CYLINDRICAL DESIGNS FOR RESPONSE SURFACE STUDIES

by

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ABSTRACT

Central Composite Designs (CCDs) with cuboidal and spherical regions are among the most popular experimental designs for studying response surfaces. Cuboidal regions are typically used when the experimenter believes the levels of one or more of the factors are bounded while a spherical region is employed when there are no restrictions on the levels of any of the factors. We propose what we call a cylindrical design in which the levels of some factors are restricted while the other factors' levels need not be. Assuming the use of a second-order model, we give the general form for the model matrix $\mathbf{X}$ of such a design and give a closed form for the determinant of the $\mathbf{X}'\mathbf{X}$ matrix as well as its inverse. We use the results for the determinant and inverse of $\mathbf{X}'\mathbf{X}$ to compare designs using the alphabetic design optimality criteria. D-efficiencies, A-efficiencies, G-efficiencies, and IV-efficiencies for CCDs will be compared with those of the cylindrical design. Graphical assessment of the maximum spherical prediction variance will also be done. It will be shown that the cylindrical design is an excellent alternative when some but not all factors have restricted levels.

INTRODUCTION

Response Surface Methodology

The results of this research are based on the ideas of response surface methodology. According to Myers et al. [11], “Response Surface Methodology (RSM) is a collection of statistical and mathematical techniques for developing, improving, and optimizing processes.” RSM combines statistical experimental design, regression modeling techniques, and optimization methods. The idea is to design an experiment in k variables, say $\xi_1, \xi_2, \ldots, \xi_k$, and from the resulting data fit a low-order polynomial that approximates the true relationship between the response, y, and the k factors. The goal is to find the levels of the k variables which produce an optimal response. Most often in RSM, the variables $\xi_1, \xi_2, \ldots, \xi_k$ are transformed to coded variables $x_1, x_2, \ldots, x_k$ which are dimensionless with mean zero and equal spread. All results in this thesis are based on the second-order regression model:

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

The second-order model is widely used in RSM because it is a flexible model able to approximate various functional forms, the parameters are easy to estimate using least squares, and practical experience has shown it to be an effective model in RSM [11]. Furthermore, we will be comparing the Central Composite Design (CCD) to the cylindrical design and the CCD is a common design for fitting second-order response surface models.

The Central Composite Design

Central composite designs were first introduced by Box and Wilson [4] and continue to be among the most popular designs for studying response surfaces. A CCD either has a cuboidal or a spherical region for its design space. The CCD is defined to consist of:

1. An $F = 2^{k-p}$ full ($p = 0$) or fractional ($p > 0$) factorial design of at least resolution V; each point is of the form $(x_1, \ldots, x_k) = (\pm 1, \ldots, \pm 1)$
2. $2k$ axial points of the form $(x_1, \ldots, x_i, \ldots, x_k) = (0, \ldots, \pm\alpha, \ldots, 0)$ for $1 \leq i \leq k$.
3. N_0 center points $(x_1, \ldots, x_k) = (0, \ldots, 0)$

There are a total of $N = F + 2k + N_0$ design points, and there are $\binom{k+2}{2}$ parameters for the quadratic model. The general form of the columns and rows of the model matrix involving two factors (x_i and x_j) for a CCD is shown in Figure 1.1.

u	x_i	x_j	$x_i x_j$	x_i^2	x_j^2	
1	1	1	1	1	1	
1	1	-1	-1	1	1	F
1	-1	1	-1	1	1	
1	-1	-1	1	1	1	
1	α	0	0	α^2	0	
1	$-\alpha$	0	0	α^2	0	
1	0	α	0	0	α^2	$2k$
1	0	$-\alpha$	0	0	α^2	
1	0	0	0	0	0	N_0

Figure 1.1: General Form of the Model Matrix **X** for a CCD

When $\alpha = 1$, the design space is cuboidal while $\alpha = \sqrt{k}$ produces a spherical design space. Values for α other than 1 or $\sqrt{k}$ are sometimes used, particularly

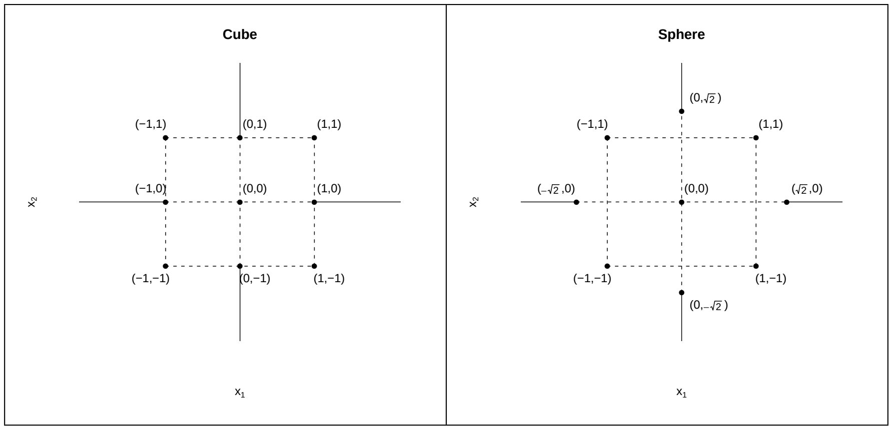

Figure 1.2: Geometric View of two-factor CCDs with cuboidal and spherical regions.

when a value for α generates a rotatable design. According to Myers et al. [11], "If the desired region of the design is spherical, the CCD that is most effective from a variance point of view is to use $\alpha = \sqrt{k}$ and three to five center runs." There are practical situations where the practitioner chooses to use either the spherical or cuboidal region. Cuboidal regions are typically employed when there are strict ranges on one or more variables, resulting in the region of interest and the region of operability being the same. If experimentation is possible beyond the ranges of the factors set by the practitioner, then a spherical region is appropriate.

