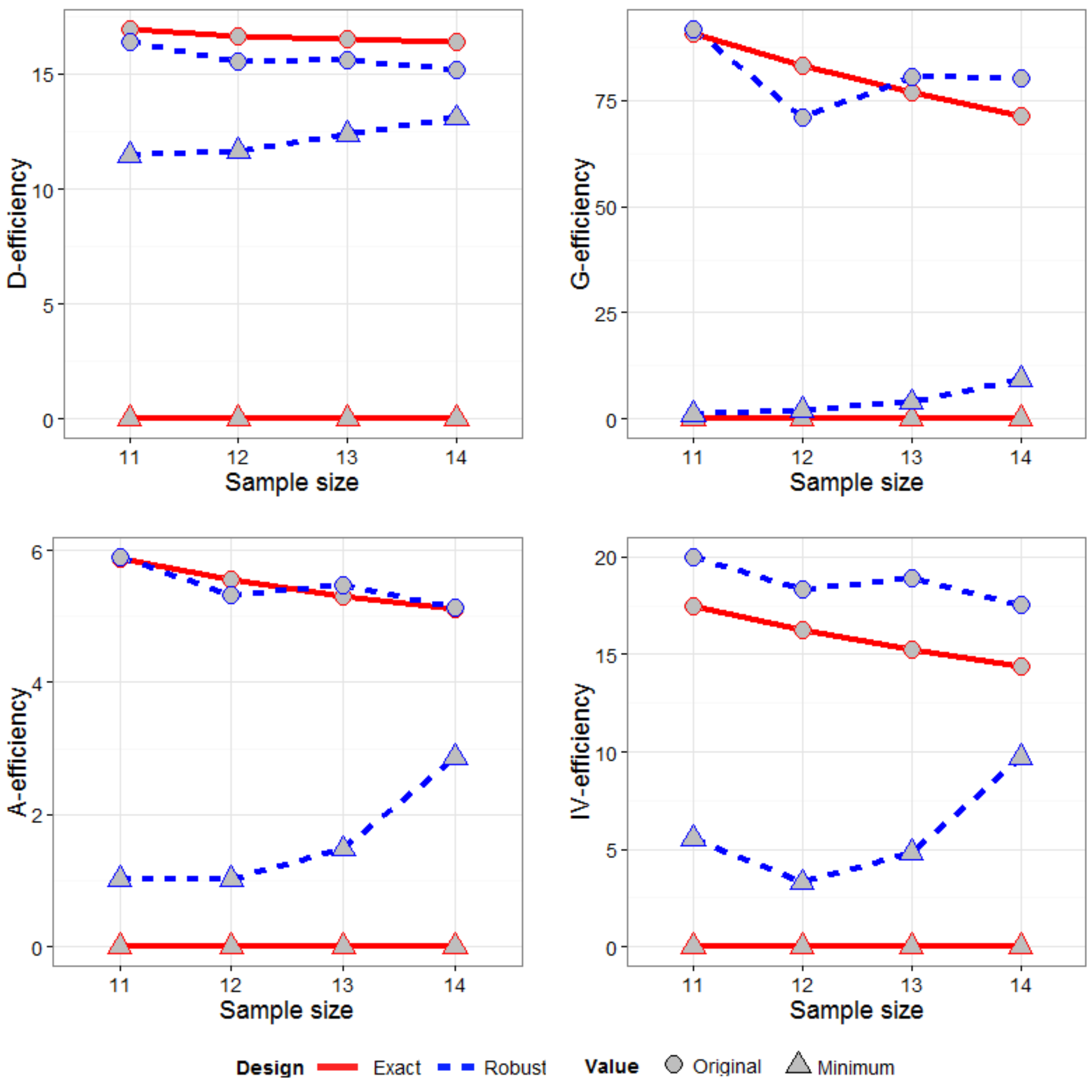



Figure 5.6: Summary of $D$-, $A$-, $G$-, $IV$-efficiencies and corresponding minimum efficiencies of four-component $D$-optimal exact and robust exact mixture designs.

# 3. $A$-Optimal Robust Exact Mixture Designs

## 3.1. Three-Component $A$-Optimal Mixture Designs

In this section, $A$-optimal robust exact designs will be constructed via the criterion (4.2) and then are compared to $A$-optimal exact designs having the same sample size. The SLD$\{3, 100\}$ and SLD$\{3, 20\}$ are used as support sets for constructing exact and robust exact designs, respectively, but in some cases, if a resulting robust exact design is near "symmetric" due to a coarseness of the grid being used, we will rerun that design using SLD$\{3, 40\}$ as a support set again. We have used a coarser grid in robust exact designs because although it is not a very time-consuming task for Min $A$ criterion, for Min $G$ and Min $IV$ it could take a few hours for only one attempt. To have robust exact mixture designs using the same support across the criteria, the SLD$\{3, 20\}$ will be used for constructing all three-component robust exact designs.

For $n = 7$, the exact mixture design contains the SLD$\{3, 2\}$ with two replicates at one midpoint. Generally, the $D$-optimal exact design is $A$-optimal, but not vice versa because for the $A$-optimal exact design, two replicates can be placed only on middles of the edges but not vertices. For the robust exact mixture design, design points are $(0, .3, .7)$, $(.7, .3, 0)$, $(.875, 0, .125)$, $(.125, 0, .875)$, $(.2, .6, .2)$, $(0, 1, 0)$, and $(.475, .05, .475)$. Five of those are on the edges of the triangle. The design points are illustrated in Figure 5.7.

Like the 7-point design, for $n = 8$, the exact mixture design is the SLD$\{3, 2\}$ with an additional replicate at two different midpoints. For the robust exact design, design points are $(.85, .15, 0)$, $(0, .15, .85)$, $(.3, .7, 0)$, $(0, .7, .3)$, $(.2, 0, .8)$, $(.8, 0, .2)$, $(0, 1, 0)$, and a centroid point. Note that the centroid point used to be $(.35, .35, .3)$, but it was changed to $(1/3, 1/3, 1/3)$ to slightly improve the Min $A$. These design points are presented in Figure 5.7. Note that design points of both designs are vertically symmetric.

Comparing all robust designs in Figure 5.7, when the sample size is small, i.e., $n = 7$ and 8, design points seem not to be at vertices, but there will be one or two design points near each vertex. When the design size is large, i.e., $n = 9$ and 10, the robust mixture design will contain points at vertices.

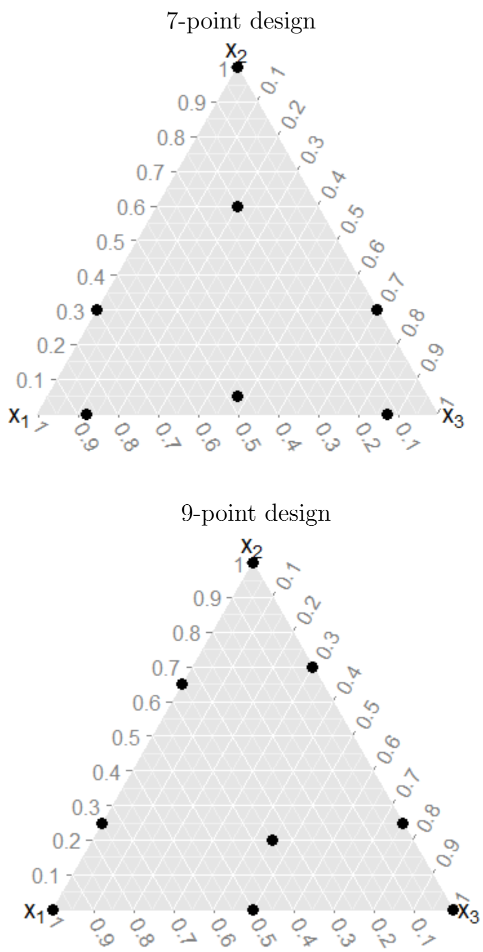



Figure 5.7: Three-component $A$-optimal robust exact mixture designs for a second-order Scheffé polynomial.

For $n = 9$, similar to the 7- and 8-point $A$-optimal designs, the exact design contains the SLD$\{3, 2\}$ points with an additional replicate at all three midpoints. For the robust exact design, design points are $(1, 0, 0)$, $(0, 1, 0)$, $(0, 0, 1)$, $(0, .7, .3)$, $(.35, .65, 0)$, $(0, .25, .75)$, $(.75, .25, 0)$, $(.5, 0, .5)$, and interior point $(.35, .2, .45)$ as shown in Figure 5.7.

For $n = 10$, the exact design contains the SLD$\{3, 2\}$ points with an additional replicate at all three midpoints and one centroid. For the robust exact design, design points are $(1, 0, 0)$, $(0, 1, 0)$, $(0, 0, 1)$, $(.75, .25, 0)$, $(0, .75, .25)$, $(.25, 0, .75)$, $(.65, 0, .35)$, $(.35, .65, 0)$, $(0, .35, .65)$, and $(.33, .33, .34)$. The boundary points in the robust exact design seems to be systematically distributed meaning that length between two consecutive points on the edges has a pattern. For example, the distance between $(0, 1, 0)$ and $(0, .75, .25)$, $(0, .75, .25)$ and $(0, .35, .65)$, and $(0, .35, .65)$ and $(0, 0, 1)$ are .25, .4, and .35, respectively. This is the same for the other two sides of the triangle.

Multiple criteria are also evaluated for both $n$-point exact and robust exact mixture designs, $n$ = 7, 8, 9, and 10, as summarized in Table 5.12. For $n = 7, 8, 9$, the exact designs are just the SLD$\{3, 2\}$ plus two replicates at different $(n-6)$ midpoints. Without an interior point, losing any unreplicated vertex leads to a design with $D$-efficiency = 0. The design efficiencies and corresponding minimum efficiencies versus the sample sizes are plotted in Figure 5.8. It is seen that the Min $A$, Min $D$, and Min $IV$ of the $A$-optimal robust exact mixture design increase as the sample size increases. When the sample sizes are 9 and 10, the $A$-efficiencies of the robust exact designs are slightly lower than those of the exact designs. The patterns of $A$- and $IV$-criteria versus the sample sizes are similar. For example, the $A$-efficiencies of the 7- and 8-point robust designs are about the same, and this is also true for the $IV$-efficiency.

Table 5.12: Properties of the 3-component $A$-optimal mixture designs for $n = 7$, 8, 9, and 10.

| | 7-point | | 8-point | | 9-point | | 10-point | |
|---|---|---|---|---|---|---|---|---|
| Criteria Evaluated | Exact | Robust | Exact | Robust | Exact | Robust | Exact | Robust |
| $D$-efficiency | 25.454 | 17.363 | 25.000 | 17.351 | 24.944 | 22.254 | 23.552 | 21.760 |
| Min $D$-efficiency | 0.000 | 11.345 | 0.000 | 13.836 | 0.000 | 17.425 | 11.908 | 17.913 |
| Leave-1-out $D$-efficiency | 7.559 | 14.077 | 12.727 | 15.639 | 16.667 | 20.323 | 20.247 | 20.423 |
| | (12.910) | (1.893) | (13.606) | (0.875) | (12.500) | (2.286) | (5.713) | (1.816) |
| Leave-2-out $D$-efficiency | | | 3.780 | 12.176 | 8.485 | 16.876 | 15.788 | 18.660 |
| | | | (9.428) | (3.348) | (12.170) | (4.888) | (8.373) | (2.526) |
| $A$-efficiency | 13.187 | 7.278 | 13.636 | 7.396 | 14.815 | 11.006 | 14.496 | 10.894 |
| Min $A$-efficiency | 0.000 | *3.245* | 0.000 | *5.005* | 0.000 | *6.958* | 1.220 | *7.987* |
| Leave-1-out $A$-efficiency | 3.810 | 3.854 | 6.593 | 5.621 | 9.091 | 8.708 | 9.988 | 9.341 |
| | (6.506) | (1.174) | (7.049) | (0.522) | (6.818) | (1.663) | (6.030) | (1.156) |
| Leave-2-out $A$-efficiency | | | 1.905 | 3.029 | 4.396 | 5.848 | 6.163 | 7.454 |
| | | | (4.751) | (1.511) | (6.305) | (2.834) | (5.958) | (1.834) |
| $G$-efficiency | 85.714 | 36.936 | 75.000 | 40.578 | 66.667 | 75.219 | 60.538 | 71.890 |
| Min $G$-efficiency | 0.000 | 3.184 | 0.000 | 11.178 | 0.000 | 9.621 | 0.597 | 13.212 |
| Leave-1-out $G$-efficiency | 28.571 | 12.068 | 42.857 | 22.074 | 50.000 | 36.718 | 47.187 | 43.299 |
| | (48.795) | (11.160) | (45.816) | (8.449) | (37.500) | (24.599) | (32.133) | (23.592) |
| Leave-2-out $G$-efficiency | | | 14.286 | 10.516 | 28.571 | 19.102 | 31.217 | 27.048 |
| | | | (35.635) | (7.643) | (40.979) | (18.944) | (36.586) | (20.711) |
| $IV$-efficiency | 25.996 | 20.569 | 27.135 | 20.424 | 29.888 | 25.368 | 30.309 | 25.429 |
| Min $IV$-efficiency | 0.000 | 9.534 | 0.000 | 13.460 | 0.000 | 16.548 | 2.652 | 20.753 |
| Leave-1-out $IV$-efficiency | 7.459 | 11.105 | 12.998 | 15.878 | 18.090 | 20.567 | 20.878 | 22.186 |
| | (12.738) | (2.175) | (13.895) | (1.346) | (13.568) | (2.585) | (12.512) | (1.598) |
| Leave-2-out $IV$-efficiency | | | 3.729 | 8.983 | 8.665 | 14.315 | 12.864 | 18.032 |
| | | | (9.303) | (4.539) | (12.428) | (6.143) | (12.353) | (3.928) |

Numbers in parentheses represent standard deviations

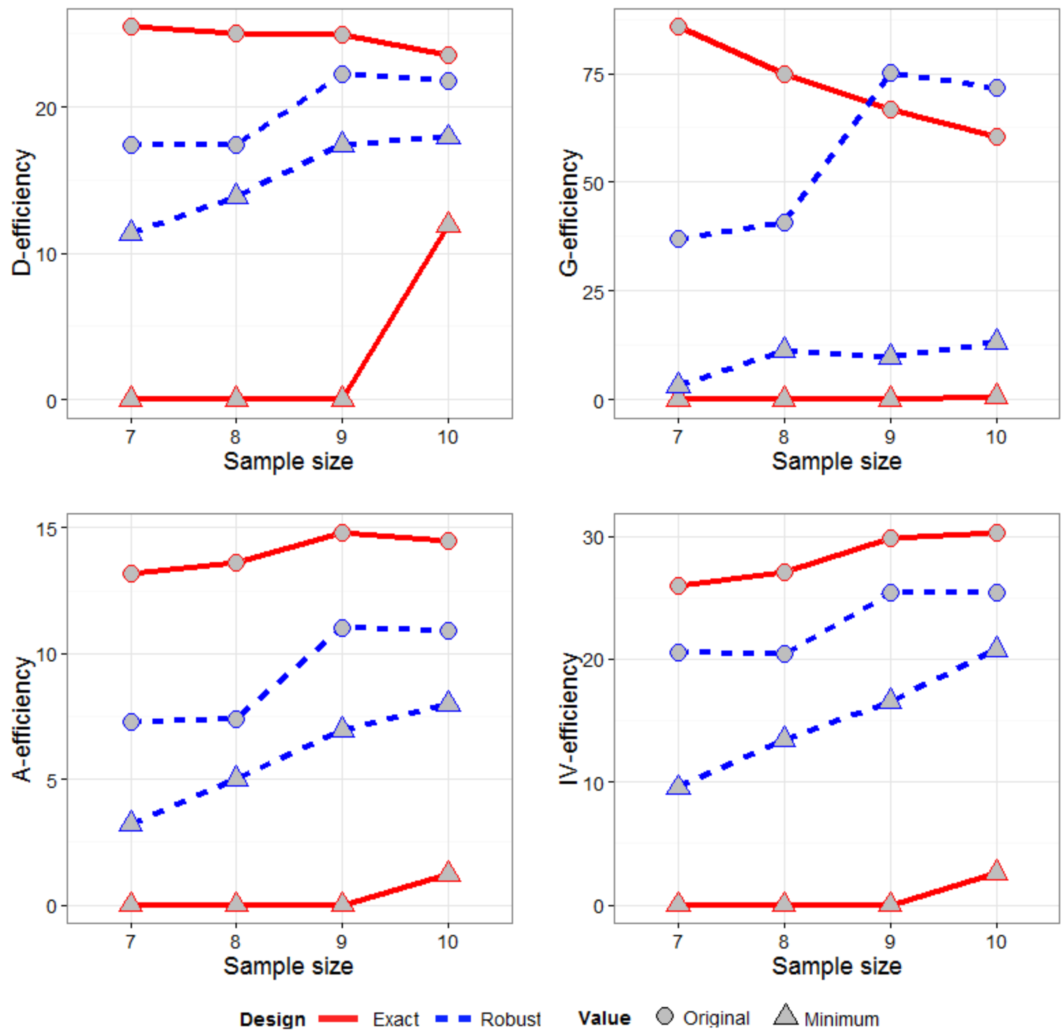



Figure 5.8: Summary of $D$-, $A$-, $G$-, $IV$-efficiencies and corresponding minimum efficiencies of three-component $A$-optimal exact and robust exact mixture designs.

## 3.2. Four-Component $A$-Optimal Mixture Designs

The study settings are the same as those in four-component $D$-optimal mixture design study. Because resulting $A$-optimal exact mixture designs are based on the SLD$\{4, 2\}$ plus two replicates at any subset of $\binom{6}{n-6}$ midpoints of the edges of the tetrahedron representing a design region, we will discuss an overall summary focusing on the robust exact mixture designs.

The design points of the robust exact mixture designs are listed in Table 5.13. Unlike the $D$-optimal robust exact designs, edge and face points seem to be more important than a vertex as the 11-point robust mixture design has only one vertex while the 13-point robustdesign has four vertices. The comparisons of criteria evaluated for both exact and robust exact mixture designs are shown in Table 5.14.

For 11-point design, the exact design has the Min $A$ of zero resulting from losing any unreplicated point. The robust exact design which aimed to maximize the Min $A$ has the Min $A$ of only 1.225. We have tried running the robust designs several times, but the Min $A$ seems difficult to maximize. The resulting design has an $A$-efficiency of only 2.5. However, the leave-1-out $D$-, $A$-, and $IV$-efficiencies are higher in the robust exact design than in the exact design.

For 12-point design, the Min $A$, leave-1-out and leave-2-out $A$-efficiencies are higher in the robust exact design than in the exact design, but the $A$-efficiency is 45% less in the robust exact design because there are not enough design points to increase both Min $A$ and $D$-efficiency, but as in 13- and 14-point design, the gap between them will decrease. If comparing the precision of predictions in both designs in terms of the $G$-efficiency, the exact design will be superior to the robust exact design.