Figure 1.2 displays the geometric view of two-factor CCDs with a cuboidal and spherical design space. Notice how the factorial points make up the corners of a square. In three dimensions, the factorial points would make up the corners of a cube and in 4 or more dimensions the factorial points would make up the corners of a hypercube. The placement of the axial points determines whether the design space is a cube or a sphere. In the cube, the axial points are on the faces of the cube, or in the case of Figure 1.2 the square. A sphere occurs when the axial distance is equal to the distance from the origin to any factorial point, i.e., the square root of the total number of factors.

Design Optimality Criteria

As different types of experimental designs have been discovered, various ways to compare the statistical properties of competing designs has advanced. The groundwork for comparing response surface designs was laid by Kiefer [8, 9] and Kiefer and Wolfowitz [10] in what is known as optimal design theory. While there are numerous ways to compare response surface designs, the focus of this research is on the alphabetic design optimality criteria. Specifically, attention is given to the D-, A-, G-, and IV-optimality criteria. Using definitions given in the OPTEX procedure in SAS [14] and definitions given by Myers et al. [11], the alphabetic design optimality criteria are given as:

1. D-criterion: minimize $|(\mathbf{X}'\mathbf{X})^{-1}|$ or maximize $|\mathbf{X}'\mathbf{X}|$

2. A-criterion: minimize trace $[(\mathbf{X}'\mathbf{X})^{-1}]$

3. G-criterion: minimize $\max_{\mathbf{x}\in\mathcal{X}} [Nf(x)'(\mathbf{X}'\mathbf{X})^{-1}f(x)]$

4. IV-criterion: minimize average $[Nf(x)'(\mathbf{X}'\mathbf{X})^{-1}f(x)]$ over $\mathbf{x}\in\mathcal{X}$

$$f(x)' = \left[\begin{array}{c|cccc|ccc|cccc} 1 & x_1 & x_2 & \ldots & x_k & x_1x_2 & \ldots & x_{k-1}x_k & x_1^2 & x_2^2 & \ldots & x_k^2 \end{array}\right]$$

where $f(x)$ is just the vector of model coefficients for the second-order model, and $\mathcal{X}$ represents the design space. D-optimality is the most popular of the four criteria for comparing designs. According to Myers et al. [11], "Under the assumption of independent normal model errors with constant variance, the determinant of $\mathbf{X}'\mathbf{X}$ is inversely proportional to the square of the volume of the confidence region on the regression coefficients." Therefore, designs that have larger determinants have smaller confidence regions and thus better estimation of the model parameters.

The A-criterion also deals with model parameter estimation. Because the trace of a matrix is just the sum of the diagonal elements of the matrix, the A-criterion seeks to minimize the sum of the individual variances of the model parameters. One problem with the A-criterion is that it ignores the covariance terms that often occur in response surface problems.

The G- and IV-criteria make use of the scaled prediction variance function $Nf(x)'(\mathbf{X}'\mathbf{X})^{-1}f(x)$. When $(\mathbf{X}'\mathbf{X})^{-1}$ is pre-multiplied by $f(x)'$ and post-multiplied by $f(x)$, the result is a polynomial function. Then the scaled prediction variance function evaluated at any $\mathbf{x} \in \mathcal{X}$ gives the scale-free variance at the point $\mathbf{x}$. There is a maximum prediction variance in the design space $\mathcal{X}$, and the design that has the smallest maximum prediction variance among competing designs is said to be best by the G-criterion.

Furthermore, one can find the average prediction variance by integrating the prediction variance function over the design space and dividing by the volume of the design space. The IV in IV-criterion stands for integrated variance because we integrate the prediction variance function over the appropriate region. Some authors (i.e. Myers et al. [11]) refer to the IV-criterion as the I-criterion. The design which has the smallest average prediction variance among competing designs is said to be best by the IV-criterion.

The statistical software package SAS evaluates and generates designs based on the design optimality criteria. SAS calculates design efficiencies based on the criteria using the following formulas assuming there are N design points and p model parameters.

$$\begin{aligned}
\text{D-efficiency} &= 100\left(\frac{|\mathbf{X}'\mathbf{X}|^{\frac{1}{p}}}{N}\right) &(1.1)\\
\text{A-efficiency} &= 100\left(\frac{p}{\text{trace}\left[N(\mathbf{X}'\mathbf{X})^{-1}\right]}\right) &(1.2)\\
\text{G-efficiency} &= 100\left(\frac{\sqrt{p/N}}{\max\limits_{x\in\mathcal{X}}\left[Nf(x)'(\mathbf{X}'\mathbf{X})^{-1}f(x)\right]}\right) &(1.3)\\
\text{IV-efficiency} &= \text{avg}\left[Nf(x)'(\mathbf{X}'\mathbf{X})^{-1}f(x)\right] \text{ over } x\in\mathcal{X} &(1.4)
\end{aligned}$$