Table 5.13: Design points of 4-component $A$-optimal robust exact mixture designs.

| Point Types | $n=11$ | | | | $n=12$ | | | | $n=13$ | | | | $n=14$ | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | $x_1$ | $x_2$ | $x_3$ | $x_4$ | $x_1$ | $x_2$ | $x_3$ | $x_4$ | $x_1$ | $x_2$ | $x_3$ | $x_4$ | $x_1$ | $x_2$ | $x_3$ | $x_4$ |
| Vertices | 0 | 0 | 1 | 0 | 1 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 1 | 0 | 0 | 0 |
| | | | | | 0 | 0 | 1 | 0 | 0 | 1 | 0 | 0 | 0 | 1 | 0 | 0 |
| | | | | | | | | | 0 | 0 | 1 | 0 | 0 | 0 | 1 | 0 |
| | | | | | | | | | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 1 |
| Edges | .6 | .4 | 0 | 0 | .7 | 0 | .3 | 0 | 0 | .3 | 0 | .7 | .3 | 0 | .7 | 0 |
| | .75 | 0 | 0 | .25 | 0 | .3 | .7 | 0 | 0 | .3 | .7 | 0 | .7 | 0 | .3 | 0 |
| | 0 | 0 | .05 | .95 | 0 | .95 | 0 | .05 | .45 | 0 | 0 | .55 | .3 | .7 | 0 | 0 |
| | 0 | .85 | 0 | .15 | .05 | 0 | 0 | .95 | 0 | 0 | .35 | .65 | 0 | .7 | 0 | .3 |
| | .85 | 0 | .15 | 0 | .6 | 0 | 0 | .4 | | | | | .4 | 0 | 0 | .6 |
| | | | | | | | | | | | | | 0 | .6 | .4 | 0 |
| Faces | .1 | .7 | .2 | 0 | .35 | .35 | 0 | .3 | .3 | .65 | 0 | .05 | .35 | .30 | 0 | .35 |
| | .25 | .3 | 0 | .45 | .25 | 0 | .5 | .25 | .35 | 0 | .5 | .15 | .30 | .35 | .35 | 0 |
| | .3 | 0 | .6 | .1 | .2 | .6 | .2 | 0 | .65 | .2 | 0 | .15 | .1 | 0 | .5 | .4 |
| | .1 | 0 | .35 | .55 | 0 | .05 | .25 | .7 | .4 | .3 | .3 | 0 | 0 | .1 | .2 | .7 |
| | 0 | .25 | .5 | .2 | 0 | .6 | .15 | .25 | 0 | .4 | .3 | .3 | | | | |

Table 5.14: Properties of the 4-component $A$-optimal mixture designs for $n = 11, 12, 13$, and 14.

| | 11-point | | 12-point | | 13-point | | 14-point | |
|---|---|---|---|---|---|---|---|---|
| Criteria Evaluated | Exact | Robust | Exact | Robust | Exact | Robust | Exact | Robust |
| $D$-efficiency | 16.964 | 10.224 | 16.667 | 11.359 | 16.489 | 13.261 | 16.410 | 13.693 |
| Min $D$-efficiency | 0.000 | 7.772 | 0.000 | 9.212 | 0.000 | 10.577 | 0.000 | 11.401 |
| Leave-1-out $D$-efficiency | 3.166 | 8.719 | 5.655 | 10.163 | 7.692 | 12.029 | 9.422 | 12.727 |
| | (7.043) | (0.559) | (8.353) | (0.714) | (8.648) | (1.080) | (8.468) | (0.955) |
| Leave-2-out $D$-efficiency | | | 1.055 | 7.894 | 2.610 | 10.301 | 4.396 | 11.339 |
| | | | (4.186) | (1.839) | (6.160) | (1.924) | (7.385) | (1.900) |
| $A$-efficiency | 6.061 | 2.557 | 5.952 | 3.295 | 5.917 | 4.442 | 5.952 | 4.621 |
| Min $A$-efficiency | 0.000 | *1.225* | 0.000 | *1.933* | 0.000 | *2.422* | 0.000 | *2.959* |
| Leave-1-out $A$-efficiency | 1.136 | 1.399 | 2.020 | 2.266 | 2.747 | 3.183 | 3.381 | 3.648 |
| | (2.528) | (0.153) | (2.984) | (0.397) | (3.089) | (0.777) | (3.039) | (0.729) |
| Leave-2-out $A$-efficiency | | | 0.379 | 1.051 | 0.932 | 1.951 | 1.570 | 2.597 |
| | | | (1.503) | (0.789) | (2.201) | (0.952) | (2.638) | (1.051) |
| $G$-efficiency | 90.909 | 30.450 | 83.333 | 26.764 | 76.923 | 45.343 | 71.429 | 60.891 |
| Min $G$-efficiency | 0.000 | 1.826 | 0.000 | 4.475 | 0.000 | 4.092 | 0.000 | 6.356 |
| Leave-1-out $G$-efficiency | 18.182 | 6.895 | 30.303 | 11.199 | 38.462 | 18.857 | 43.956 | 27.651 |
| | (40.452) | (3.730) | (44.761) | (7.125) | (43.240) | (15.929) | (39.504) | (22.264) |
| Leave-2-out $G$-efficiency | | | 6.061 | 4.407 | 13.986 | 7.958 | 21.978 | 13.452 |
| | | | (24.044) | (4.504) | (33.012) | (8.787) | (36.925) | (14.101) |
| $IV$-efficiency | 18.545 | 12.117 | 18.464 | 13.180 | 18.649 | 16.671 | 19.119 | 16.915 |
| Min $IV$-efficiency | 0.000 | 5.047 | 0.000 | 7.825 | 0.000 | 9.226 | 0.000 | 10.919 |
| Leave-1-out $IV$-efficiency | 3.437 | 6.872 | 6.182 | 9.578 | 8.522 | 12.520 | 10.657 | 13.847 |
| | (7.646) | (1.214) | (9.131) | (1.213) | (9.580) | (2.365) | (9.577) | (2.062) |
| Leave-2-out $IV$-efficiency | | | 1.146 | 4.633 | 2.853 | 8.055 | 4.870 | 10.261 |
| | | | (4.545) | (3.356) | (6.735) | (3.552) | (8.181) | (3.605) |

Numbers in parentheses represent standard deviations

For 13-point design, like previous designs, the Min $A$ of zero in the exact design is a result of losing one of the unreplicated points. The Min $A$ is increased from 0 to 2.4 while the $A$-efficiency is decreased from 5.9 to 4.4 when using the robust exact design instead of the exact design. The leave-1-out and leave-2-out $A$-efficiencies are also higher in the robust design than in the exact design. As expected, the $G$-efficiency is very sensitive to a point changing; however, the average precision of predictions in both designs are not much different as the $IV$-efficiencies of exact and robust exact designs are 18.6 and 16.7, respectively. Overall, the robust exact design, which is slightly less optimal in terms of $D$-, $A$-, and $IV$-optimality, should be used in an experimentation because its robustness against one and two missing runs is improved.

For 14-point design, the Min $A$ markedly increases from 0 to 2.96. The Min $A$ of 2.96 is not very low as it is about 50% of the original $A$-efficiency of the exact design. The previous $A$-optimal robust exact designs, in general, have very low values of the $G$-efficiency, but in this case, the robust exact design has very high value of the $G$-efficiency, about 85% of that of the exact design.

All design efficiencies and corresponding minimum efficiencies for the $A$-optimal exact and robust exact mixture designs are plotted against the sample sizes as illustrated in Figure 5.9. The Min $A$, Min $D$, Min $G$, $A$-, $D$-, and $G$-efficiencies of the robust exact design increase as the sample sizes increase. If one of the unreplicated points is lost in the exact design, the model will be not estimable, i.e. Min $A$, Min $D$, Min $G$, and Min $IV$ are all zero.

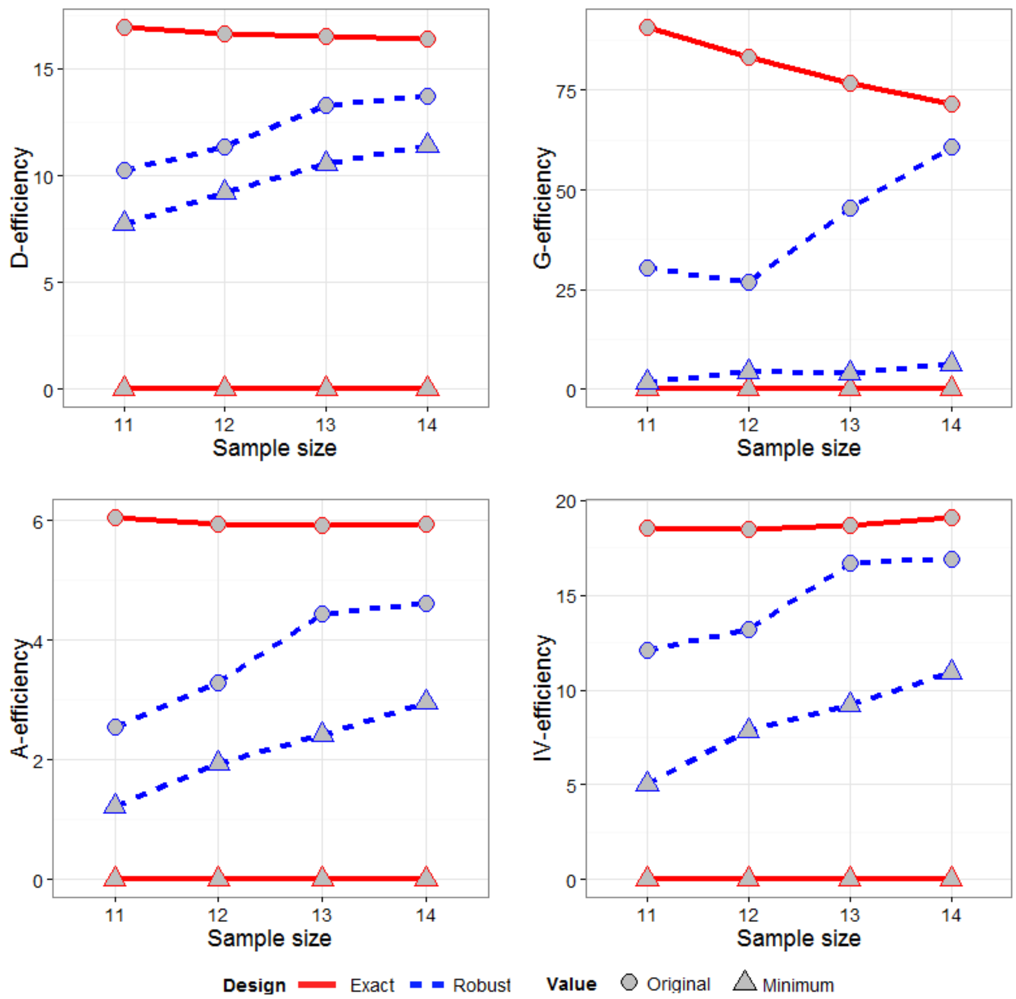



Figure 5.9: Summary of $D$-, $A$-, $G$-, $IV$-efficiencies and corresponding minimum efficiencies of four-component $A$-optimal exact and robust exact mixture designs.

## 4. $G$-Optimal Robust Exact Mixture Designs

### 4.1. Three-Component $G$-Optimal Mixture Designs

The $G$-optimal robust exact designs will be constructed via criterion (4.3), and the resulting designs will be compared to the $G$-optimal exact design having the same sample size. The OPTEX procedure in SAS software (SAS Institute Inc., 2013) will only optimize the $D$- and $A$-optimality criteria. Even though $G$-optimal designs could be one of many tries which are generated by $D$ criterion with the highest $G$-efficiency (SAS Institute Inc., 2014), from our experience this usually does not give the exact $G$-optimal design. Therefore, a Matlab program (MATLAB, 2014) was written to generate both exact and robust exact designs in this study.

4.1.1. The 7-Point Design: The design points of exact and robust exact mixture designs are illustrated in Figure 5.10. The exact design contains all vertices, $(.5, 0, .5)$, $(0, .39, .61)$, $(.61, .39, 0)$, and interior point $(.21, .58, .21)$. Also, those points are vertically symmetric. The SPVs are high for design points near vertices and the middles of the edges. For the robust exact design, the design points are $(.85, .15, 0)$, $(.85, 0, .15)$, $(0, .85, .15)$, $(.2, .8, 0)$, $(.05, 0, .95)$, $(.4, .2, .4)$, and interior point $(.05, .15, .8)$. The robust exact design has no design points at vertices but has two points in a neighborhood for each vertex. Therefore, when one of the two points is lost, there is still one point left to help the prediction at the vertex. However, a design having no point at vertices is usually not very optimal. Thus, overall the SPVs are larger in the robust design as shown in Figure 5.10.

The exact design has the Min $G$ of 1.91 as shown in Table 5.15 and this is a result of losing point $(.5, 0, .5)$. However, losing any vertices also gives very low value of $G$-efficiency, less than 2.5. Its $G$-efficiency is as high as 87.4 while it is only 29.5 for the robust exact mixture design. The Min $G$ is considerably improved from 1.9 to 9.9 in the robust exact design by having two design points near the vertices. In this study, the $G$-efficiency is found to be extremely sensitive to a point changing. In this case, a sample size is the smallest and to maximize the Min $G$ , it seems to produce a very poor design. Not only the $G$-efficiency, but other criteria in Table 5.15 also indicate the exact design is, generally, superior to the robust exact mixture design.

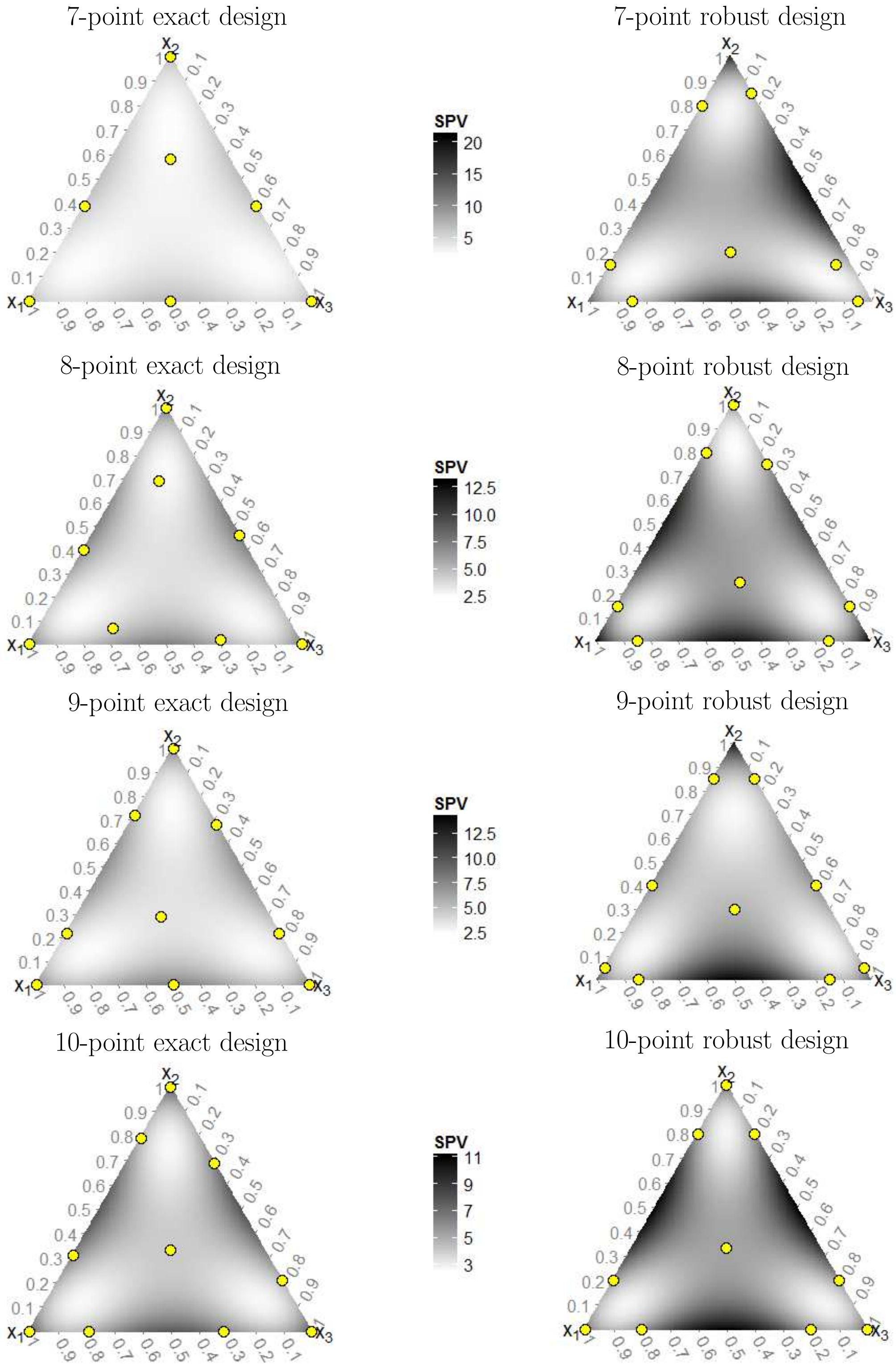



Figure 5.10: The three-component $G$-optimal exact and robust exact mixture designs for a second-order Scheffé polynomial.

Table 5.15: Properties of the 3-component $G$-optimal mixture designs for $n = 7$, 8, 9, and 10.

| | 7-point | | 8-point | | 9-point | | 10-point | |
|---|---|---|---|---|---|---|---|---|
| Criteria Evaluated | Exact | Robust | Exact | Robust | Exact | Robust | Exact | Robust |
| $D$-efficiency | 23.875 | 13.886 | 21.937 | 16.248 | 21.761 | 17.641 | 20.895 | 18.797 |
| Min $D$-efficiency | 14.355 | 10.909 | 16.004 | 14.309 | 17.787 | 15.693 | 18.061 | 17.045 |
| Leave-1-out $D$-efficiency | 17.833 | 11.570 | 18.808 | 14.728 | 19.942 | 16.487 | 19.746 | 17.886 |
| | (4.415) | (0.828) | (3.115) | (0.265) | (2.043) | (0.539) | (1.292) | (0.585) |
| Leave-2-out $D$-efficiency | | | 13.714 | 11.767 | 16.732 | 14.566 | 18.187 | 16.643 |
| | | | (4.385) | (2.206) | (4.598) | (1.875) | (1.929) | (1.035) |
| $A$-efficiency | 11.887 | 4.138 | 10.449 | 6.003 | 10.299 | 7.118 | 9.545 | 7.100 |
| Min $A$-efficiency | 0.920 | 1.657 | 2.931 | 3.265 | 4.594 | 4.803 | 7.593 | 6.073 |
| Leave-1-out $A$-efficiency | 4.888 | 2.357 | 6.824 | 4.647 | 8.273 | 6.028 | 8.355 | 6.333 |
| | (3.681) | (0.541) | (2.775) | (0.622) | (1.761) | (0.889) | (0.775) | (0.132) |
| Leave-2-out $A$-efficiency | | | 3.132 | 2.547 | 5.645 | 4.321 | 6.823 | 5.327 |
| | | | (2.750) | (1.381) | (2.575) | (1.555) | (1.406) | (0.701) |
| $G$-efficiency | 87.351 | 29.542 | 80.444 | 46.449 | 78.165 | 42.387 | 77.105 | 54.671 |
| Min $G$-efficiency | 1.910 | *9.910* | 6.221 | *20.024* | 12.936 | *23.397* | 19.005 | *27.954* |
| Leave-1-out $G$-efficiency | 18.703 | 11.827 | 26.398 | 21.974 | 35.664 | 25.020 | 39.923 | 32.283 |
| | (31.289) | (1.956) | (26.740) | (1.871) | (23.914) | (1.866) | (19.110) | (6.130) |
| Leave-2-out $G$-efficiency | | | 8.312 | 12.086 | 18.369 | 18.667 | 25.952 | 25.435 |
| | | | (13.384) | (8.028) | (16.215) | (7.997) | (14.916) | (7.864) |
| $IV$-efficiency | 26.096 | 13.291 | 24.417 | 16.697 | 24.258 | 18.946 | 22.925 | 17.913 |
| Min $IV$-efficiency | 1.909 | 3.843 | 7.145 | 7.481 | 11.128 | 12.003 | 18.535 | 13.005 |
| Leave-1-out $IV$-efficiency | 11.068 | 7.898 | 16.516 | 13.300 | 19.943 | 16.262 | 20.403 | 16.221 |
| | (7.076) | (2.065) | (5.251) | (2.554) | (3.584) | (2.469) | (1.525) | (1.363) |
| Leave-2-out $IV$-efficiency | | | 8.064 | 7.630 | 14.108 | 11.927 | 16.955 | 13.879 |
| | | | (6.167) | (4.517) | (5.903) | (4.566) | (3.415) | (2.511) |

Numbers in parentheses represent standard deviations

<u>4.1.2. The 8-Point Design:</u> The exact mixture design contains all vertices and $(.6, .4, 0)$, $(.18, .69, .13)$, $(0, .46, .54)$, $(.66, .07, .27)$, and $(.29, .02, .69)$. Three of them are interior points. The robust exact mixture design contains $(.15, 0, .85)$, $(.85, 0, .15)$, $(0, .15, .85)$, $(.85, .15, 0)$, $(0, .75, .25)$, $(.2, .8, 0)$, vertex point $(0, 1, 0)$, and interior point $(.35, .25, .4)$. One might observe that the $G$-optimal exact and robust exact mixture designs do not usually have replicated points like we saw in $D$- and $A$-optimal exact designs. The robust exact design has very high SPVs at points near the middles of edges as well as points $(1, 0, 0)$ and $(0, 0, 1)$.