For the research in this thesis, we used these same formulas to calculate design efficiencies for both CCDs and cylindrical designs. Note that the D-, A-, and G-efficiencies are each multiplied by the value 100. For these criteria, the efficiency is given as a percentage where a design with 100% efficiency indicates that the design is optimal by that criterion. The IV-efficiency is not given as a percentage, but is simply the value of the average prediction variance for a design. Thus, in comparing designs using the IV-efficiency, the design with the smallest average prediction variance would be chosen based on the IV-efficiency. Because CCDs have been in existence for some time now, the design efficiencies for CCDs have been calculated before, and we compared our results with previous ones and found them in agreement. Table 1.1 on page 7 gives the design efficiencies for central composite designs with both cuboidal and spherical regions with either 1 or 2 center points. For the present research, we consider designs which have between 3 and 10 factors.

Let CCD(s) and CCD(c) denote a CCD with spherical and cuboidal design regions, respectively. For both the D-efficiency and the A-efficiency, the CCD(s) has higher design efficiency than the CCD(c) regardless of the number of center points. For fewer numbers of factors, the CCD(c) tends to have a higher G-efficiency than the CCD(s) when 1 center point is utilized, but when 2 center points are used, the CCD(s) has significantly higher G-efficiency for all numbers of factors. For a CCD(s) with no

Table 1.1: D-, A-, and G-efficiencies and IV criterion values for CCDs with cuboidal and spherical regions with 1 and 2 center points for k = 3 to 10 factors.

Factors	N_0	Region	D-eff (pct)	A-eff (pct)	G-eff (pct)	IV value
3	1	Cube	46.22	31.29	83.62	5.51
3	1	Sphere	71.13	32.40	66.67	8.12
3	2	Cube	43.00	30.68	78.55	5.45
3	2	Sphere	71.47	44.93	94.59	6.83
4	1	Cube	44.52	25.49	77.98	8.44
4	1	Sphere	76.73	31.65	60.00	12.15
4	2	Cube	43.30	24.91	75.08	8.45
4	2	Sphere	77.26	45.40	98.90	10.47
5	1	Cube	42.69	25.30	74.91	10.97
5	1	Sphere	80.02	36.95	77.78	16.13
5	2	Cube	41.42	24.47	72.25	11.17
5	2	Sphere	79.75	49.83	87.64	14.94
6	1	Cube	44.80	18.98	62.52	17.30
6	1	Sphere	83.84	33.72	62.22	22.02
6	2	Cube	43.98	18.64	61.22	17.47
6	2	Sphere	84.07	48.24	96.95	20.21
7	1	Cube	46.01	12.88	44.17	30.03
7	1	Sphere	85.47	28.06	45.57	29.42
7	2	Cube	45.54	12.75	43.67	30.15
7	2	Sphere	86.04	42.76	84.72	26.56
8	1	Cube	46.86	13.40	47.23	35.29
8	1	Sphere	87.87	32.32	55.56	36.18
8	2	Cube	46.36	13.25	46.71	35.53
8	2	Sphere	88.14	47.46	99.78	33.89
9	1	Cube	47.73	8.46	30.11	64.73
9	1	Sphere	87.94	24.87	37.41	49.11
9	2	Cube	47.47	8.41	29.92	64.90
9	2	Sphere	88.46	39.18	72.45	45.30
10	1	Cube	49.06	8.87	32.04	73.26
10	1	Sphere	89.99	28.31	44.30	55.37
10	2	Cube	48.77	8.82	31.84	73.54
10	2	Sphere	90.33	43.36	83.92	52.17

center points, the $\mathbf{X'X}$ matrix is either singular or near-singular and adding one center point still results in a large prediction variance at the center of the design [11]. As more center runs are included, the prediction variance stabilizes and we see that the CCD(s) is more G-efficient than the CCD(c). Finally, the average prediction variance is lower for the CCD(c) than the CCD(s) for between 3 and 6 factors regardless of whether one or two center points are utilized. The average prediction variance is only slightly lower for the CCD(c) than the CCD(s) with 8 factors and one center point. Other than the above mentioned, the CCD(s) has lower average prediction variance than the CCD(c).

Thus, when an experimenter has strict ranges on one or more of the factors and decides to utilize a CCD with a cuboidal region, design efficiency can be lost. It is important to note that when even just one factor needs strict bounds, the use of a cuboidal region in essence bounds all factors between -1 and 1 in coded version. Our new design, the cylindrical design allows the experimenter to bound only the factors that should be and allow the other factors to stretch beyond the coded values of -1 and 1. Furthermore, as will be shown, the cylindrical design tends to have higher efficiency than the CCD with a cuboidal region among the design optimality criteria.

The Cylindrical Design

A **cylindrical design** consists of $C \geq 1$ cuboidal factors (bounded between -1 and 1) and $S \geq 2$ spherical factors (not bounded between -1 and 1) and has the following components:

1. An $F = 2^{C+S-p}$ full ($p = 0$) or fractional ($p > 0$) factorial design of at least resolution V; each point is of the form
   $(x_1, \ldots, x_C, z_1, \ldots, z_S) = (\pm 1, \ldots, \pm 1 | \pm 1, \ldots, \pm 1)$

2. $2C$ axial points of the form

   $(x_1, \ldots, x_i, \ldots, x_C, z_1, \ldots, z_S) = (0, \ldots, \pm 1, \ldots, 0|0, \ldots, 0)$

3. $2S$ axial points of the form

   $(x_1, \ldots, x_C, z_1, \ldots, z_k, \ldots, z_S) = (0, \ldots, 0|0, \ldots, \pm\alpha, \ldots, 0)$ where $\alpha = \sqrt{S}$.

4. N_0 center points $(x_1, \ldots, x_C, z_1, \ldots, z_S) = (0, \ldots, 0|0, \ldots, 0)$

where the | notation indicates the location of the separation between the cuboidal and spherical factors.

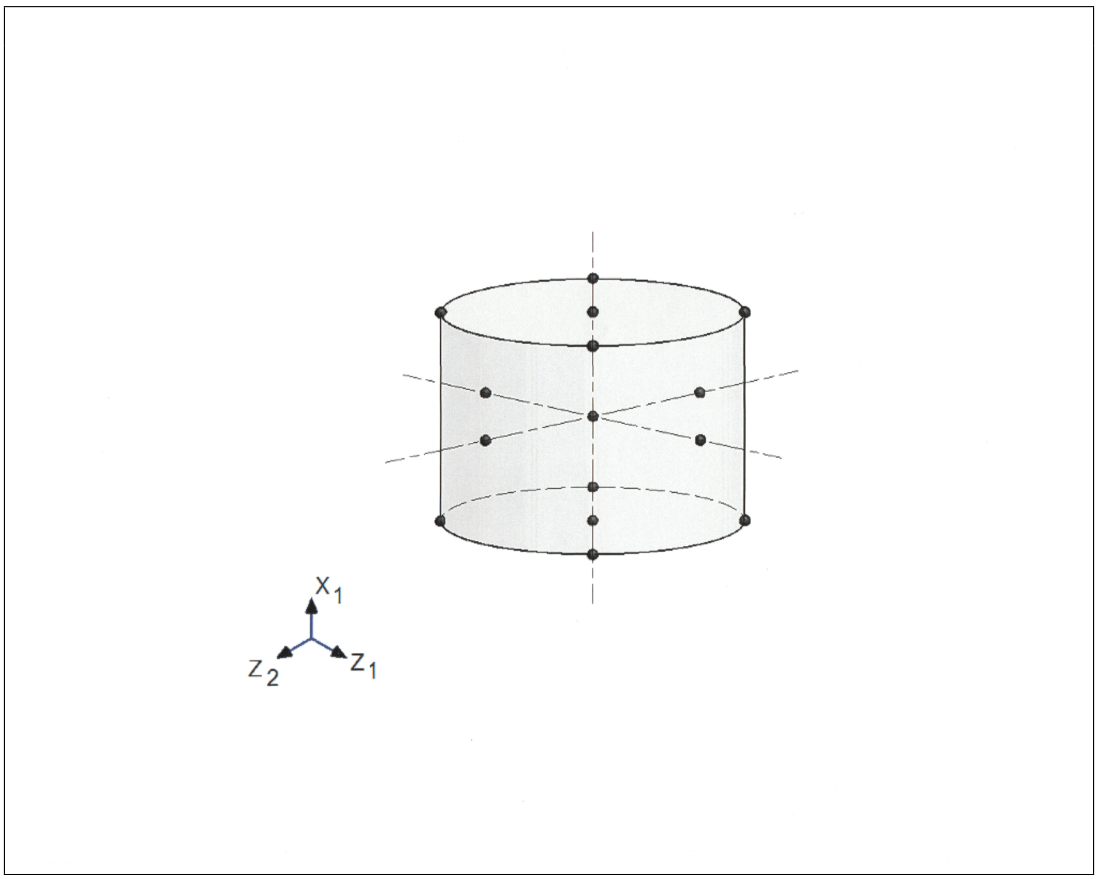

Figure 1.3: Design Space for 3-factor Cylindrical Design (1 Cuboidal Factor and 2 Spherical Factors)

For a cylindrical design, there are a total of $N = F + 2(C + S) + N_0$ design points. Figure 1.3 shows the design space for a cylindrical design in 3 factors. Note that the space is actually a three-dimensional cylinder which is why we gave this class of designs the name. The points shown in the plot represent the design points. The factorial points are the ones on the outer edge of the circles on the top and bottom of the cylinder. The cuboidal axial points are in the center of the circles on top and bottom of the cylinder. The spherical axial points are on the sides of the cylinder (with axial distance equal to $\sqrt{2}$). Finally, the point in the center of the cylinder represents where the center points would be located.

In order to study the design efficiencies for a cylindrical design, it is necessary to find closed forms for the determinant and the inverse of the $\mathbf{X}'\mathbf{X}$ matrix. First, we need to know the general structure for the model matrix $\mathbf{X}$. Figure 1.4 displays the general form of the model matrix for a cylindrical design for any two cuboidal factors and any two spherical factors.