Vertices of the exact design seem more important than the others because if one of them is missing, the $G$-efficiency will drop to $6 - 7$ as shown in Table 5.15. The Min $G$ is more than three times improved in the robust exact design, but its $G$-efficiency is low. As illustrated in Figure 5.10, we can determine the design region having very poor prediction. Overall, the robust exact design is inferior to the exact design in regard to many criteria.

<u>4.1.3. The 9-Point Design:</u> The design points of the exact design are $(1, 0, 0)$, $(0, 1, 0)$, $(0, 0, 1)$, $(.28, .72, 0)$, $(.78, .22, 0)$, $(0, .22, .78)$, $(0, .68, .32)$, $(.5, 0, .5)$, and $(.4, .29, .31)$. Unlike the exact design, the robust exact design has no vertices, but there are two points near each vertex. The design points are $(0, .4, .6)$, $(.6, .4, 0)$, $(.15, .85, 0)$, $(.15, 0, .85)$, $(.85, 0, .15)$, $(0, .85, .15)$, $(.95, .05, 0)$, $(0, .05, .95)$, and $(.35, .3, .35)$. The SPVs of the exact design are high when the prediction are made at the vertices and middles of the edges. The robust exact design improved the Min $G$ by having two points near each vertex, but this usually results to a sub-optimal design.

If one of vertices and $(.5, 0, .5)$ is missing in the exact design, the $G$-efficiency will drop to around $13 - 14$ as summarized in Table 5.15. The Min $G$ is doubled in the robust design, but its $G$-efficiency is about a half of that of the exact design. In our experience, the alphabetic optimal designs generally contain points at vertices, so if any designs have no vertices, they likely have low values of optimality criteria. In this case, the robust exact design is inferior to the exact design in regard to many criteria except for the Min $G$.

4.1.4. The 10-Point Design: The exact mixture design contains $(1,0,0)$, $(0,1,0)$, $(0,0,1)$, $(.79,0,.21)$, $(0,.21,.79)$, $(.21,.79,0)$, $(.69,.31,0.0)$, $(0.0,.69,.31)$, $(.31,0.0,.69)$, and $(.33,.33,.34)$ as depicted in Figure 5.10. Is is observed that points on the boundary of the triangle are systematically distributed. For example, the lengths between $(0,1,0)$ and $(0,.69,.31)$, $(0,.69,.31)$ and $(0,.21,.79)$, and $(0,.21,.79)$ and $(0,0,1)$ are .31, .48, and .21, respectively. This is also the case for other two sides. Likewise, the robust exact design contains a centroid point and boundary points which are also systematically distributed. Its design points are $(1,0,0)$, $(0,1,0)$, $(0,0,1)$, $(.2,.8,0)$, $(.2,0,.8)$, $(.8,0,.2)$, $(.8,.2,0)$, $(0,.2,.8)$, $(0,.8,.2)$, and $(.33,.33,34)$. The SPVs are very high when predictions at points near vertices and middles of the edges.

For the exact design, the Min $G$ of 19 is a result of losing one of the vertices. Like other $G$-optimal robust exact designs, an amount of the Min $G$ improved is less than the difference between $G$-efficiencies of both designs. However, this 10-point robust exact design is different from other previous robust exact design as it has all vertices. Also, the differences between $D$-, $A$-, $G$-, and $IV$-efficiencies of both designs are smaller compared to 7-, 8-, 9-point $G$-optimal designs.

From Figure 5.11, it is seen that the Min $G$ might not be a good criterion to be used for constructing the robust exact mixture. Although the Min $G$ and Min $D$ of the robust exact designs increase as the sample sizes increase, the $G$-efficiencies are still low compared to those of the exact designs. In aspects of $D$-, $A$-, and $IV$-criteria, the $G$-optimal robust exact mixture designs are also poor meaning that the minima of those efficiencies are not improved, and without a missing point, the efficiencies of the robust designs are much lower compared to the exact designs. The situation will get better when the sample size increases.

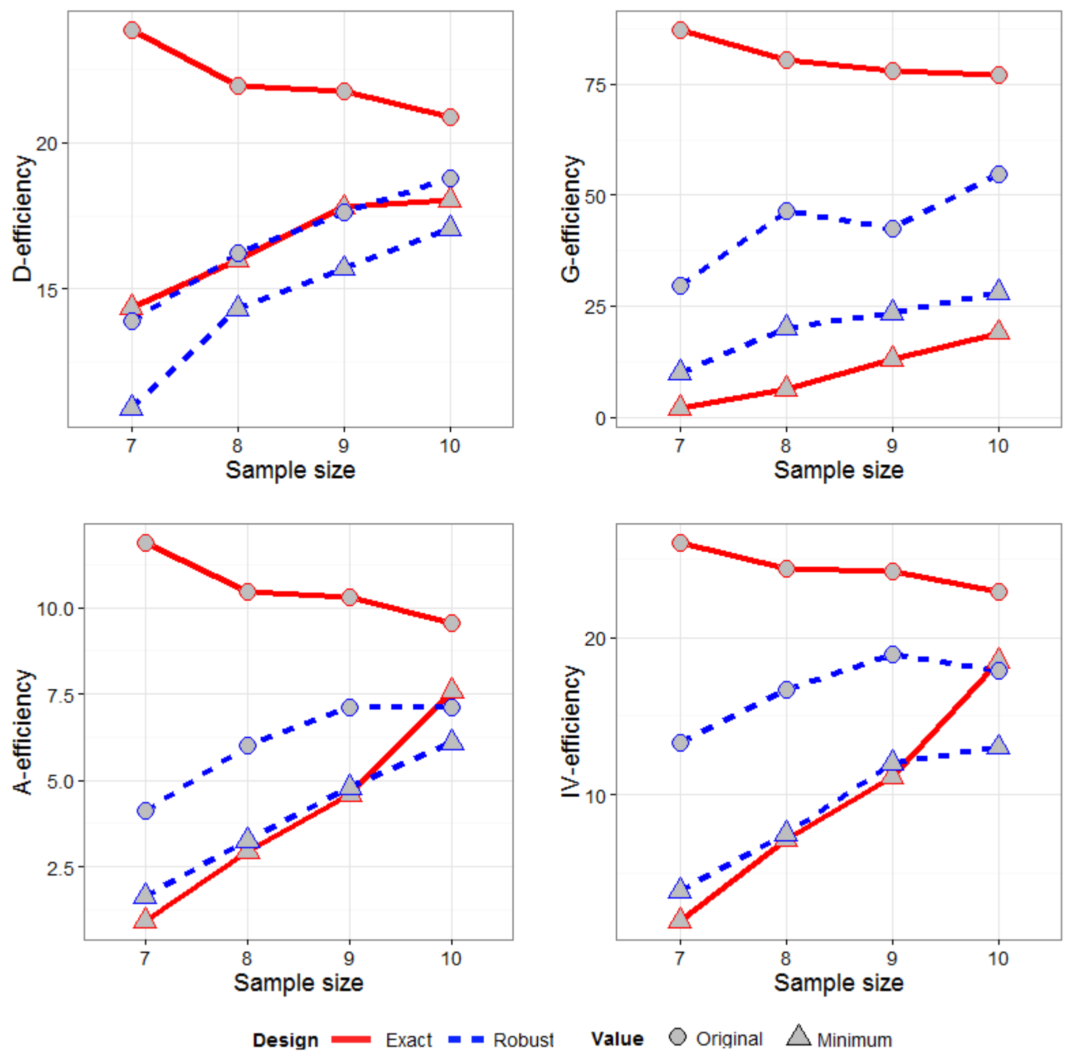



Figure 5.11: Summary of $D$-, $A$-, $G$-, $IV$-efficiencies and corresponding minimum efficiencies of three-component $G$-optimal exact and robust exact mixture designs.

## 4.2. Four-Component $G$-Optimal Mixture Designs

For four components, robust exact designs were constructed by applying criterion (4.3) and then compared to the $G$-optimal exact designs having the same sample size. The SLD$\{4, 50\}$ and SLD$\{4, 20\}$ are used as supports for constructing exact and robust exact designs, respectively. A Matlab program (MATLAB, 2014) was written to generate both exact and robust exact mixture designs in this study.

### 4.2.1. The 11-Point Design:

Design points of exact and robust exact designs are listed in Table 5.16. The exact design has an unreplicated point at each vertex, at middles of the edges, and at the centroid of the design region while the robust exact design puts most points on the faces of the tetrahedron and has no vertices.

We observed that the design maximizing the Min $G$ seems not to have any high values of other criteria especially when the design size is very small compared to the number of parameter to be estimated in the model. In this case, there are only 11 points where none of them are at vertices. This will, however, maximize only the Min $G$ but give very low values of the usual optimality criteria. From Table 5.18, the Min $G$ is slightly increased by 3.4 when using the robust exact design instead of the exact design, but the $G$-efficiency substantially drops. In this case, the exact mixture design is obviously superior to the robust exact design in many aspects, e.g., $D$-, $A$-, $IV$-efficiencies.

Table 5.16: Design points of the 11-point 4-component $G$-optimal exact and robust exact mixture designs.

| Point Types | Exact Design on SLD$\{4,50\}$ | | | | Robust Design on SLD$\{4,20\}$ | | | |
|---|---|---|---|---|---|---|---|---|
| | $x_1$ | $x_2$ | $x_3$ | $x_4$ | $x_1$ | $x_2$ | $x_3$ | $x_4$ |
| Vertices | All vertices | | | | | | | |
| Edges | All middles of the edges | | | | 0 | .2 | 0 | .8 |
| | | | | | .3 | .7 | 0 | 0 |
| | | | | | 0 | .7 | .3 | 0 |
| Faces | | | | | .05 | .9 | 0 | .05 |
| | | | | | .1 | .2 | .7 | 0 |
| | | | | | .6 | .05 | 0 | .35 |
| | | | | | .2 | 0 | .1 | .7 |
| | | | | | .8 | .15 | .05 | 0 |
| | | | | | 0 | .10 | .7 | .2 |
| | | | | | .7 | 0 | .25 | .05 |
| Interior | .25 | .25 | .25 | .25 | .1 | .3 | .2 | .4 |

Table 5.17: Design points of the 12-point 4-component $G$-optimal exact and robust exact mixture designs.

| Point Types | Exact Design on SLD$\{4,50\}$ | | | | Robust Design on SLD$\{4,20\}$ | | | |
|---|---|---|---|---|---|---|---|---|
| | $x_1$ | $x_2$ | $x_3$ | $x_4$ | $x_1$ | $x_2$ | $x_3$ | $x_4$ |
| Vertices | All vertices | | | | | | | |
| Edges | All middles of the edges | | | | .8 | 0 | .2 | 0 |
| | | | | | .8 | .2 | 0 | 0 |
| | | | | | 0 | .8 | 0 | .2 |
| | | | | | .2 | .8 | 0 | 0 |
| | | | | | 0 | .7 | .3 | 0 |
| | | | | | .7 | 0 | 0 | .3 |
| | | | | | 0 | 0 | .1 | .9 |
| | | | | | 0 | 0 | .9 | .1 |
| Faces | | | | | 0 | .35 | .35 | .3 |
| | | | | | .35 | 0 | .3 | .35 |
| | | | | | .1 | .1 | 0 | .8 |
| | | | | | .1 | .1 | .8 | 0 |
| Interior | .25 | .25 | .25 | .25 | | | | |
| | .25 | .25 | .25 | .25 | | | | |

Table 5.18: Properties of the 4-component $G$-optimal mixture designs for $n = 11$, 12, 13, and 14.

| | 11-point | | 12-point | | 13-point | | 14-point | |
|---|---|---|---|---|---|---|---|---|
| Criteria Evaluated | Exact | Robust | Exact | Robust | Exact | Robust | Exact | Robust |
| $D$-efficiency | 16.413 | 7.696 | 15.451 | 9.400 | 14.582 | 9.915 | 14.045 | 10.124 |
| Min $D$-efficiency | 11.487 | 6.261 | 11.192 | 8.256 | 10.843 | 9.093 | 11.783 | 9.508 |
| Leave-1-out $D$-efficiency | 12.957 | 6.635 | 12.895 | 8.542 | 12.764 | 9.269 | 12.901 | 9.614 |
| | (1.698) | (0.208) | (1.818) | (0.247) | (1.722) | (0.133) | (1.163) | (0.108) |
| Leave-2-out $D$-efficiency | | | 4.055 | 6.434 | 10.529 | 8.318 | 11.531 | 8.901 |
| | | | (6.029) | (2.345) | (2.472) | (0.637) | (1.559) | (0.567) |
| $A$-efficiency | 5.902 | 1.677 | 5.525 | 2.063 | 5.254 | 2.464 | 4.730 | 2.497 |
| Min $A$-efficiency | 1.015 | 0.583 | 1.367 | 1.374 | 1.513 | 1.430 | 2.066 | 1.648 |
| Leave-1-out $A$-efficiency | 1.862 | 0.925 | 2.497 | 1.501 | 3.119 | 2.019 | 3.503 | 2.156 |
| | (1.493) | (0.182) | (1.629) | (0.114) | (1.599) | (0.195) | (1.013) | (0.156) |
| Leave-2-out $A$-efficiency | | | 0.526 | 0.765 | 1.592 | 1.406 | 2.373 | 1.707 |
| | | | (0.989) | (0.446) | (1.267) | (0.461) | (1.085) | (0.424) |
| $G$-efficiency | 91.908 | 13.637 | 84.746 | 27.683 | 78.752 | 31.034 | 77.705 | 40.864 |
| Min $G$-efficiency | 1.099 | *4.414* | 1.541 | *11.370* | 1.981 | *15.842* | 6.899 | *22.834* |
| Leave-1-out $G$-efficiency | 11.970 | 5.137 | 19.078 | 14.882 | 24.647 | 17.590 | 28.435 | 24.220 |
| | (29.245) | (1.167) | (34.097) | (3.056) | (31.499) | (1.730) | (28.452) | (1.335) |
| Leave-2-out $G$-efficiency | | | 2.475 | 6.577 | 7.348 | 11.974 | 12.114 | 18.461 |
| | | | (12.312) | (5.093) | (15.466) | (5.567) | (15.894) | (6.518) |
| $IV$-efficiency | 20.007 | 8.957 | 20.101 | 8.893 | 19.239 | 11.170 | 17.887 | 10.268 |
| Min $IV$-efficiency | 5.572 | 2.514 | 7.751 | 5.002 | 5.150 | 4.739 | 7.702 | 4.699 |
| Leave-1-out $IV$-efficiency | 6.937 | 5.234 | 9.806 | 6.634 | 12.127 | 9.440 | 13.947 | 9.119 |
| | (3.974) | (1.315) | (4.765) | (0.817) | (4.820) | (1.548) | (3.230) | (1.325) |
| Leave-2-out $IV$-efficiency | | | 2.026 | 3.460 | 6.634 | 6.857 | 9.957 | 7.471 |
| | | | (3.388) | (2.029) | (4.179) | (2.604) | (3.901) | (2.273) |

Numbers in parentheses represent standard deviations

4.2.2. The 12-point Design: The design points of exact and robust exact mixture designs are listed in Table 5.17. Like the 11-point $G$-optimal exact design, all design points are the SLD$\{4, 2\}$ plus two centroids. For the robust exact mixture design, all points are lying on the edges and faces of the design region. Similar to $G$-optimal robust exact designs with a small sample size, no vertices are included.

From Table 5.18, the Min $G$ of 1.541 of the exact design is a result of losing one of the vertices. The Min $G$ considerably increases from 1.541 to 11.37 when using the robust exact design instead of the exact design; however, its $G$-efficiency is low. This is due to the fact that the robust design, aiming to maximize the Min $G$, has no vertices which usually increase values of all optimality criteria. Nevertheless, the difference between two $G$-efficiencies is narrower than that in the 11-point $G$-optimal designs.

4.2.3. The 13-Point Design: Design points of exact and robust exact mixture designs are listed in Table 5.19. Unlike 11- or 12-point $G$-optimal exact designs, only three of six midpoints are included in the 13-point exact design. If the design points were the same as those in the 12-point exact design with an added centroid point, the $G$-efficiency would be 78.5146, slightly less than the $G$-efficiency of the current exact design. Most design points of the robust exact design are lying on the edge of the tetrahedron, and no vertices.