By using matrix multiplication, the general form of the $\mathbf{X}'\mathbf{X}$ matrix has been derived and is shown in Figure 1.5. This general form will be used in finding the determinant of the $\mathbf{X}'\mathbf{X}$ matrix in the next chapter.

u	x_i	x_j	z_k	z_l	x_ix_j	x_iz_k	x_iz_l	x_jz_k	x_jz_l	z_kz_l	${x_i}^2$	${x_j}^2$	${z_k}^2$	${z_l}^2$
1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
1	1	1	1	-1	1	1	-1	1	-1	-1	1	1	1	1
1	1	1	-1	1	1	-1	1	-1	1	-1	1	1	1	1
1	1	1	-1	-1	1	-1	-1	-1	-1	1	1	1	1	1
1	1	-1	1	1	-1	1	1	-1	-1	1	1	1	1	1
1	1	-1	1	-1	-1	1	-1	-1	1	-1	1	1	1	1
1	1	-1	-1	1	-1	-1	1	1	-1	-1	1	1	1	1
1	1	-1	-1	-1	-1	-1	-1	1	1	1	1	1	1	1
1	-1	1	1	1	-1	-1	-1	1	1	1	1	1	1	1
1	-1	1	1	-1	-1	-1	1	1	-1	-1	1	1	1	1
1	-1	1	-1	1	-1	1	-1	-1	1	-1	1	1	1	1
1	-1	1	-1	-1	-1	1	1	-1	-1	1	1	1	1	1
1	-1	-1	1	1	1	-1	-1	-1	-1	1	1	1	1	1
1	-1	-1	1	-1	1	-1	1	-1	1	-1	1	1	1	1
1	-1	-1	-1	1	1	1	-1	1	-1	-1	1	1	1	1
1	-1	-1	-1	-1	1	1	1	1	1	1	1	1	1	1
1	1	0	0	0	0	0	0	0	0	0	1	0	0	0
1	-1	0	0	0	0	0	0	0	0	0	1	0	0	0
1	0	1	0	0	0	0	0	0	0	0	0	1	0	0
1	0	-1	0	0	0	0	0	0	0	0	0	1	0	0
1	0	0	α	0	0	0	0	0	0	0	0	0	α^2	0
1	0	0	$-\alpha$	0	0	0	0	0	0	0	0	0	α^2	0
1	0	0	0	α	0	0	0	0	0	0	0	0	0	α^2
1	0	0	0	$-\alpha$	0	0	0	0	0	0	0	0	0	α^2
1	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Figure 1.4: General Form of the Model Matrix **X** for a Cylindrical Design

	u	x_i	x_j	z_k	z_l	x_ix_j	x_iz_k	x_iz_l	x_jz_k	x_jz_l	z_kz_l	x_i^2	x_j^2	z_k^2	z_l^2
u	N	0	0	0	0	0	0	0	0	0	0	F_1	F_1	F_2	F_2
x_i	0	F_1	0	0	0	0	0	0	0	0	0	0	0	0	0
x_j	0	0	F_1	0	0	0	0	0	0	0	0	0	0	0	0
z_k	0	0	0	F_2	0	0	0	0	0	0	0	0	0	0	0
z_l	0	0	0	0	F_2	0	0	0	0	0	0	0	0	0	0
x_ix_j	0	0	0	0	0	F	0	0	0	0	0	0	0	0	0
x_iz_k	0	0	0	0	0	0	F	0	0	0	0	0	0	0	0
x_iz_l	0	0	0	0	0	0	0	F	0	0	0	0	0	0	0
x_jz_k	0	0	0	0	0	0	0	0	F	0	0	0	0	0	0
x_jz_l	0	0	0	0	0	0	0	0	0	F	0	0	0	0	0
z_kz_l	0	0	0	0	0	0	0	0	0	0	F	0	0	0	0
x_i^2	F_1	0	0	0	0	0	0	0	0	0	0	F_1	F	F	F
x_j^2	F_1	0	0	0	0	0	0	0	0	0	0	F	F_1	F	F
z_k^2	F_2	0	0	0	0	0	0	0	0	0	0	F	F	F_3	F
z_l^2	F_2	0	0	0	0	0	0	0	0	0	0	F	F	F	F_3

$$F_1 = F + 2$$
$$F_2 = F + 2\alpha^2$$
$$F_3 = F + 2\alpha^4$$

Figure 1.5: The $\mathbf{X'X}$ Matrix for a Cylindrical Design

THE DETERMINANT OF $\mathbf{X'X}$ AND THE D-CRITERION

Introduction

The goal of this chapter is to derive a closed form for the determinant of the $\mathbf{X'X}$ matrix so that D-efficiencies can be calculated. By a closed form, we mean that the formula for $\mathbf{X'X}$ should involve only C, S, F, α, and N where C is the number of cuboidal factors, S is the number of spherical factors, F is the number of factorial points used, α is the axial distance for the spherical factors, and $N = F+2(C+S)+N_0$ is the total number of design points. If a closed form for the determinant can be found, the model matrix will not need to be written out for every combination of cuboidal and spherical factors. The same approach will be used in finding a closed form for the inverse matrix in chapter 3.