The properties of exact and robust exact designs are summarized in Table 5.18. The Min $G$ is considerably improved in the robust exact design, yet its $G$-efficiency is still low compared to that of the exact design. Again, since the robust exact design does not contain any vertices, $D$-, $A$-, $G$-, and $IV$-efficiencies will usually be low. However, the gap between $G$-efficiencies of both designs is now only 47.7, and

Table 5.19: Design points of the 13-point 4-component $G$-optimal exact and robust exact mixture designs.

| Point Types | Exact Design on SLD$\{4,50\}$ | | | | Robust Design on SLD$\{4,20\}$ | | | |
|---|---|---|---|---|---|---|---|---|
| | $x_1$ | $x_2$ | $x_3$ | $x_4$ | $x_1$ | $x_2$ | $x_3$ | $x_4$ |
| Vertices | All vertices | | | | | | | |
| Edges | .5 | 0 | 0 | .5 | .2 | 0 | .8 | 0 |
| | 0 | .5 | 0 | .5 | .2 | .8 | 0 | 0 |
| | 0 | .5 | .5 | 0 | .8 | .2 | 0 | 0 |
| | | | | | .8 | 0 | 0 | .2 |
| | | | | | 0 | .2 | 0 | .8 |
| | | | | | 0 | .8 | .2 | 0 |
| | | | | | 0 | 0 | .8 | .2 |
| | | | | | 0 | 0 | .2 | .8 |
| | | | | | 0 | .7 | 0 | .3 |
| Faces | 0 | .2 | .2 | .6 | .35 | .05 | 0 | .6 |
| | .6 | .2 | .2 | 0 | .05 | .3 | .65 | 0 |
| | .02 | 0 | .5 | .48 | .65 | 0 | .3 | .05 |
| | .48 | 0 | .5 | .02 | | | | |
| | .46 | .5 | 0 | .04 | | | | |
| Interior | .22 | .24 | .24 | .30 | .2 | .2 | .3 | .3 |

if compared to designs with sample sizes of 11 and 12 whose differences between $G$-efficiencies of exact and robust exact designs are 78.3 and 57, respectively.

4.2.4. The 14-Point Design: Design points of exact and robust exact mixture designs are listed in Table 5.20. The exact design has points scattered all over the boundary. It is interesting that most points of the robust exact design are on the edges, and they are the combinations of .8, .2, and two 0's. As presented in Table 5.18, the Min $G$ is increased by 15.9 when using the robust exact design instead of the exact design while the $G$-efficiency is dropped by 36.8. As previously mentioned, as the sample size increases, the difference between $G$-efficiencies of exact and robust exact designs decreases. However, this is not the case for the Min $G$. So far, the difference of Min $G$'s of 11-, 12-, 13-, and 14-point exact and robust exact designs are

3.3, 9.9, 13.8, and 15.9, respectively. The differences between $G$-efficiencies in 11-, 12-, 13-, and 14-point designs are 78.3, 57, 47.7, and 36.8, respectively. Thus, as the sample size increases, the resulting robust exact mixture design will be more robust to a missing point and closer to the $G$-optimal exact design.

Table 5.20: Design points of the 14-point 4-component $G$-optimal exact and robust exact mixture designs.

| Point Types | Exact Design on SLD$\{4, 50\}$ | | | | Robust Design on SLD$\{4, 20\}$ | | | |
|---|---|---|---|---|---|---|---|---|
| | $x_1$ | $x_2$ | $x_3$ | $x_4$ | $x_1$ | $x_2$ | $x_3$ | $x_4$ |
| Vertices | All vertices | | | | | | | |
| Edges | .6 | 0 | 0 | .4 | 0 | .8 | .2 | 0 |
| | .32 | 0 | .68 | 0 | 0 | .8 | 0 | .2 |
| | .48 | .52 | 0 | 0 | 0 | 0 | .2 | .8 |
| | 0 | .38 | 0 | .62 | 0 | 0 | .8 | .2 |
| | 0 | .5 | .5 | 0 | .8 | .2 | 0 | 0 |
| | | | | | .8 | 0 | .2 | 0 |
| | | | | | .8 | 0 | 0 | .2 |
| | | | | | .2 | .8 | 0 | 0 |
| | | | | | .2 | 0 | .8 | 0 |
| | | | | | .2 | 0 | 0 | .8 |
| | | | | | 0 | .2 | .8 | 0 |
| | | | | | 0 | .05 | 0 | .95 |
| faces | .66 | .12 | .22 | 0 | | | | |
| | .16 | 0 | .18 | .66 | | | | |
| | 0 | .7 | .12 | .18 | | | | |
| | 0 | 0 | .58 | .42 | | | | |
| Interior | .28 | .22 | .26 | .24 | .35 | .25 | .30 | .15 |
| | | | | | .05 | .30 | .05 | .6 |

Figure 5.12 shows plots of all four alphabetic efficiencies and corresponding minimums of exact and robust exact mixture designs against sample sizes. Not only the $G$-efficiency and Min $G$, but other criteria of the robust exact designs are very low compared to those of the exact designs. The $D$-efficiencies of the robust exact designs are even lower than the Min $D$'s of the exact mixture designs. In conclusion, the Min $G$ is not a good criterion to construct the robust exact mixture designs.

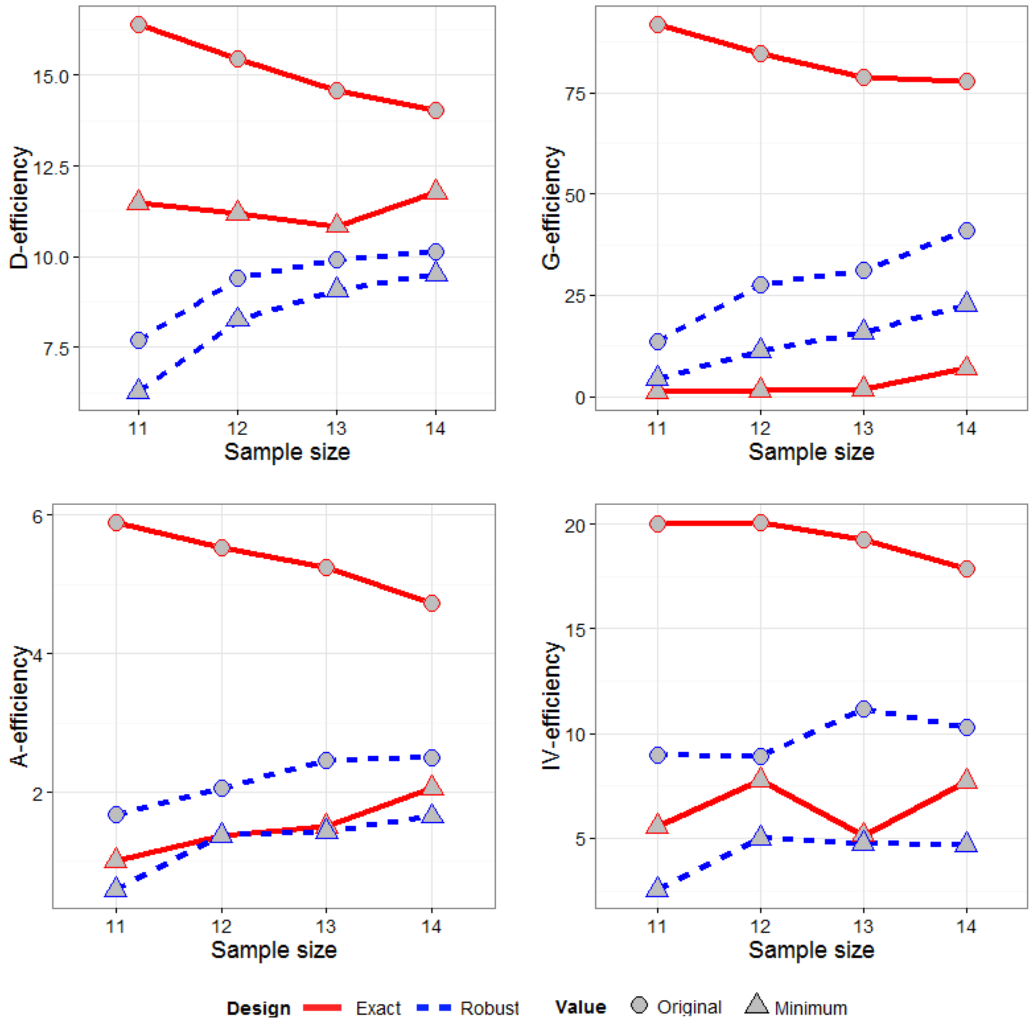



Figure 5.12: Summary of $D$-, $A$-, $G$-, $IV$-efficiencies and corresponding minimum efficiencies of four-component $G$-optimal exact and robust exact mixture designs.

# 5. $IV$-Optimal Robust Exact Mixture Designs

## 5.1. Three-Component $IV$-Optimal Mixture Designs

In this section, the $IV$-optimal robust exact designs will be constructed by using criterion (4.4), and will be compared to the corresponding exact mixture design having the same sample size. A Matlab program (MATLAB, 2014) was written to find both exact and robust exact designs by using support SLD$\{3, 100\}$ and SLD$\{3, 20\}$, respectively.

5.1.1. The 7-Point Design: The exact design contains the SLD$\{3, 2\}$ points as illustrated in Figure 5.13. For the robust exact design, points are $(0, .3, .7)$, $(.7, .3, 0)$, $(.875, 0, .125)$, $(.125, 0, .875)$, $(.2, .6, .2)$, $(0, 1, 0)$, and $(.475, .05, .475)$. They are the same as the $A$-optimal exact robust design points. The design points are vertically symmetric. Both exact and robust exact designs do not include any replicated points. It is also seen that the robust exact mixture design has very high SPVs at points near or at $(1, 0, 0)$ and $(0, 0, 1)$.

A comparison of criteria evaluated for exact and robust exact mixture design are summarized in Table 5.21. The Min $IV$ increases from 3.3 to 9.5, but the $IV$-efficiency drops from 28.2 to 20.5. As expected, the robust design will have a lower $IV$-efficiency because only one vertex is included.

5.1.2. The 8-Point Design: Design points of the exact design are similar to those of the 7-point $IV$-optimal design. Its design points are $(1, 0, 0)$, $(0, 1, 0)$, $(0, 0, 1)$, two $(.5, 0, .5)$'s, $(.51, .49, 0)$, $(0, .49, .51)$, and $(.27, .45, .28)$ as illustrated in Figure 5.13. The interior point is not at the centroid as in the 7-point design. If the interior point were at the centroid, the Min $IV$ would be lower compared to the current design. The robust exact mixture design contains points $(0, 1, 0)$, $(.75, 0, .25)$, $(.25, 0, .75)$, $(.8, .2, 0)$, $(.3, .7, 0)$, $(0, .15, .85)$, $(0, .65, .35)$, and $(.3, .35, .35)$. Seven of these are lying on the boundary of the design region. Design points of the robust exact design are similar to those of the 8-point $A$-optimal design. Without a missing point, the minimum and mean of SPVs of the exact design are 2.33 and 3.53, respectively, and for the robust exact design, the minimum and mean of SPVs are 2.63 and 4.6, respectively.

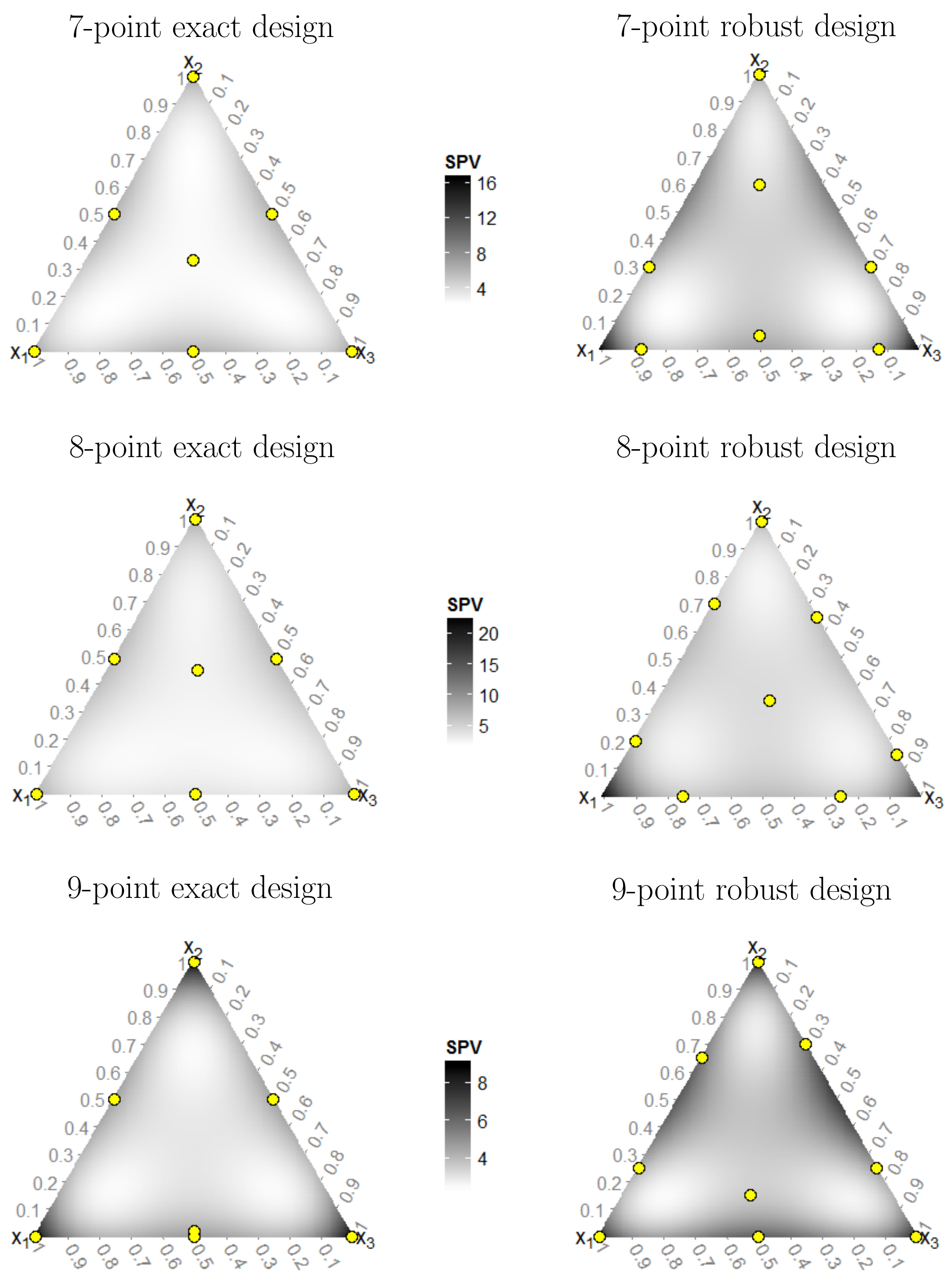



Figure 5.13: The three-component $IV$-optimal exact and robust exact mixture designs for a second-order Scheffé polynomial. Numbers represent the number of replications.

Table 5.21: Properties of the 3-factor $IV$-optimal mixture designs for $n = 7$, 8, and 9.

| | 7-point | | 8-point | | 9-point | |
|---|---|---|---|---|---|---|
| Criteria Evaluated | Exact | Robust | Exact | Robust | Exact | Robust |
| $D$-efficiency | 24.600 | 17.363 | 24.007 | 17.180 | 24.784 | 22.349 |
| Min $D$-efficiency | 12.719 | 11.345 | 8.347 | 13.246 | 5.350 | 17.463 |
| Leave-1-out $D$-efficiency | 17.884 | 14.077 | 18.610 | 15.411 | 18.492 | 20.418 |
| | (5.315) | (1.893) | (6.480) | (1.141) | (9.529) | (2.298) |
| Leave-2-out $D$-efficiency | | | 8.040 | 12.126 | 10.877 | 16.855 |
| | | | (9.661) | (2.808) | (10.673) | (4.971) |
| $A$-efficiency | 13.050 | 7.278 | 13.157 | 7.774 | 14.717 | 11.012 |
| Min $A$-efficiency | 1.575 | 3.245 | 0.148 | 4.670 | 0.008 | 6.614 |
| Leave-1-out $A$-efficiency | 4.778 | 3.854 | 6.782 | 5.821 | 9.023 | 8.705 |
| | (4.170) | (1.174) | (5.523) | (0.723) | (6.757) | (1.616) |
| Leave-2-out $A$-efficiency | | | 2.221 | 3.101 | 4.363 | 5.792 |
| | | | (3.801) | (1.587) | (6.242) | (3.026) |
| $G$-efficiency | 86.369 | 36.936 | 75.060 | 26.877 | 66.670 | 75.099 |
| Min $G$-efficiency | 0.763 | 3.184 | 0.068 | 8.919 | 0.004 | 9.486 |
| Leave-1-out $G$-efficiency | 20.524 | 12.068 | 36.352 | 17.808 | 49.341 | 36.680 |
| | (35.646) | (11.160) | (41.375) | (7.562) | (37.051) | (23.892) |
| Leave-2-out $G$-efficiency | | | 10.060 | 8.719 | 27.814 | 19.700 |
| | | | (26.141) | (6.351) | (39.924) | (19.465) |
| $IV$-efficiency | 28.185 | 20.569 | 28.157 | 21.615 | 29.905 | 25.193 |
| Min $IV$-efficiency | 3.299 | *9.534* | 0.319 | *15.617* | 0.018 | *17.971* |
| Leave-1-out $IV$-efficiency | 10.265 | 11.105 | 14.501 | 16.441 | 18.107 | 20.430 |
| | (8.216) | (2.175) | (11.461) | (0.879) | (13.555) | (2.194) |
| Leave-2-out $IV$-efficiency | | | 4.764 | 9.149 | 8.681 | 14.089 |
| | | | (7.828) | (4.592) | (12.415) | (6.534) |

Numbers in parentheses represent standard deviations

As shown in Table 5.21, the Min $IV$ is much higher in the robust exact design than in the exact design. For the exact design, if one of the vertices is missing, the $IV$-efficiency will be less than 1. Note that different missing vertices will give different $IV$-efficiencies, but all corresponding values are very small ($< 1$). The leave-1-out and leave-2-out $IV$-efficiencies indicate that the robust exact design is more robust to one and two missing points than the exact design.

5.1.3. The 9-Point Design: The design points of exact and robust exact mixture designs are illustrated in Figure 5.13. Unlike the 7- and 8-point $G$-optimal exact designs, the 9-point exact design does not have points close to the centroid, and most design points are lying on the boundary of the design region. Design points are the SLD$\{3, 2\}$ and $(.49, .02, .49)$, and they are also vertically symmetric. Two replicates are at the middles of the triangle. For the robust exact design, it contains all vertices, as well as $(.45, .15, .4)$, $(0, .7, .3)$, $(.5, 0, .5)$, $(0, .25, .75)$, $(.75, .25, 0)$, and $(.35, .65, 0)$. A pattern of design points is similar to those of the 9-point $A$-optimal exact design as shown in Figure 5.7. As shown in Figure 5.13, the SPVs of the exact design are high at points near or at vertices, and for the robust exact design, predictions near or at the vertices and middles of edges are poor compared to the rest of the design space.

A comparison of properties of exact and robust exact designs are presented in Table 5.21. The resulting robust exact design is impressive because of the high values of Min $IV$ and $IV$-efficiency. The Min $IV$ increases from 0.02 to 18 while the $IV$-efficiency drops slightly from 29.9 to 25.2 when using the robust exact mixture design instead of the exact mixture design. According to the leave-1-out and leave-2-out $IV$-efficiencies, the robust exact design is also more robust to one and two missing points.