Deriving $|\mathbf{X'X}|$

In his Ph.D. dissertation, Borkowski [1] used an adjusted model matrix to find the determinant for the $\mathbf{X'X}$ matrix of a mixed resolution design. Using a similar approach, we find the determinant of the $\mathbf{X'X}$ matrix for a cylindrical design. The proof of deriving the closed form for $|\mathbf{X'X}|$ follows the proceeding steps:

1. Define matrices $\mathbf{X}_{\boldsymbol{\Delta}}$ and $\mathbf{A}$ such that $\mathbf{XA} = \mathbf{X}_{\boldsymbol{\Delta}}$ and $|\mathbf{A}| = 1$.

2. Show $|\mathbf{X'X}| = |\mathbf{X'}_{\boldsymbol{\Delta}}\mathbf{X}_{\boldsymbol{\Delta}}|$.

3. Calculate $|\mathbf{X'}_{\boldsymbol{\Delta}}\mathbf{X}_{\boldsymbol{\Delta}}|$.

First, the general form of the adjusted model matrix $\mathbf{X}_{\boldsymbol{\Delta}}$ is shown in Figure 2.1.

u	x_i	x_j	z_k	z_l	x_ix_j	x_iz_k	x_iz_l	x_jz_k	x_jz_l	z_kz_l	x_i^2	x_j^2	z_k^2	z_l^2
1	1	1	1	1	1	1	1	1	1	1	$1-\delta_1$	$1-\delta_1$	$1-\delta_2$	$1-\delta_2$
1	1	1	1	-1	1	1	-1	1	-1	-1	$1-\delta_1$	$1-\delta_1$	$1-\delta_2$	$1-\delta_2$
1	1	1	-1	1	1	-1	1	-1	1	-1	$1-\delta_1$	$1-\delta_1$	$1-\delta_2$	$1-\delta_2$
1	1	1	-1	-1	1	-1	-1	-1	-1	1	$1-\delta_1$	$1-\delta_1$	$1-\delta_2$	$1-\delta_2$
1	1	-1	1	1	-1	1	1	-1	-1	1	$1-\delta_1$	$1-\delta_1$	$1-\delta_2$	$1-\delta_2$
1	1	-1	1	-1	-1	1	-1	-1	1	-1	$1-\delta_1$	$1-\delta_1$	$1-\delta_2$	$1-\delta_2$
1	1	-1	-1	1	-1	-1	1	1	-1	-1	$1-\delta_1$	$1-\delta_1$	$1-\delta_2$	$1-\delta_2$
1	1	-1	-1	-1	-1	-1	-1	1	1	1	$1-\delta_1$	$1-\delta_1$	$1-\delta_2$	$1-\delta_2$
1	-1	1	1	1	-1	-1	-1	1	1	1	$1-\delta_1$	$1-\delta_1$	$1-\delta_2$	$1-\delta_2$
1	-1	1	1	-1	-1	-1	1	1	-1	-1	$1-\delta_1$	$1-\delta_1$	$1-\delta_2$	$1-\delta_2$
1	-1	1	-1	1	-1	1	-1	-1	1	-1	$1-\delta_1$	$1-\delta_1$	$1-\delta_2$	$1-\delta_2$
1	-1	1	-1	-1	-1	1	1	-1	-1	1	$1-\delta_1$	$1-\delta_1$	$1-\delta_2$	$1-\delta_2$
1	-1	-1	1	1	1	-1	-1	-1	-1	1	$1-\delta_1$	$1-\delta_1$	$1-\delta_2$	$1-\delta_2$
1	-1	-1	1	-1	1	-1	1	-1	1	-1	$1-\delta_1$	$1-\delta_1$	$1-\delta_2$	$1-\delta_2$
1	-1	-1	-1	1	1	1	-1	1	-1	-1	$1-\delta_1$	$1-\delta_1$	$1-\delta_2$	$1-\delta_2$
1	-1	-1	-1	-1	1	1	1	1	1	1	$1-\delta_1$	$1-\delta_1$	$1-\delta_2$	$1-\delta_2$
1	1	0	0	0	0	0	0	0	0	0	$1-\delta_1$	$-\delta_1$	$-\delta_2$	$-\delta_2$
1	-1	0	0	0	0	0	0	0	0	0	$1-\delta_1$	$-\delta_1$	$-\delta_2$	$-\delta_2$
1	0	1	0	0	0	0	0	0	0	0	$-\delta_1$	$1-\delta_1$	$-\delta_2$	$-\delta_2$
1	0	-1	0	0	0	0	0	0	0	0	$-\delta_1$	$1-\delta_1$	$-\delta_2$	$-\delta_2$
1	0	0	α	0	0	0	0	0	0	0	$-\delta_1$	$-\delta_1$	$\alpha^2-\delta_2$	$-\delta_2$
1	0	0	$-\alpha$	0	0	0	0	0	0	0	$-\delta_1$	$-\delta_1$	$\alpha^2-\delta_2$	$-\delta_2$
1	0	0	0	α	0	0	0	0	0	0	$-\delta_1$	$-\delta_1$	$-\delta_2$	$\alpha^2-\delta_2$
1	0	0	0	$-\alpha$	0	0	0	0	0	0	$-\delta_1$	$-\delta_1$	$-\delta_2$	$\alpha^2-\delta_2$
1	0	0	0	0	0	0	0	0	0	0	$-\delta_1$	$-\delta_1$	$-\delta_2$	$-\delta_2$

$$\delta_1 = \frac{F+2}{N}$$

$$\delta_2 = \frac{F+2\alpha^2}{N}$$

Figure 2.1: General Form of the Adjusted Model Matrix X_Δ.