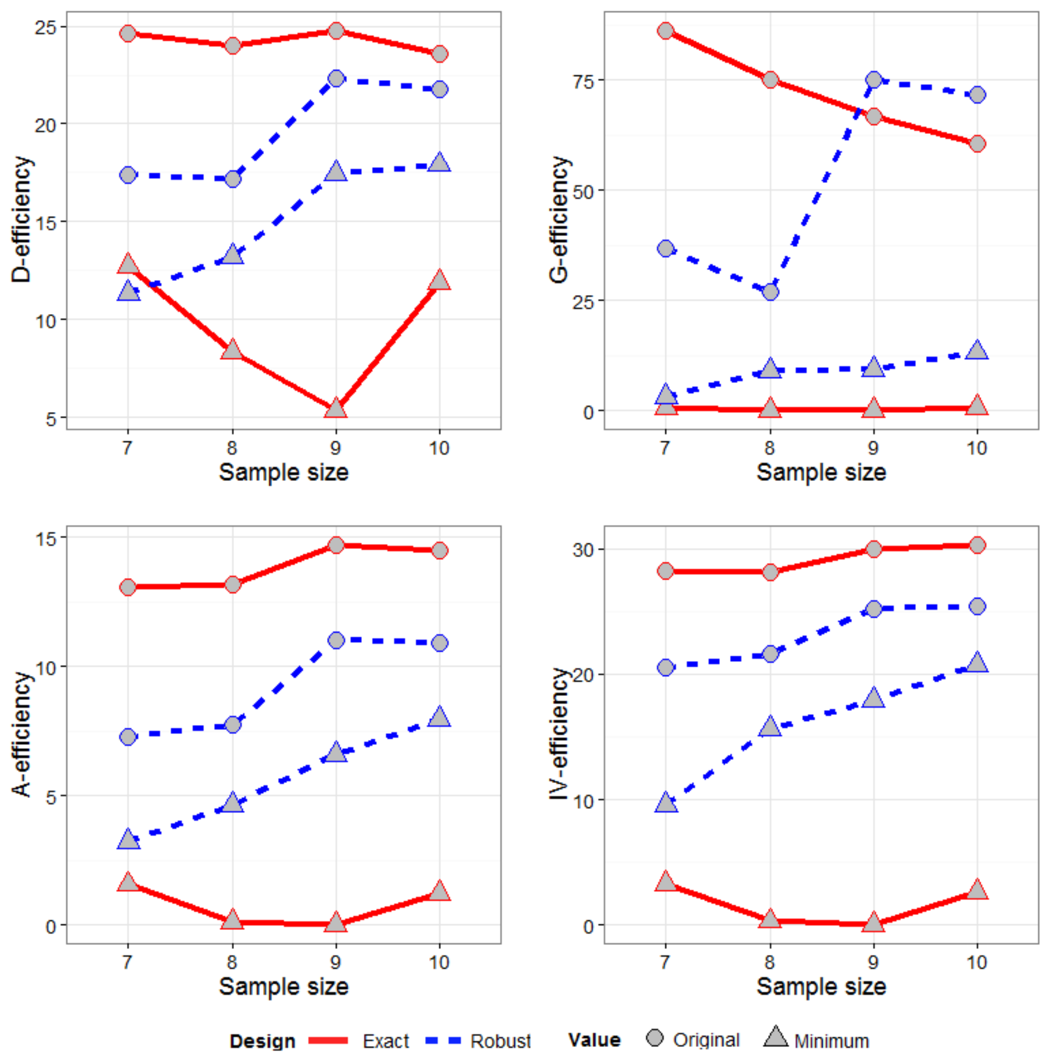



Figure 5.14: Summary of $D$-, $A$-, $G$-, $IV$-efficiencies and corresponding minimum efficiencies of three-component $IV$-optimal exact and robust exact mixture designs.

5.1.4. The 10-Point Design: The exact mixture design is the same as the $A$-optimal exact design, and the robust exact design is the same as the $A$-optimal robust exact design. In Figure 5.14, all efficiencies of the $A$-optimal exact and robust exact designs are plotted against the sample sizes. The Min $A$, Min $D$, and Min $IV$ increase as the sample sizes increase. The patterns of criteria response related to $A$- and $IV$-

criteria are about the same. For example, when the sample size increases from 7 to 8, the Min $A$ and Min $IV$ of the exact mixture design decrease, and then the Min $A$ and Min $IV$ slightly decrease when $n$ increases from 9 to 10.

## 5.2. Four-Component $IV$-Optimal Mixture Designs

The Matlab (MATLAB, 2014) program was written to find both exact and robust exact designs by using supports SLD$\{4, 50\}$ and SLD$\{4, 20\}$, respectively. We use a coarser grid for robust exact mixture designs because criterion (4.4) itself is heavily time-consuming. The sample sizes in this study are 11, 12, 13, and 14.

### 5.2.1. The 11-Point Design:

Design points of exact and robust exact designs are listed in Table 5.22. The $IV$-optimal design is exactly the same as the $G$-optimal exact design, but this is not the case for the robust exact design. The robust exact design has no vertices and pattern of design points. This is what we actually expected because the sample size of 11 is very small, and to maximize the Min $IV$ or Min $G$, prediction criteria, the vertices seem not to be the most important as we saw in the three-component $IV$- and $G$-optimal robust exact mixture designs.

The properties of both exact and robust exact designs are summarized in Table 5.23. In this case, the MIN $IV$ is slightly improved when using the robust exact design instead of the exact design, but the $IV$-efficiency drops considerably from 13.2 to 5.9. We would recommend using the exact design because many criteria values are much higher than those in the robust exact design. Like near-saturated $G$-optimal robust exact design, the 11-point $IV$-optimal robust design is very poor in both parameter estimation and precision of the prediction.

5.2.2. The 12-Point Design: The exact mixture design contain the SLD$\{4, 2\}$ points, face point $(1/3, 1/3, 1/3, 0)$, and interior point $(.21, .21, .21, .37)$. The robust exact mixture design has only one vertex, and most design points are lying on the boundary of the design region as listed in Table 5.22. The robust exact design does not have very low $IV$-efficiency compared to that of the exact design. The Min $IV$, Min $A$, and Min $G$ are improved, but the corresponding leave-1-out efficiency is lower in the robust exact design than in the exact design.

5.2.3. The 13-Point Design: The exact mixture designs contains the SLD$\{4, 2\}$ points and face points $(.38, .24, .38, 0)$, $(.38, .24, 0, .38)$, $(0, .24, .38, .38)$. If one of the vertices is missing, the $IV$-efficiency will drop to 4.6 as shown in Table 5.23. However, losing vertex point $(0, 1, 0, 0)$ does not cause the lowest $IV$-efficiency because points on the faces all have .24 in the second component while other component values are 0 and .38.

Because the sample size is larger, the difference between $IV$-efficiencies of both exact and robust designs is smaller than that of the 11- or 12-point designs. The Min $IV$ increases from 4.6 to 10.8, but leave-1-out and leave-2-out $IV$-efficiencies are not much changed. Overall, the robust exact design can be an alternative which is more robust to a missing point but less $IV$-optimal. Considering criteria related to $D$- and $A$-criteria, both designs have about the same precision of parameter estimation and robustness to one and two missing points.

Table 5.22: Design points of 4-component $IV$-optimal robust exact mixture designs.

| Point Types | $n=11$ | | | | $n=12$ | | | | $n=13$ | | | | $n=14$ | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | $x_1$ | $x_2$ | $x_3$ | $x_4$ | $x_1$ | $x_2$ | $x_3$ | $x_4$ | $x_1$ | $x_2$ | $x_3$ | $x_4$ | $x_1$ | $x_2$ | $x_3$ | $x_4$ |
| Vertices | | | | | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 1 | 0 | 1 | 0 | 0 |
| | | | | | | | | | 0 | 1 | 0 | 0 | 0 | 0 | 1 | 0 |
| | | | | | | | | | | | | | 0 | 0 | 0 | 1 |
| Edges | .3 | 0 | .7 | 0 | 0 | .9 | .1 | 0 | .9 | 0 | 0 | .1 | 0 | .35 | 0 | .65 |
| | .7 | .3 | 0 | 0 | .7 | .3 | 0 | 0 | .05 | 0 | .95 | 0 | .9 | 0 | 0 | .1 |
| | 0 | .7 | 0 | .3 | 0 | .3 | .7 | 0 | 0 | .3 | 0 | .7 | .4 | 0 | 0 | .6 |
| | 0 | 0 | .4 | .6 | .35 | 0 | 0 | .65 | 0 | .7 | .3 | 0 | .6 | 0 | .4 | 0 |
| | .5 | 0 | 0 | .5 | .6 | 0 | .4 | 0 | .7 | .3 | 0 | 0 | .7 | .3 | 0 | 0 |
| | .1 | .9 | 0 | 0 | .8 | 0 | 0 | .2 | .6 | 0 | .4 | 0 | 0 | 0 | .5 | .5 |
| | | | | | | | | | 0 | 0 | .5 | .5 | | | | |
| | | | | | | | | | .5 | 0 | 0 | .5 | | | | |
| Faces | .9 | 0 | .05 | .05 | .5 | 0 | .85 | .1 | 0 | .2 | .7 | .1 | 0 | .4 | .4 | .2 |
| | .1 | .15 | 0 | .75 | 0 | .3 | .2 | .5 | .25 | .5 | 0 | .25 | .1 | .2 | .7 | 0 |
| | .05 | .45 | .5 | 0 | .1 | .7 | 0 | .2 | .3 | 0 | .4 | .3 | .3 | 0 | .4 | .3 |
| | 0 | .1 | .8 | .1 | .1 | 0 | .4 | .5 | | | | | .3 | .4 | 0 | .3 |
| | | | | | | | | | | | | | .15 | .70 | .15 | 0 |
| Interior | .3 | .2 | .3 | .2 | .35 | .25 | .3 | .1 | | | | | | | | |

Table 5.23: Properties of the 4-factor $IV$-optimal mixture designs for $n = 11$, 12, 13, and 14.

| | 11-point | | 12-point | | 13-point | | 14-point | |
|---|---|---|---|---|---|---|---|---|
| Criteria Evaluated | Exact | Robust | Exact | Robust | Exact | Robust | Exact | Robust |
| $D$-efficiency | 16.413 | 10.143 | 15.746 | 10.654 | 15.472 | 13.188 | 14.974 | 12.974 |
| Min $D$-efficiency | 11.487 | 8.023 | 10.406 | 8.374 | 10.517 | 10.753 | 10.830 | 10.705 |
| Leave-1-out $D$-efficiency | 12.957 | 8.606 | 13.232 | 9.531 | 13.513 | 12.042 | 13.459 | 12.057 |
| | (1.698) | (0.520) | (1.966) | (0.644) | (2.073) | (0.926) | (1.846) | (0.909) |
| Leave-2-out $D$-efficiency | | | 8.078 | 7.662 | 10.584 | 10.180 | 11.825 | 10.928 |
| | | | (5.004) | (1.393) | (3.874) | (2.218) | (2.276) | (1.272) |
| $A$-efficiency | 5.902 | 2.635 | 5.764 | 2.940 | 5.884 | 4.141 | 5.930 | 4.331 |
| Min $A$-efficiency | 1.015 | 0.959 | 0.612 | 1.515 | 0.813 | 2.005 | 1.452 | 2.435 |
| Leave-1-out $A$-efficiency | 1.862 | 1.315 | 2.792 | 2.007 | 3.568 | 3.018 | 4.064 | 3.433 |
| | (1.493) | (0.286) | (1.754) | (0.341) | (1.928) | (0.724) | (1.806) | (0.640) |
| Leave-2-out $A$-efficiency | | | 0.921 | 0.936 | 1.810 | 1.841 | 2.577 | 2.494 |
| | | | (1.122) | (0.599) | (1.614) | (0.994) | (1.648) | (0.813) |
| $G$-efficiency | 91.908 | 14.640 | 83.892 | 22.904 | 77.658 | 43.613 | 72.788 | 44.291 |
| Min $G$-efficiency | 1.099 | 1.735 | 0.609 | 3.562 | 0.796 | 5.159 | 1.464 | 5.763 |
| Leave-1-out $G$-efficiency | 11.970 | 5.399 | 20.653 | 10.702 | 28.050 | 19.323 | 32.350 | 22.659 |
| | (29.245) | (2.762) | (33.306) | (5.929) | (32.544) | (15.168) | (31.295) | (14.904) |
| Leave-2-out $G$-efficiency | | | 3.822 | 4.245 | 9.600 | 8.849 | 14.142 | 12.061 |
| | | | (12.547) | (4.195) | (18.197) | (9.283) | (20.617) | (9.951) |
| $IV$-efficiency | 20.007 | 13.238 | 20.159 | 14.223 | 20.620 | 16.171 | 21.126 | 17.401 |
| Min $IV$-efficiency | 5.572 | *5.885* | 3.589 | *8.724* | 4.561 | *10.825* | 7.395 | *12.599* |
| Leave-1-out $IV$-efficiency | 6.937 | 6.964 | 10.317 | 9.935 | 12.850 | 12.314 | 14.870 | 14.285 |
| | (3.974) | (0.902) | (5.042) | (1.025) | (5.619) | (1.677) | (5.250) | (1.491) |
| Leave-2-out $IV$-efficiency | | | 3.619 | 4.788 | 6.883 | 7.896 | 9.740 | 10.776 |
| | | | (3.556) | (2.912) | (4.991) | (3.583) | (5.025) | (2.846) |

Numbers in parentheses represent standard deviations

5.2.4. The 14-Point Design: The exact mixture design contains the SLD$\{4, 2\}$ points, face points $(1/3, 1/3, 1/3, 0)$ and its three variations. For the robust exact mixture design, there are three vertices. It is seen from Table 5.22, the number of vertices in the robust design increases as the sample size increases. The robust exact design has very high $IV$-efficiency compared to that of the exact design, and the Min $IV$ increases from 7.4 to 12.6. The leave-1-out $IV$-efficiencies, as well as leave-2-out $IV$-efficiencies, are about the same in both exact and robust exact designs. Considering criteria related to the $D$- and $A$-optimality, the precision of parameter estimation in the robust exact design is slightly less than that of the exact design.

As illustrated in Figure 5.15, the Min $IV$, Min $A$, and $IV$- and $A$-efficiencies of the $IV$-optimal robust exact mixture design increase as the sample sizes increase. When sample size is 11 (smallest design), the robust exact design is very poor. However, when the sample size is large, i.e. $n = 13, 14$, the Min $IV$ criterion can improve the robustness with small loss in an $IV$-efficiency.

## 6. An Example of a Constrained Mixture Experiment

To illustrate the construction of a robust mixture design against a missing value, consider a problem studied by Tabarestani and Tehrani (2014). They investigated the influence of the different mixtures of fat replacers on the physicochemical properties of low-fat hamburger: texture, color, cooking yield, cooking loss, shrinkage, fat retention, moisture retention, and juiciness. The fat replacer is composed of a combination of soy flour ($x_1$), split-pea flour ($x_2$), and starch. If the fat replacer could replace the original fat without any decrease in physical properties, the resulting healthier hamburger would be attractive to people. The 13-run mixture experiment design used in their study is listed in Table 5.24.

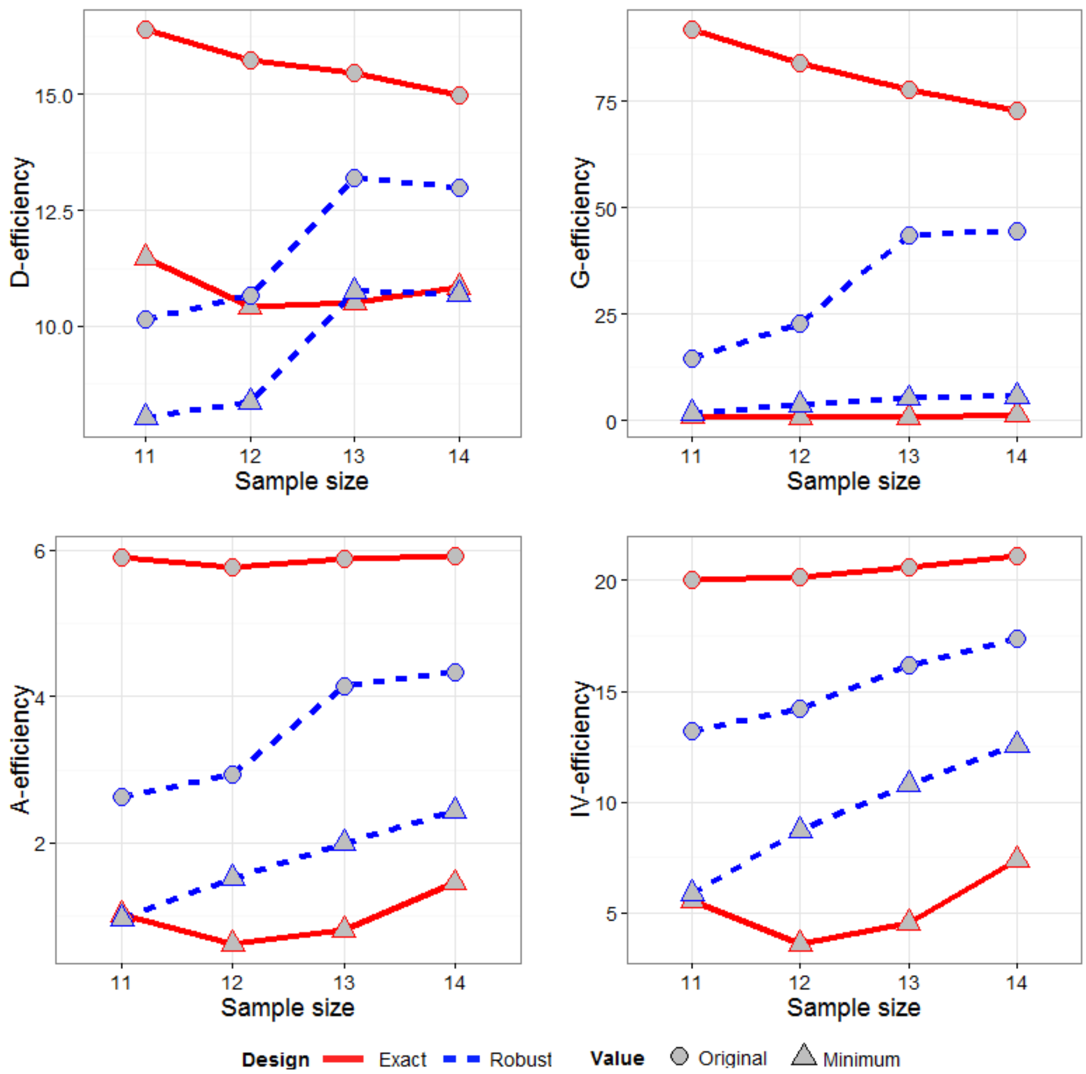



Figure 5.15: Summary of $D$-, $A$-, $G$-, $IV$-efficiencies and corresponding minimum efficiencies of four-component $IV$-optimal exact and robust exact mixture designs.

Note that a sum of fat replacer components in raw data in Table 5.24 equals 15% of all ingredients of low-fat beef burger. The actual components are calculated by dividing each component value by 15. Also, based on the subject-matter knowledge and preliminary experiments, constraints on the mixture components are $0 < q_1 < \frac{2}{3}$, $0 < q_2 < \frac{2}{3}$, and $0 < q_3 < \frac{1}{3}$. The thirteen runs of actual component values are illustrated in Figure 5.16. We have used the Xvert function in R package mixexp (Lawson, 2014) to find the extreme vertices. The Xvert function applies the XVERT algorithm proposed by Snee and Marquardt (1974), and it was published in FORTRAN code by Piepel (1988). As shown in Figure 5.16, the design region is a trapezoid whose vertices are $(\frac{2}{3}, \frac{1}{3}, 0)$, $(\frac{2}{3}, 0, \frac{1}{3})$, $(0, \frac{2}{3}, \frac{1}{3})$, and $(\frac{1}{3}, \frac{2}{3}, 0)$. The design points in their study consists four vertices, four midpoints of the edges, a center point, and four interior points. The method to select those design points was not mentioned in the article, but it is actually an augmented simplex lattice design. This design was used to optimize multiple responses simultaneously. We have evaluated their design as if the second-order model were fitted. Its $D$-efficiency and Min $D$ are 3.669 and 2.892, respectively.

Table 5.24: Experimental design with three components: soy flour, split-pea flour and starch.

| Raw Component Data (grams) | | | Actual Component | | |
|---|---|---|---|---|---|
| Soy ($x_1$) | Split-pea ($x_2$) | Starch ($x_3$) | Soy ($q_1$) | Split-pea ($q_2$) | Starch ($q_3$) |
| 6.25 | 6.25 | 2.50 | .4167 | .4167 | .1666 |
| 8.13 | 5.63 | 1.24 | .5420 | .3753 | .0827 |
| 10.00 | 2.50 | 2.50 | .6666 | .1667 | .1667 |
| 5.00 | 5.00 | 5.00 | .3333 | .3333 | .3334 |
| 10.00 | 5.00 | 0.00 | .6667 | .3333 | .0000 |
| 5.63 | 8.13 | 1.24 | .3753 | .5420 | .0827 |
| 10.00 | 0.00 | 5.00 | .6667 | .0000 | .3333 |
| 8.13 | 3.13 | 3.74 | .5420 | .2087 | .2493 |
| 7.50 | 7.50 | 0.00 | .5000 | .5000 | .0000 |
| 5.00 | 10.00 | 0.00 | .3333 | .6667 | .0000 |
| 2.50 | 10.00 | 2.50 | .1667 | .6666 | .1667 |
| 3.13 | 8.13 | 3.74 | .2087 | .5420 | .2493 |
| 0.00 | 10.00 | 5.00 | .0000 | .6667 | .3333 |

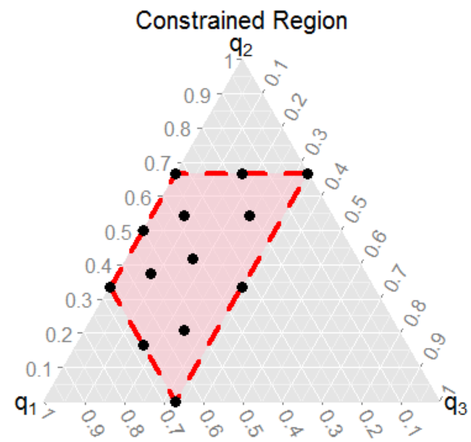



Figure 5.16: Data from Tabarestani and Tehrani (2014).

Suppose we want to consider $D$-optimal mixture designs having the sample size of less than or equal to 13 to fit a second-order Scheffé polynomial. The $D$-optimal exact and robust exact designs can be constructed in the usual way. The support for searching exact and robust exact mixture designs is SLD$\{3, 100\}$ with aforementioned upper bound constraints. The component values of .33 and .66 may be replaced by $\frac{1}{3}$ and $\frac{2}{3}$, respectively if the $D$-efficiency and/or Min $D$ are improved.

For $n = 7$, the exact design contains points lying only on the boundary of the design region as shown in Figure 5.17. Those are vertices: $(\frac{2}{3}, 0, \frac{1}{3})$, $(0, \frac{2}{3}, \frac{1}{3})$, $(\frac{2}{3}, \frac{1}{3}, 0)$, and $(\frac{1}{3}, \frac{2}{3}, 0)$ and midpoints: $(\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$, $(\frac{4}{6}, \frac{1}{6}, \frac{1}{6})$, and $(\frac{1}{6}, \frac{4}{6}, \frac{1}{6})$. Its $D$-efficiency is as high as 4.717, but if point $(\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$ is missing, the $D$-efficiency will drop to zero. For the robust exact design, all design points are the same as those in the exact design, but only midpoint $(0, \frac{2}{3}, \frac{1}{3})$ is moved to (.17, .58, .25). This causes the new design to have the $D$-efficiency of 4.442 and Min $D$ of 3.206.

For $n = 8$, the exact design points are the same as those of the 7-point $D$-optimal exact design but with an additional point (.4, .4, .2). Its $D$-efficiency is 4.637, and the Min $D$ of 3.441 results from losing one of points $(\frac{2}{3}, 0, \frac{1}{3})$ and $(0, \frac{2}{3}, \frac{1}{3})$. The robust exact design has all vertices as well as $(.66, .14, .2)$, $(.42, .42, .16)$, $(.14, .66, .20)$, and $(\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$. Its $D$-efficiency and Min $D$ are 4.538 and 3.650, respectively.

For $n = 9$, the exact design as shown in Figure 5.19 (top) is composed of vertices and midpoints with two replicates at $(0, \frac{2}{3}, \frac{1}{3})$ and $(\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$. Its $D$-efficiency and Min $D$ are 4.607 and 3.057, respectively. The minimum $D$-efficiency is a result of losing point $(\frac{2}{3}, 0, \frac{1}{3})$. For the robust exact mixture design, design points are $(1, 0, 0)$, $(0, 1, 0)$, $(0, 0, 1)$, $(.66, .2, .14)$, $(.32, .35, .33)$, $(.2, .66, .14)$, $(.55, .12, .33)$, and 2 $(0, \frac{2}{3}, \frac{1}{3})$'s. The $D$-efficiency and Min $D$ respectively are 4.407 and 3.755.

For $n = 10$, as illustrated in Figure 5.18 design points of the exact design are the same as those of the 9-point exact design, but an additional replicate is added to $(\frac{2}{3}, 0, \frac{1}{3})$. Its $D$-efficiency and Min $D$ are 4.637 and 3.843, respectively. The robust exact design has also three points at vertices with two replicates at $(\frac{2}{3}, 0, \frac{1}{3})$ and $(0, \frac{2}{3}, \frac{1}{3})$. Other points on the boundary are $(.66, .23, .11)$, $(.23, .66, .11)$, $(\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$, and $(.35, .65, 0)$. The only interior point is $(.39, .38, .23)$. This design has the $D$-efficiency of 4.482 and Min $D$ of 3.919.

For $n = 11$, the exact design has the same pattern as that of the 10-point exact design. It contains (1) vertices with two replicates at $(\frac{2}{3}, \frac{1}{3}, 0)$, $(\frac{2}{3}, 0, \frac{1}{3})$, and $(0, \frac{2}{3}, \frac{1}{3})$; (2) boundary points $(\frac{2}{3}, \frac{1}{6}, \frac{1}{6})$ and 2 $(\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$'s; and (3) interior point $(.19, .66, .16)$. The design have a $D$-efficiency of 4.662 and Min $D$ of 3.945. For the robust exact design, a pattern of design points is similar to that of the 10-point robust exact design. There are four vertices with two replicates, and other points are $(.66, .20, .14)$, $(\frac{1}{6}, \frac{2}{3}, \frac{1}{6})$, $(.49, .51, 0)$, $(\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$, and $(.37, .37, .26)$. Its $D$-efficiency and Min $D$ are 4.496 and 4.145, respectively.

For $n = 12$, the exact design contains two replicates in each vertex, two replicates at $(\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$, and midpoints $(\frac{1}{6}, \frac{2}{3}, \frac{1}{6})$, $(\frac{2}{3}, \frac{1}{6}, \frac{1}{6})$. The design has $D$-efficiency of 4.718 and Min $D$ of 4.361. Like the exact design. the robust exact design has two replicates at all vertices and one replicate at midpoints $(\frac{1}{6}, \frac{2}{3}, \frac{1}{6})$, $(\frac{2}{3}, \frac{1}{6}, \frac{1}{6})$, and the last two points are $(\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$ and $(.35, .36, .29)$. Its $D$-efficiency and Min $D$ are 4.670 and 4.367, respectively.

For $n = 13$, the design points of exact and robust exact are exactly the same. Both contain two replicates at all vertices, two replicates at $(\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$, and also midpoints $(\frac{1}{6}, \frac{2}{3}, \frac{1}{6})$, $(\frac{2}{3}, \frac{1}{6}, \frac{1}{6})$. Interior point $(.41, .41, .18)$ is also included. The design points are presented in Figure 5.19. The $D$-efficiency and Min $D$ are 4.778 and 4.629, respectively.

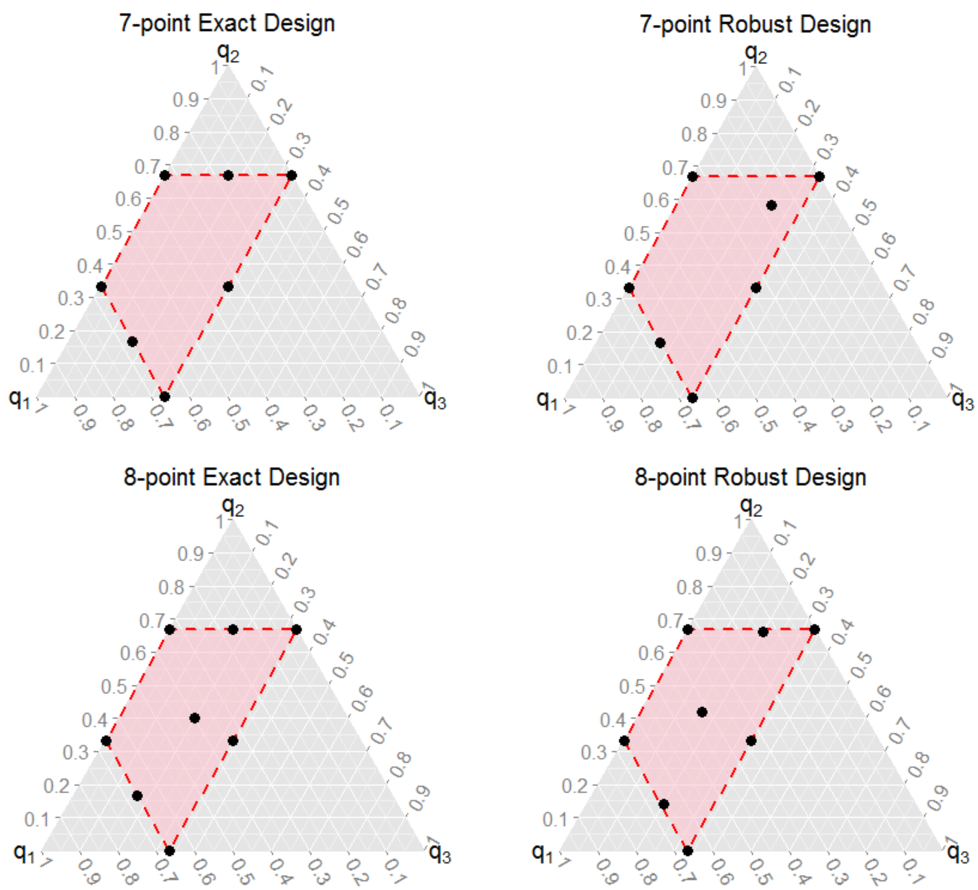



Figure 5.17: The 7- and 8-point exact and robust exact designs for a low-fat hamburger experiment. Numbers represent the number of replications.

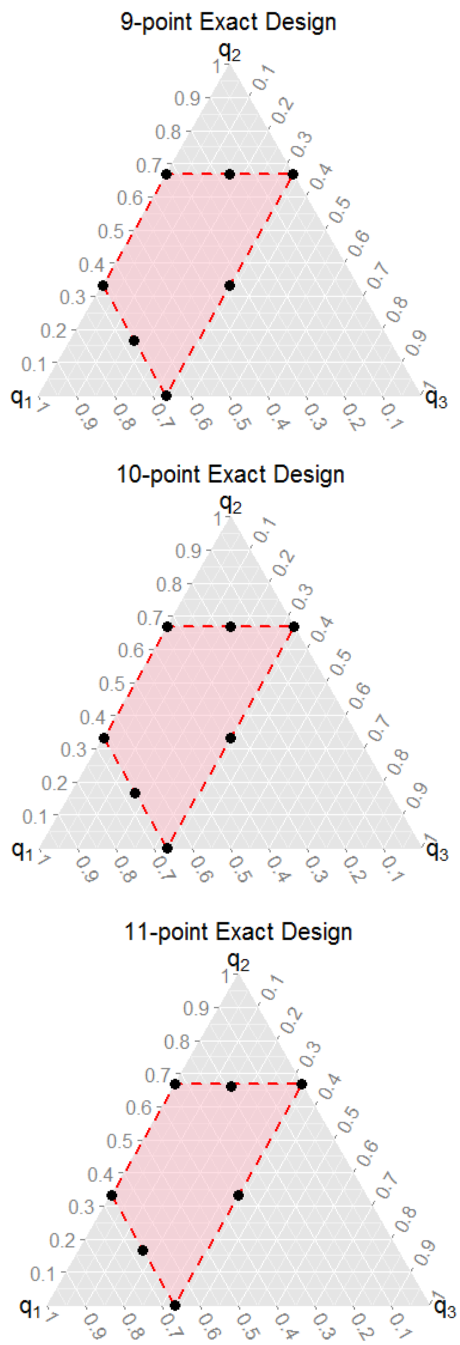



Figure 5.18: The 9-, 10-, and 11-point exact and robust exact designs for a low-fat hamburger experiment. Numbers represent the number of replications.

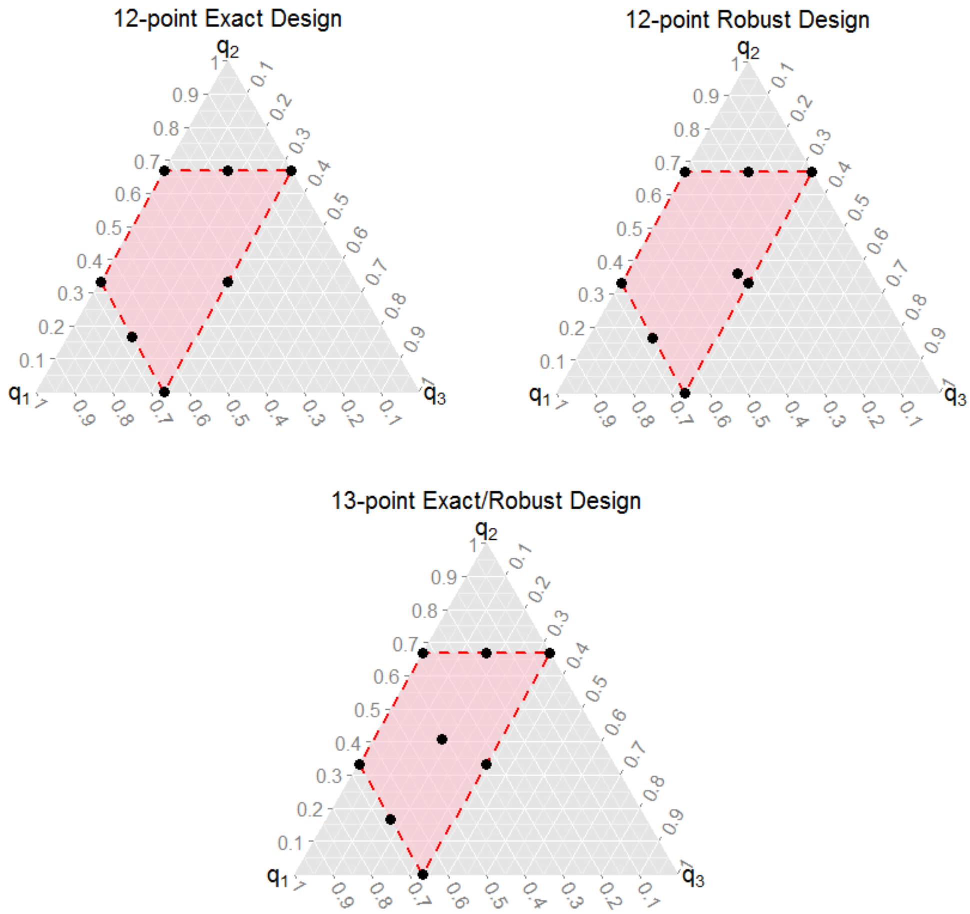



Figure 5.19: The 12- and 13-point exact and robust exact designs for a low-fat hamburger experiment.

# CHAPTER 6

# ADAPTIVE EXPERIMENTS

## 1. Introduction

Suppose a researcher has a well-planned experimental design, but it is not robust to a missing observation. However, when running the experiment, the response at $\mathbf{x}_i$ is uncollectible. It is natural to repeat this failed trial if additional resources are available. The cause of a failed trial is very important and should be explored. If it is a technical mishap such as an accidentally broken apparatus or randomly failing machine, then repeating the trial is feasible. On the other hand, a failed trial may result from infeasible operating settings or an unsuspected feature of the system being studied, in which case the initially defined experimental region $\mathcal{X}$ cannot be exhaustively studied. Such a missing point cannot be repeated. That point accordingly could be ignored, and the experimenter could continue collecting the data for the remaining experimental runs in the design. A serious problem, however, arises if the missing point appreciably affects the variances of estimates or the prediction variances. In extreme cases, this might make $\mathbf{X}^{\mathrm{T}}\mathbf{X}$ singular. To protect against such a problem, the rest of the design points after missing point $\mathbf{x}_i$ could be reconstructed according to a certain criterion, e.g., $D$-, $A$-, $G$-, and $IV$-optimality criteria. Different missing points will lead to selecting different sets of remaining design points. Thus, the design is changing in real time once one trial has failed, and the new design is referred to as an adaptive design. In this chapter, we will give examples of adaptive designs generated by $D$-, $A$-, $G$-, and $IV$-criteria. For each criterion, we will discuss potential improvement in the value of the criterion of the resulting design compared to the original exact design.

## 2. Examples of $D$-Optimal Adaptive Designs

Suppose the $(N_0 + N + 1)$-point experimental design has been planned, but when collecting responses in a random order, the $(N_0 + 1)$th point response is uncollectible and cannot be repeated. Furthermore, we have resources for only $N$ additional runs. Let $\mathbf{M}(\xi_0)$ denote the moment matrix of the $N_0$ design points whose responses were already collected and $\mathbf{M}(\xi)$ denote the moment matrix of the additional reconstructed $N$ design points. The $(N_0 + N)$-point $D$-optimal adaptive design is constructed in a way to maximize the determinant of

$$(N_0 + N)\mathbf{M}(\widetilde{\xi}) = N_0\mathbf{M}(\xi_0) + N\mathbf{M}(\xi)\,, \tag{6.1}$$

where $\mathbf{M}(\widetilde{\xi})$ is the combined moment matrix of the design points being collected before trial $\mathbf{x}_i$ is lost and new design points generated.

Suppose a researcher conducted an experiment using an 8-point $D$-optimal exact design, and the order of collecting data is illustrated in Figure 6.1. The responses at coordinates $(-1, 1)$, $(0, -.215)$, $(1, .082)$, $(0, 1)$, $(1, 1)$, $(1, -1)$, $(-1, -1)$, and $(-1, .082)$ are to be sequentially collected. The adaptive design will be constructed based on the support $\{-1, -.9, \ldots, .9, 1\}^2$.