Let the $N \times N$ matrix $\mathbf{A}$ be defined as:

$$\mathbf{A} = \begin{bmatrix} 1 & 0 & 0 & 0 & -\delta_1\mathbf{J}'_\mathbf{C} & -\delta_2\mathbf{J}'_\mathbf{S} \\ 0 & \mathbf{I_C} & 0 & 0 & 0 & 0 \\ 0 & 0 & \mathbf{I_S} & 0 & 0 & 0 \\ 0 & 0 & 0 & \mathbf{I_{CS}} & 0 & 0 \\ 0 & 0 & 0 & 0 & \mathbf{I_C} & 0 \\ 0 & 0 & 0 & 0 & 0 & \mathbf{I_S} \end{bmatrix}.$$

	u	x_i	x_j	z_k	z_l	x_ix_j	x_iz_k	x_iz_l	x_jz_k	x_jz_l	z_kz_l	x_i^2	x_j^2	z_k^2	z_l^2
u	N	0	0	0	0	0	0	0	0	0	0	0	0	0	0
x_i	0	$F+2$	0	0	0	0	0	0	0	0	0	0	0	0	0
x_j	0	0	$F+2$	0	0	0	0	0	0	0	0	0	0	0	0
z_k	0	0	0	$F+2\alpha^2$	0	0	0	0	0	0	0	0	0	0	0
z_l	0	0	0	0	$F+2\alpha^2$	0	0	0	0	0	0	0	0	0	0
x_ix_j	0	0	0	0	0	F	0	0	0	0	0	0	0	0	0
x_iz_k	0	0	0	0	0	0	F	0	0	0	0	0	0	0	0
x_iz_l	0	0	0	0	0	0	0	F	0	0	0	0	0	0	0
x_jz_k	0	0	0	0	0	0	0	0	F	0	0	0	0	0	0
x_jz_l	0	0	0	0	0	0	0	0	0	F	0	0	0	0	0
z_kz_l	0	0	0	0	0	0	0	0	0	0	F	0	0	0	0
x_i^2	0	0	0	0	0	0	0	0	0	0	0	a_1	a_2	a_5	a_5
x_j^2	0	0	0	0	0	0	0	0	0	0	0	a_2	a_1	a_5	a_5
z_k^2	0	0	0	0	0	0	0	0	0	0	0	a_5	a_5	a_3	a_4
z_l^2	0	0	0	0	0	0	0	0	0	0	0	a_5	a_5	a_4	a_3

$$a_1 = F + 2 - \frac{(F+2)^2}{N} \quad (2.1)$$

$$a_2 = F - \frac{(F+2)^2}{N} \quad (2.2)$$

$$a_3 = F + 2\alpha^4 - \frac{(F+2\alpha^2)^2}{N} \quad (2.3)$$

$$a_4 = F - \frac{(F+2\alpha^2)^2}{N} \quad (2.4)$$

$$a_5 = F - \frac{(F+2)(F+2\alpha^2)}{N} \quad (2.5)$$

Figure 2.2: The General Form of $\mathbf{X}'_{\mathbf{\Delta}}\mathbf{X}_{\mathbf{\Delta}}$

$\mathbf{I_C}$ and $\mathbf{I_S}$ are $C-$ and $S-$dimensional identity matrices. $\mathbf{I_{CS}}$ is a $\left[\binom{C}{2} + \binom{S}{2} + CS\right]-$dimensional identity matrix, and $\mathbf{J_C}$ and $\mathbf{J_S}$ are $C \times 1$ and $S \times 1$ unit vectors.

By using matrix multiplication, it is readily seen that $\mathbf{X_\Delta} = \mathbf{XA}$. Furthermore, because $\mathbf{A}$ is an upper triangular matrix with diagonal entries equal to 1, the determinant $|\mathbf{A}| = 1$. Then

$$\begin{aligned} |\mathbf{X}'_{\mathbf{\Delta}}\mathbf{X}_{\mathbf{\Delta}}| &= |(\mathbf{XA})'(\mathbf{XA})| \\ &= |\mathbf{A}'\mathbf{X}'\mathbf{XA}| \\ &= |\mathbf{A}'||\mathbf{X}'\mathbf{X}||\mathbf{A}| \end{aligned}$$

$$= \quad |\mathbf{X}'\mathbf{X}|$$

Hence, $|\mathbf{X}'\mathbf{X}|$ can be found simply by finding $|\mathbf{X}'_{\boldsymbol{\Delta}}\mathbf{X}_{\boldsymbol{\Delta}}|$. The general form for $\mathbf{X}'_{\boldsymbol{\Delta}}\mathbf{X}_{\boldsymbol{\Delta}}$ is shown in Figure 2.2.