First, suppose the first trial has failed and cannot be repeated. In this case, $N_0$ equals zero. As illustrated in Figure 6.2 with $N_0 = 0$, the adaptive design still has three points at vertices like the original exact design but also has point $(-1, .9)$ near to the missing point. The adaptive design points are listed in Table 6.1. The $D$-efficiencies of adaptive and exact designs are 44.542 and 39.849. The $D$-efficiency of the 7-point $D$-optimal exact design generated by a genetic algorithm (Borkowski,

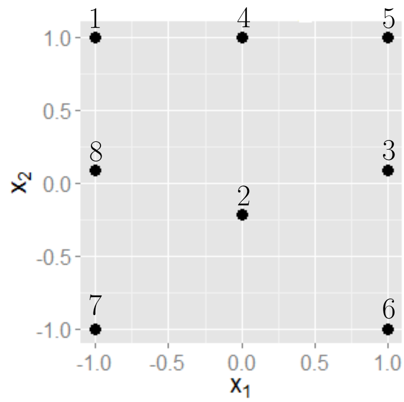



Figure 6.1: The random order of collecting responses in the eight-point $D$-optimal exact designs for a second-order model in two factors.

2003b) is 45.029. Thus, the adaptive design is just slightly inferior with respect to $D$-efficiency.

Suppose, the second response at $(0, -.215)$ is not collectible and cannot be repeated. The adaptive design corresponds to the design having $N_0 = 1$ in Figure 6.2. Also, Figure 6.2 with $N_0 = 2$ corresponds to the situation where the response at $(1, .082)$ was failed to be collected. In this case, the adaptive and exact designs are similar. The adaptive design respectively has points $(-1, .1)$ and $(-.1, 1)$ instead of $(-1, .082)$ and $(0, 1)$. The $D$-efficiencies of adaptive and exact designs are 44.890 and 44.873, respectively.

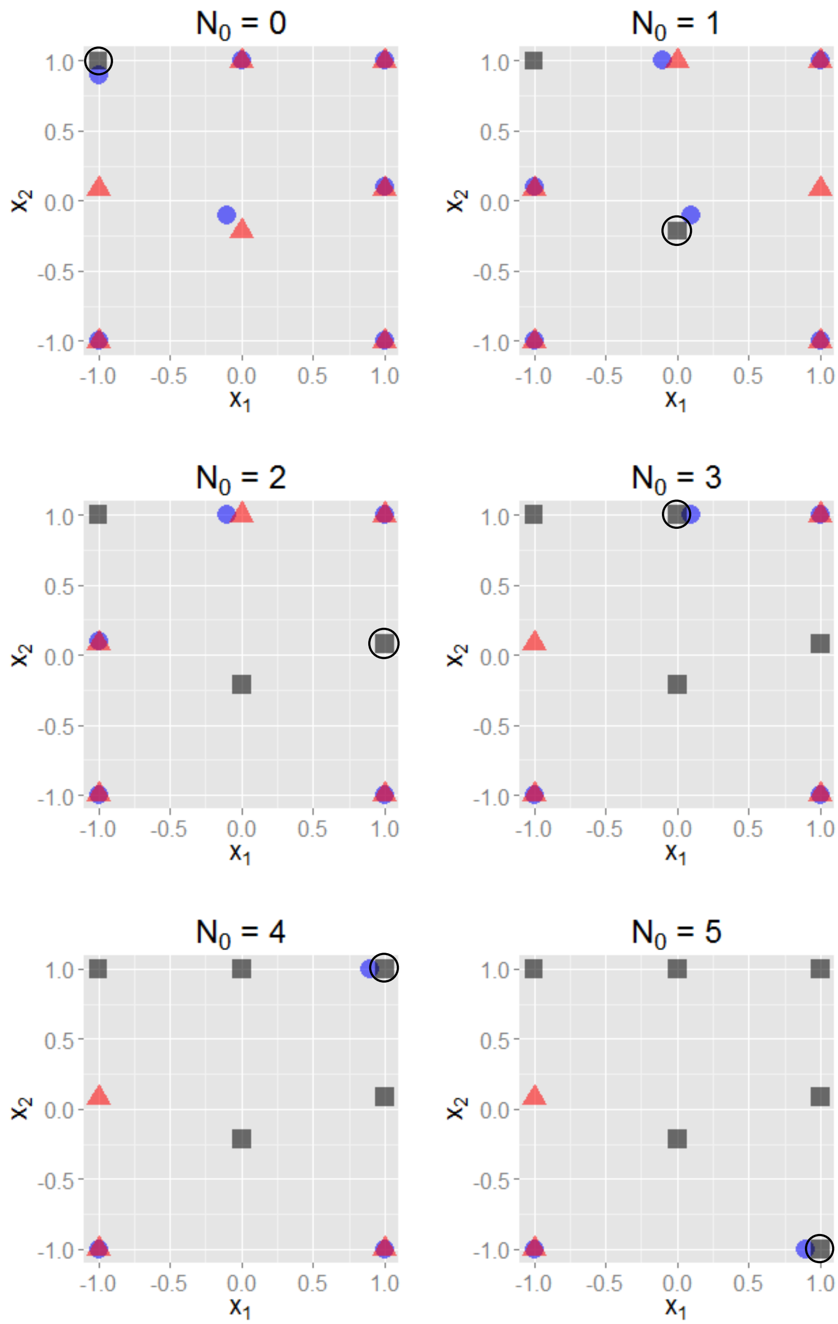



Figure 6.2: Seven-point $D$-optimal adaptive designs for a second-order model in 2 factors. Solid squares correspond the responses being collected and squares within a circle correspond to the failed response. Solid triangles correspond to the remaining design points not collected in the exact design and solid circles correspond to the adaptive design points.

Table 6.1: Seven-point $D$-optimal adaptive designs.

| Order | Original | | $N_0=0$ | | $N_0=1$ | | $N_0=2$ | | $N_0=3$ | | $N_0=4$ | | $N_0=5$ | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | $x_1$ | $x_2$ | $x_1$ | $x_2$ | $x_1$ | $x_2$ | $x_1$ | $x_2$ | $x_1$ | $x_2$ | $x_1$ | $x_2$ | $x_1$ | $x_2$ |
| 1 | -1 | 1 | | | -1 | 1 | -1 | 1 | -1 | 1 | -1 | 1 | -1 | 1 |
| 2 | 0 | -.215 | -.1 | .1 | | | 0 | -.215 | 0 | -.215 | 0 | -.215 | 0 | -.215 |
| 3 | 1 | .082 | 1 | .1 | .1 | -.1 | | | 1 | .082 | 1 | .082 | 1 | .082 |
| 4 | 0 | 1 | 0 | 1 | -.1 | 1 | -.1 | 1 | | | 0 | 1 | 0 | 1 |
| 5 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | | | 1 | 1 |
| 6 | 1 | -1 | 1 | -1 | 1 | -1 | 1 | -1 | 1 | -1 | 1 | -1 | | |
| 7 | -1 | -1 | -1 | -1 | -1 | -1 | -1 | -1 | -1 | -1 | -1 | -1 | -1 | -1 |
| 8 | -1 | .082 | -1 | .9 | -1 | .1 | -1 | .1 | .1 | 1 | .9 | 1 | .9 | -1 |

Table 6.2: Six-point $A$-optimal adaptive designs.

| Order | Original | | $N_0=0$ | | $N_0=1$ | | $N_0=2$ | | $N_0=3$ | | $N_0=4$ | | $N_0=5$ | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | $x_1$ | $x_2$ | $x_1$ | $x_2$ | $x_1$ | $x_2$ | $x_1$ | $x_2$ | $x_1$ | $x_2$ | $x_1$ | $x_2$ | $x_1$ | $x_2$ |
| 1 | -1 | .478 | | | -1 | .478 | -1 | .478 | -1 | .478 | -1 | .478 | -1 | .478 |
| 2 | 1 | .478 | 1 | .4 | | | 1 | .478 | 1 | .478 | 1 | .478 | 1 | .478 |
| 3 | 0 | -.218 | 0 | -.2 | 0 | -.2 | | | 0 | -.218 | 0 | -.218 | 0 | -.218 |
| 4 | 1 | -1 | 1 | -1 | 1 | -1 | 1 | -1 | | | 1 | -1 | 1 | -1 |
| 5 | 0 | 1 | .1 | 1 | -.1 | 1 | 0 | 1 | 0 | 1 | | | 0 | 1 |
| 6 | 0 | -.218 | -1 | .6 | 1 | .6 | 0 | -.3 | .9 | -1 | -.1 | 1 | | |
| 7 | -1 | -1 | -1 | -1 | -1 | -1 | -1 | -1 | -1 | -1 | -1 | -1 | -1 | -1 |

When the fourth response at point $(0, 1)$ has failed to be collected ($N_0 = 3$), the adaptive design attempts to repeat that response by having nearby point $(.1, 1)$ in the design. If the response is allowed to repeat at $(0, 1)$, the adaptive design will have that point instead of $(.1, 1)$. This may not be practically useful if data collection in the design space near $(0, 1)$ cannot be conducted. However, this indicates that point $(0, 1)$ is more important than point $(-1, .082)$ in terms of the $D$-efficiency, so that the adaptive design chose to place a point near $(0, 1)$ instead of $(-1, .082)$. The design points are illustrated in Figure 6.2 ($N_0 = 3$). The $D$-efficiencies of adaptive and exact designs are 44.896 and 43.150, respectively.

Figure 6.2 ($N_0 = 4$) corresponds to the situation where the response at the fifth design point has failed to be collected. The design points of the adaptive design are similar to those of the exact design. Instead of having a point close to $(-1, .082)$, the adaptive design has point $(.9, 1)$ which is near missing point $(1, 1)$. The $D$-efficiencies of the adaptive and exact designs are 43.769 and 39.849, respectively, so it is seen that the vertices are more important than the midpoints of the edges in terms of the $D$-efficiency.

If the sixth response has failed to be collected and cannot be repeated, conducting the experiment of the remaining design points in the exact design will yield the $D$-efficiency of 33.648. The adaptive design attempts to collect a response close to the missing point $(1, -1)$ by including point $(.9, -1)$ into the design, and the corresponding $D$-efficiency is 44.291.

From aforementioned adaptive designs, it is seen that only the design point for the missing response is removed from the candidate set. Thus, the adaptive design may include a point very close to the missing design point.

## 3. Examples of $A$-Optimal Adaptive Designs

Suppose an $(N_0 + N + 1)$-run experiment was conducted. When collecting the data, the $(N_0 + 1)$th trial has failed and cannot be repeated, and we have resources for only $N$ runs, for such a situation, we propose to apply the $A$-optimality criterion to find the set of $N$ points that maximizes the $A$-criterion. The set of $N$ points will be searched so that

$$\text{trace}\left[(N_0 + N)^{-1}\mathbf{M}^{-1}(\widetilde{\xi})\right] = \text{trace}\left[N_0\mathbf{M}(\xi_0) + N\mathbf{M}(\xi)\right]^{-1} \tag{6.2}$$

will be minimized. The resulting $(N_0 + N)$-point design will be referred to as the $A$-optimal adaptive design.

Suppose the 7-point $A$-optimal exact design whose design points are $(\pm 1, -1)$, $(0, 1)$, $(\pm 1, .478)$, and two $(0, -.218)$'s is planned to be used in the experimentation. These design points were found in Borkowski (2003b). The order of responses to be collected is illustrated in Figure 6.3. The adaptive design will be constructed based on the support $\{-1, -.9, \ldots, .9, 1\}^2$.

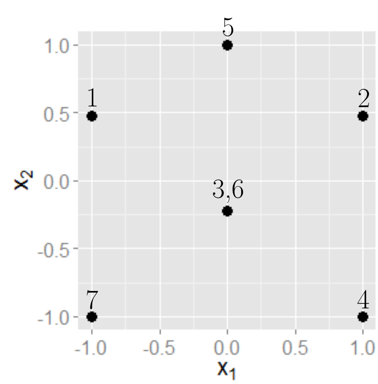



Figure 6.3: The random order of collecting responses in the seven-point $A$-optimal exact designs for a second-order model in two factors.

Figure 6.4 illustrates the adaptive designs when $N_0$ equals 0, 1, 2, 3, 4, and 5. If the first response at $(-1, .478)$ has failed to be collected, maximizing (6.2) results in an adaptive design that still has a point close to the missing point. This indicates that the missing point is important for the $A$-efficiency. The $A$-efficiencies of the adaptive and exact designs are 24.888 and 0, respectively. Hence, in this case conducting the experiment using the remaining points in the exact design is not very useful as the second-order model will not be estimable.

When $N_0 = 1$, the adaptive design contains point $(1, .6)$ close to missing point $(1, .478)$. The $A$-efficiencies of the adaptive and robust designs are 24.904 and 0, respectively. Thus, in this case a new set of adaptive design points is mandatory. Otherwise, the model parameters are not estimable.

For $N_0 = 2$, as illustrated in Figure 6.4, the third response at $(0, -.218)$ cannot be observed. However, the sixth response is also be collected at this point again. If $(0, -.218)$ is still in a set of candidate points, the adaptive and exact designs will be exactly the same having the $A$-efficiency of 24.932. Suppose point $(0, -.218)$ cannot be repeated, and point $(0, -.2)$ is excluded from the set of candidate points, the adaptive design will select nearby point $(0, -.3)$ instead of $(0, -.2)$, and the corresponding $A$-efficiency is 24.835.

For $N_0 = 3$, suppose experimenter determines not to allow any points in the neighboring region formed by $.8 \leq x_1 \leq 1$ and $-1 \leq x_2 \leq -.8$ to be included in the adaptive design. The adaptive design will collect the remaining responses at $(.7, -1)$, $(.1, 1)$, and $(-1, -1)$. It is seen that $(.7, -1)$ is still as close as possible to the missing response. The $A$-efficiencies of adaptive and exact designs are 23.077 and 0, respectively. As mentioned in Chapter 4, Section 4.1, if one of the boundary points in 7-point $A$-optimal exact design is missing, the $A$-efficiency $= 0$.

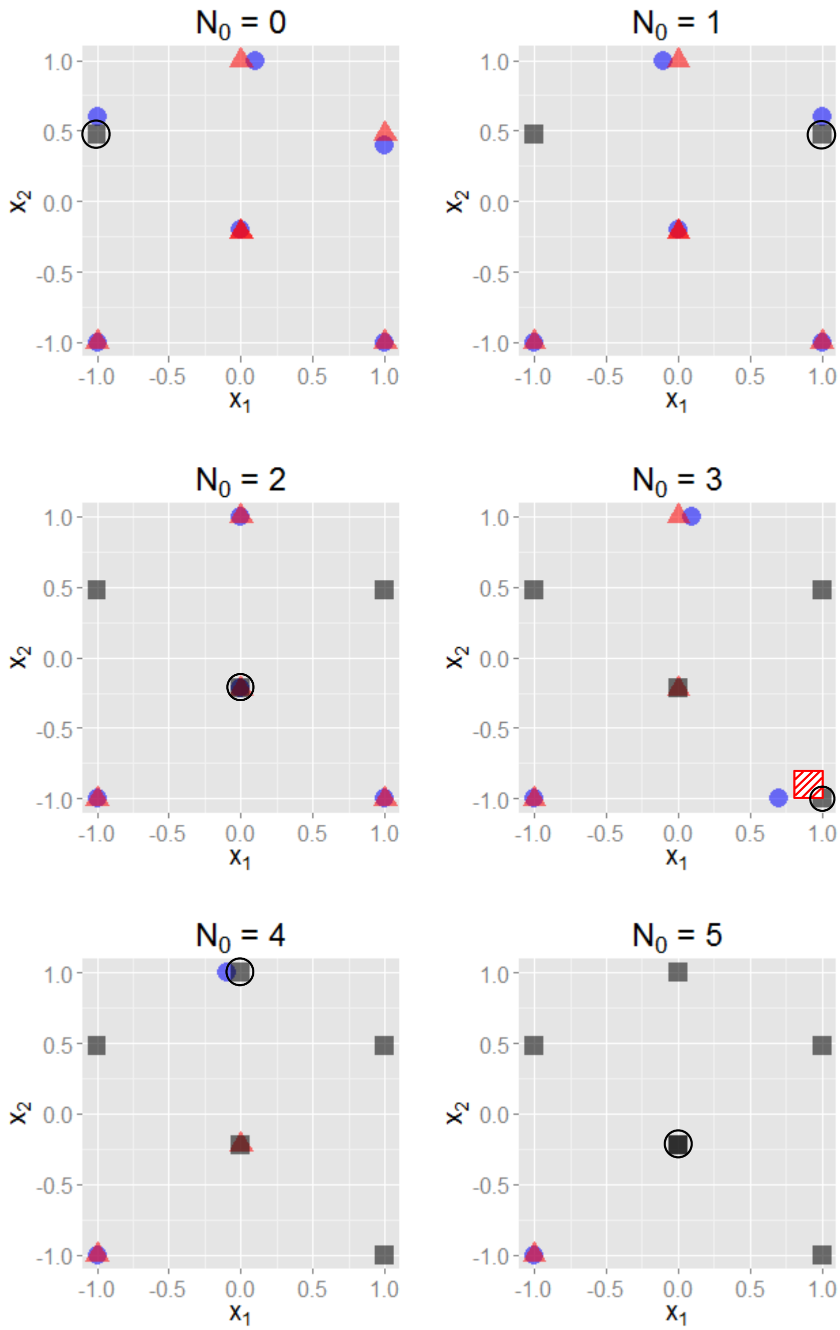



Figure 6.4: Six-point $A$-optimal adaptive designs for a second-order model in 2 factors. Solid squares correspond the responses being collected and squares within a circle correspond to the failed response. Solid triangles correspond to the remaining design points not collected in the exact design and solid circles correspond to the adaptive design points.

If the fifth response at $(0, 1)$ is missing, the adaptive design ($N_0 = 4$) will include only one replicate at points $(0, -.218)$ and $(-1, -1)$. The corresponding $A$-efficiency is 24.864. The exact design with missing point $(0, 1)$ has the $A$-efficiency $= 0$.

If the sixth point is missing, the last design point maximizing equation (6.2) will be $(-1, -1)$. This is the same for the exact design, and both designs have $A$-efficiency $= 24.931$. Hence, in this case the vertex is more important to the $A$-efficiency, so that the adaptive design chose not to include another point near $(0, -.218)$, the missing point.

## 4. Examples of $G$-Optimal Adaptive Designs

We can also apply the $G$-optimality criterion for reconstructing the design once the $(N_0 + 1)$th response is missing. Suppose the $(N_0 + N + 1)$-run experiment is employed, but when collecting responses in the order being randomly assigned, the $(N_0 + 1)$th observed value fails and cannot be repeated. Also, we have resources for only $N$ experimental runs. Instead of continuing collecting data at remaining design points, a set of points could be constructed to minimize

$$\max_{\mathbf{x} \in \mathcal{X}} \left[ (N_0 + N)^{-1} \mathbf{x}^{\mathrm{T}(m)} \mathbf{M}^{-1}(\widetilde{\xi}) \mathbf{x}^{(m)} \right], \tag{6.3}$$

where $(N_0 + N)\mathbf{M}(\widetilde{\xi}) = N_0 \mathbf{M}(\xi_0) + N\mathbf{M}(\xi)$. The resulting design will be referred to as the $(N_0 + N)$-point $G$-optimal adaptive design.

Suppose the seven-point three-component $G$-optimal exact mixture design was used. The design points have been searched in 5.4.1 and are illustrated in Figure 5.10. Note that the design points are $(1, 0, 0)$, $(0, 1, 0)$, $(0, 0, 1)$, $(.5, 0, .5)$, $(0, .39, .61)$, $(.61, .39, 0)$, and $(.21, .58, .21)$. The order of collecting responses are shown in Figure 6.5. The support used for constructing the adaptive designs is the SLD$\{3, 20\}$.

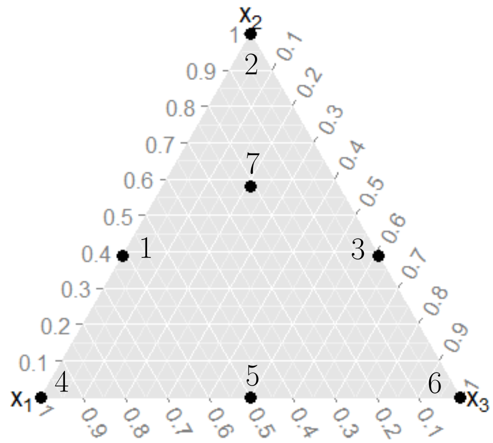



Figure 6.5: The random order of collecting responses in the seven-point $G$-optimal exact designs for a second-order model in three-component experiment.

If the first response has failed to be collected and cannot be repeated at $(.61, .39, 0)$, the set of six experimental runs that minimizes (6.3) is composed of $(1, 0, 0)$, $(0, 1, 0)$, $(0, 0, 1)$, $(.5, .5, 0)$, $(.5, 0, .5)$, and $(0, .5, .5)$, and the corresponding $G$-efficiency is 100. The design points are illustrated in Figure 6.6 ($N_0 = 0$). If using the remaining six design points of the exact design, this will give the $G$-efficiency $= 17.395$.

If the second observation at $(0, 1, 0)$ is missing, the adaptive design will include $(0, .95, .05)$ which is close to the missing point. Other points of the adaptive design are $(.4, 0, .6)$, $(0, .35, .65)$ and two vertices which are also in the exact design. The $G$-efficiencies of adaptive and exact designs are 73.172 and 2.005, respectively.

For $N_0 = 2$, the adaptive design contains $(1, 0, 0)$, $(0, 0, 1)$, $(.45, 0, .55)$, and $(0, .45, .55)$. The last point is close to the missing point, so this indicates that the missing point is important to the $G$-efficiency, so that the adaptive design does not include any interior points. The $G$-efficiencies of the adaptive and exact designs are 87.747 and 17.395, respectively.

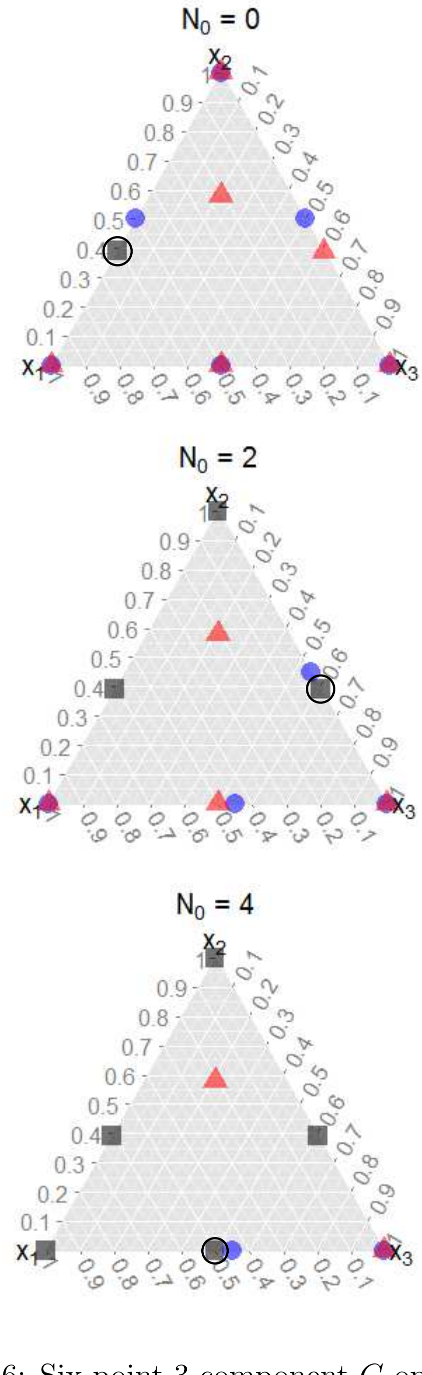



Figure 6.6: Six-point 3-component $G$-optimal adaptive mixture designs for a second-order model. Solid squares correspond the responses being collected and squares within a circle correspond to the failed response. Solid triangles correspond to the remaining design points not collected in the exact design and solid circles correspond to the adaptive design points.

When the fourth response has failed, the adaptive design contains points $(0,0,1)$, $(.35,0,.65)$, and $(.95,0,.05)$. It is seen that point $(.95,0,.05)$ is close to the missing $(1,0,0)$, so this suggests the vertices are very important to the $G$-efficiency. Like previous adaptive designs, there is no interior point. The $G$-efficiencies of the adaptive and exact designs are 73.172 and 2.234, respectively.

For $N_0 = 4$ and $N_0 = 5$, the adaptive designs have a design point next to the missing point. If the missing point can be repeated, this will give the highest $G$-efficiency. It is seen that if we have limited resources, an interior point is not very important to the $G$-efficiency. For $N_0 = 4$, the $G$-efficiencies of the adaptive and exact designs are 87.747 and 1.910, respectively, and for $N_0 = 5$, the $G$-efficiencies of the adaptive and exact designs are 70.417 and 1.910, respectively.

## 5. Examples of $IV$-Optimal Adaptive Designs

Suppose an $(N_0 + N + 1)$-run experiment was conducted, but when collecting the data, the $(N_0 + 1)$th trial is uncollectible and cannot be repeated, and we have resources for only $N$ runs. For such a situation, the $IV$-optimality criterion can be employed to find a new set of $N$ points so that

$$\frac{N_0 + N}{A} \operatorname{trace}\left[\mathbf{M}^{-1}(\widetilde{\xi}) \int_{\mathcal{X}} \mathbf{x}^{\mathrm{T}(m)} \mathbf{x}^{(m)} \, d\mathbf{x}^{(m)}\right] \tag{6.4}$$

will be minimized. Note that $A$ is the volume of design space $\mathcal{X}$ and $(N_0 + N)\mathbf{M}(\widetilde{\xi}) = N_0\mathbf{M}(\xi_0) + N\mathbf{M}(\xi)$.

Suppose the seven-point $IV$-optimal exact design was used. The design points are illustrated in Figure 4.21 (left). Note that the design points are $(1,-1), (-1,1)$, $(-1,-.004)$, $(.004,1)$, $(1,.768)$, $(-.768,-1)$, and two $(.095,-.095)$'s. The order of collecting responses is shown in Figure 6.7.

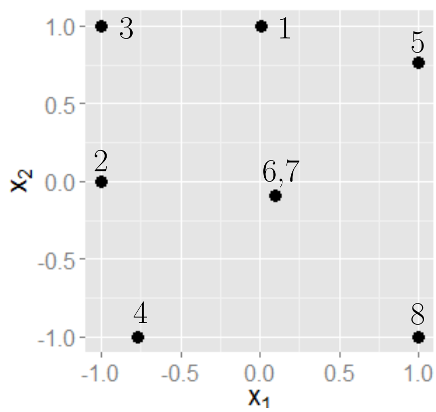



Figure 6.7: The random order of collecting responses in the eight-point $IV$-optimal exact designs for a second-order model in three-component experiment.

First, suppose the first response has failed to be collected. Thus, the adaptive design points are $(-1, .3)$, $(-.3, 1)$, $(1, .9)$, $(-.8, -1)$, $(1, -1)$, and two $(.2, -.1)$'s. Once the response at $(0.004, 1)$ is missing, the adaptive design does not include vertex $(-1, 1)$. As illustrated in Figure 6.8 ($N_0 = 0$), two points of exact and adaptive designs have about the same coordinates. This is probably due to the grid used to construct the adaptive design. If a finer grid was used, those two points could be the same. The $IV$-efficiencies of the exact and adaptive designs are 21.611 and 24.654, respectively.

Suppose, the second response at $(-1, -.004)$ is missing and cannot be repeated. The adaptive design contains points $(-.1, -.2)$, $(0, -.2)$, $(-1, -1)$, $(1, .5)$, $(.9, -1)$, and $(-1, .6)$, and its $IV$-efficiency is 24.694. The design points are rather different from those of the exact design whose the $IV$-efficiency is 20.816.

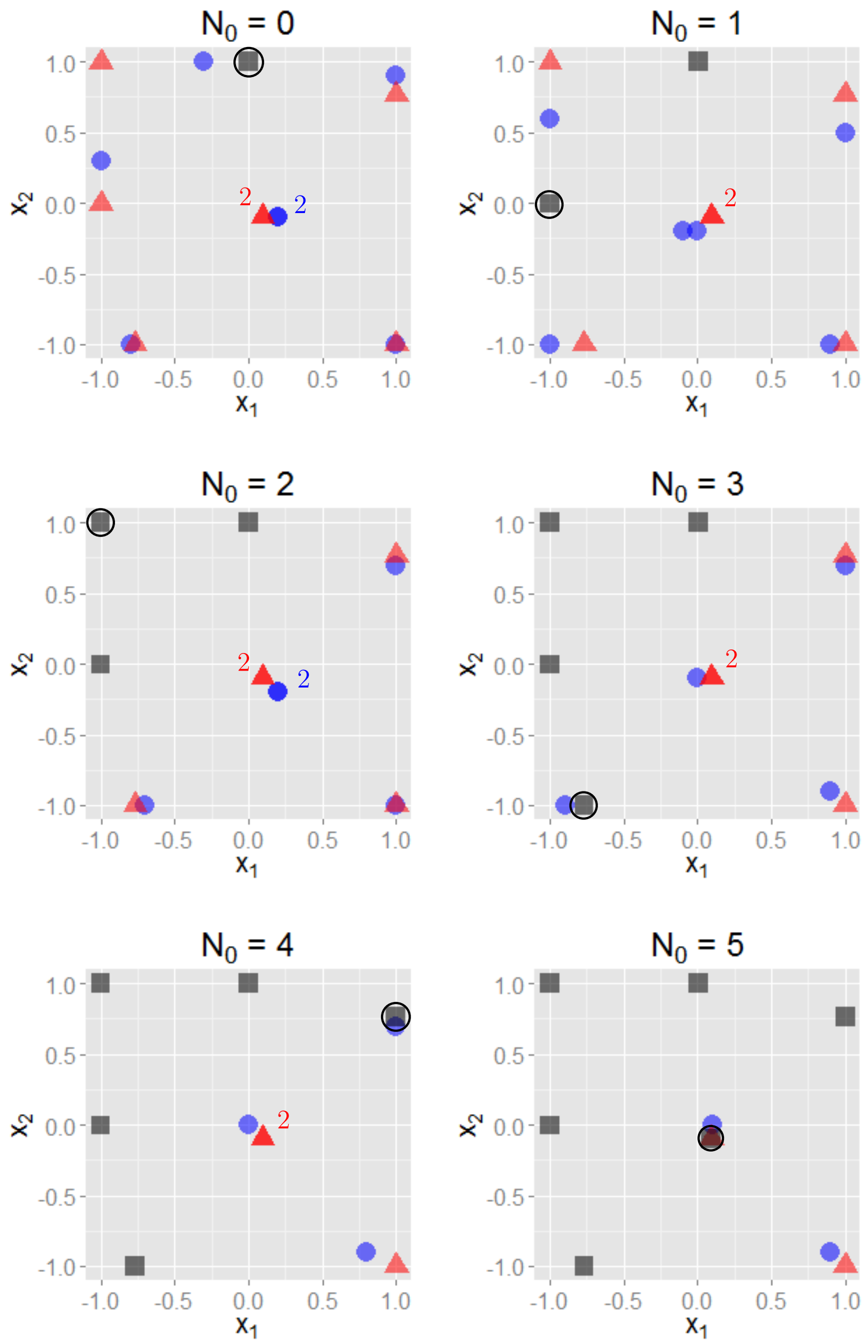



Figure 6.8: Seven-point $IV$-optimal adaptive designs for a second-order model in 2 factors. Solid squares correspond the responses being collected and squares within a circle correspond to the failed response. Solid triangles correspond to the remaining design points not collected in the exact design and solid circles correspond to the adaptive design points.

For $N_0 = 2$, the design points of the adaptive designs are similar to those of the exact design, but two replicates of the adaptive design are closer to the origin. Besides points already collected, the adaptive design contains points $(1, .7)$, $(1, -1)$, $(-.7, -1)$, and two $(.2, -.2)$'s. Notice that even though the vertical point $(-1, 1)$ is missing, the adaptive design does not contain any points close to it. The $IV$-efficiencies of the exact and adaptive designs are 21.972 and 22.367, respectively, thus the $IV$-efficiency is just improved slightly.

For $N_0 = 3$ and 4, the adaptive designs have one design point close to the origin and one point close to the missing point. If the experiment can be repeated at the missing point, it will be included into the adaptive designs. For $N_0 = 3$, the $IV$-efficiencies of the exact and adaptive designs are 5.457 and 22.641, respectively, and for $N_0 = 4$, the $IV$-efficiencies of the exact and adaptive designs are 5.878 and 22.315, respectively. It seems points $(-.768, -1)$ and $(1, .768)$ are very important so that the adaptive design chose to include a point near the missing point and not to replicate the point close to the origin.

When the sixth response is missing at $(.095, -.095)$. the adaptive design will include points $(.9, -.9)$ and $(.1, 0)$. The latter point is close to missing point $(.095, -.095)$, but this is because of the coarseness of the set of candidate points which does not include point $(.095, -.095)$; otherwise, the adaptive design would have this point. In this case, the $IV$-efficiency is slightly improved as the $IV$-efficiencies of the exact and adaptive designs are 22.405 and 22.554, respectively.

## 6. Summary and Discussion

In conclusion, once a response is missing and only this design point is removed from the candidate set, the resulting adaptive sometimes includes a design point very close to the missing design point. In previous examples of $IV$-optimal adaptive designs, when $N_0 = 0$, 1, and 2, the adaptive designs did not include a design point very close to the missing point, but for $A$- and $G$-optimal adaptive designs the resulting designs always include a design point close to the missing point. If the response was missing at random, then the point can still be included in the candidate set. In our examples, the $D$-optimal adaptive design with $N_0 = 3$ included point $(.1, 1)$ very close to missing $(0, 1)$, and if we are allowed to have $(0, 1)$ in the candidate set, the adaptive design will have point $(0, 1)$ instead of $(.1, 1)$. However, as shown in Figure 6.2 ($N_0 = 3$), both designs are still different because the adaptive design will not include any point close to $(-1, .082)$. Finally, if it is determined that an infeasible region exist in the neighborhood of the failed point, then all points in this infeasible region will be excluded from the candidate set.

# CHAPTER 7

# CONCLUSIONS AND FUTURE RESEARCH

When small second-order response surface designs are used due to limited resources or the expensive nature of an experiment, if one response fails, it can substantially affect the quality of the parameter estimation and/or precision of the prediction. The goal of the dissertation is to assess the after effects of having a missing run and to discover robust exact designs.

The CCDs, HSCDs, PBCDs, hybrid designs, BBDs, and alphabetic optimal designs were studied to assess their robustness to an arbitrary missing point via the variants of the $D$-efficiency: the Avg $\ell(\xi_N)$, Max $\ell(\xi_N)$, and Min $D$. These are useful when comparing designs with different sample sizes and also reveal the precision of the parameter estimation in a design when a missing point occurs. The new VdgRsm package in R makes the VDGs and FDS plots not only for designs in a spherical region, but also in a cuboidal region. The VdgRsm package is able to generate a contour plot of SPVs which helps researches to locate the design region whose precision of predictions are unacceptably poor. The procedures for generating random points uniformly inside a $k$-dimensional hypersphere and on the surface of a hypercube were also discussed in Chapter 2.

The behaviors of the $D$-, $A$-, $G$-, and $IV$-efficiencies of CCDs with different values of axial distance were studied in Chapter 3. The robust axial distance guarantees that despite a CCD having a missing factorial, axial, or center point, the desired efficiency is still maximized. The robust CCDs based on the Min $D$, Min $A$, Min $G$, or Min $IV$ are usually not rotatable which can be observed from the VDG. The axial distance resulting from the Min $D$ is the highest and, respectively, followed by those obtained from the Min $G$, Min $IV$, and Min $A$ criteria. The resulting robust CCDs were compared to the corresponding spherical CCDs.

Computer-generated designs are often referred to as tailor-made designs which experimenters can specify the number of experimental runs, constraints, and model to be fitted. In Chapter 4, the modified optimality criteria were proposed and employed to construct exact designs robust to a single missing observation in a cuboidal region. The point-exchange algorithm based on the grid search was modified in regard to the generation of the starting design. The new robust criteria themselves, especially the modified $G$- and $IV$-criteria, are computationally expensive, and the computational time sizably increased as the dimension of the experimental region and/or the number of design points increased. The resulting $D$-, $A$-, $G$-, and $IV$-optimal robust exact designs with a certain number of design points were compared to the corresponding exact designs. Their robustness against one and two missing points were evaluated by the leave-1-out and leave-2-out efficiencies, respectively. In the conclusion of Chapter 4, the Min $D$, Min $IV$, and Min $A$ were preferable to the Min $G$ because the resulting designs are not only robust to a missing point, but also satisfied the other criteria not being used to construct the design. The Min $G$ criterion seems to be poorly maximized, and for small numbers of design points this criterion usually leads to unsatisfactory designs in regard the precision of parameter estimation and prediction.

The efficient algorithms together with the Min $D$, Min $A$, Min $G$, or Min $IV$ to construct the robust exact designs are still needed, especially for designs with three or more factors. Future research could be using the global optimization methods such as simulated annealing and genetic algorithms for constructing the robust design against a missing point. Furthermore, the mechanism of missing completely at random (MCAR) was made for the work in this dissertation, but if we know the probability of losing points in a design, incorporating this knowledge to construct the robust exact design in an experiment with two or more factors should be explored.

The newly proposed robust criteria in Chapter 4 were also employed for constructing the robust exact mixture designs in Chapter 5. The length of computational time is lessened in constructing exact mixture designs because there is at least one constraint that all component values must sum to one. The $D$- and $A$-optimal exact mixture designs for the second-order mixture model do not usually include an interior point, and the design points include points in the simplex lattice $\{q, 2\}$ designs. If one of the unreplicated points on the boundary is missing, the second-order model will not be estimable. Thus, the exact mixture designs are generally very sensitive to a missing point. Our proposed criteria led to generating exact designs which still have high precision of parameter estimation and prediction, but also are robust against a missing point. Like robust exact designs in Chapter 4, the Min $G$ criterion still gave relatively poor robust exact mixture designs as their robustness are only slightly improved, but the $G$-efficiencies are very low compared to the exact mixture designs.

The adjustment can be made in a real time for the remaining design points when one response fails to be observed. The exact optimal designs were augmented by regenerated design points so that the desired optimality criterion is maximized. This approach is useful for any experimental designs, and not only for the optimal exact designs given in Chapter 6 as examples.

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