Note how $\mathbf{X}'_{\boldsymbol{\Delta}}\mathbf{X}_{\boldsymbol{\Delta}}$ is a $p \times p$ diagonal matrix except for a $(C+S)\times(C+S)$ submatrix $\mathbf{K_Q}$ where p is the number of model parameters. The submatrix $\mathbf{K_Q}$ corresponds to the intersection of the rows and columns of the quadratic terms and has the form

$$\mathbf{K_Q} = \left[\begin{array}{cccc|cccc} a_1 & a_2 & \dots & a_2 & a_5 & a_5 & \dots & a_5 \\ a_2 & a_1 & \dots & a_2 & a_5 & a_5 & \dots & a_5 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ a_2 & a_2 & \dots & a_1 & a_5 & a_5 & \dots & a_5 \\ \hline a_5 & a_5 & \dots & a_5 & a_3 & a_4 & \dots & a_4 \\ a_5 & a_5 & \dots & a_5 & a_4 & a_3 & \dots & a_4 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ a_5 & a_5 & \dots & a_5 & a_4 & a_4 & \dots & a_3 \end{array}\right]$$

which can be written as:

$$\begin{bmatrix} \mathbf{K_1} & \mathbf{K_2} \\ \mathbf{K_3} & \mathbf{K_4} \end{bmatrix} = \left[\begin{array}{c|c} a\mathbf{I_C} + b\mathbf{J_C}\mathbf{J}'_{\mathbf{C}} & f\mathbf{J_C}\mathbf{J}'_{\mathbf{S}} \\ \hline f\mathbf{J_S}\mathbf{J}'_{\mathbf{C}} & d\mathbf{I_S} + e\mathbf{J_S}\mathbf{J}'_{\mathbf{S}} \end{array}\right]$$

$$\begin{aligned} a &= a_1 - a_2 = 2 \\ b &= a_2 \\ d &= a_3 - a_4 = 2\alpha^4 \\ e &= a_4 \\ f &= a_5 \end{aligned}$$

Also, $\mathbf{I_C}$ is a $C \times C$ identity matrix, $\mathbf{I_S}$ is an $S \times S$ identity matrix, and $\mathbf{J_C}$ and $\mathbf{J_S}$ are $C \times 1$ and $S \times 1$ unit vectors. Furthermore, note how $|\mathbf{X'_\Delta X_\Delta}|$ is just the product of the diagonal terms times the determinant of the submatrix $\mathbf{K_Q}$. In other words,

$$|\mathbf{X'X}| = |\mathbf{X'_\Delta X_\Delta}| = N(F+2)^C(F+2\alpha^2)^S F^{\binom{C}{2}+\binom{S}{2}+CS}|\mathbf{K_Q}|.$$

From Hocking [7] we have that

$$det\left(\begin{bmatrix} \mathbf{K_1} & \mathbf{K_2} \\ \mathbf{K_3} & \mathbf{K_4} \end{bmatrix}\right) = |\mathbf{K_1}||\mathbf{K_4} - \mathbf{K_3 K_1^{-1} K_2}|. \tag{2.6}$$

We also make frequent use the following two identities found in Searle [15]:

$$(a\mathbf{I_n} + b\mathbf{J_n J'_n})^{-1} = \frac{1}{a}\left(\mathbf{I_n} - \frac{b}{a+nb}\mathbf{J_n J'_n}\right) \tag{2.7}$$

and

$$|a\mathbf{I_n} + b\mathbf{J_n J'_n}| = a^{n-1}(a+nb) \tag{2.8}$$

So, to find $|\mathbf{K_Q}|$ first note that $\mathbf{K_1^{-1}} = (a\mathbf{I_C} + b\mathbf{J_C J'_C})^{-1} = \frac{1}{a}(\mathbf{I_C} - \frac{b}{a+Cb}\mathbf{J_C J'_C})$. Next we pre-multiply by $\mathbf{K_3}$ to obtain

$$\begin{aligned}
\mathbf{K_3 K_1^{-1}} &= f\mathbf{J_S J'_C}\left[\frac{1}{a}\left(\mathbf{I_C} - \frac{b}{a+Cb}\mathbf{J_C J'_C}\right)\right] \\
&= \frac{f}{a}\left(\mathbf{J_S J'_C} - \frac{b}{a+Cb}\mathbf{J_S J'_C J_C J'_C}\right) = \frac{f}{a}\left(\mathbf{J_S J'_C} - \frac{Cb}{a+Cb}\mathbf{J_S J'_C}\right) \\
&= \frac{f}{a}\left(\frac{a}{a+Cb}\right)\mathbf{J_S J'_C}.
\end{aligned}$$

Now we post-multiply by $\mathbf{K_2}$ and we have

$$\begin{aligned}
\mathbf{K_3 K_1^{-1} K_2} &= \left(\frac{f}{a}\left(\frac{a}{a+Cb}\right)\mathbf{J_S J'_C}\right) f\mathbf{J_C J'_S} \\
&= \frac{f^2}{a}\left(\frac{Ca}{a+Cb}\right)\mathbf{J_S J'_S} \\
&= \frac{Cf^2}{(a+Cb)}\mathbf{J_S J'_S}.
\end{aligned}$$

Next, we find

$$\begin{aligned}\mathbf{K_4} - \mathbf{K_3}\mathbf{K_1^{-1}}\mathbf{K_2} &= (d\mathbf{I_S} + e\mathbf{J_S}\mathbf{J_S'}) - \frac{Cf^2}{(a+Cb)}\mathbf{J_S}\mathbf{J_S'} \\ &= d\mathbf{I_S} + \left(e - \frac{Cf^2}{(a+Cb)}\right)\mathbf{J_S}\mathbf{J_S'}.\end{aligned}$$

Then, $|\mathbf{K_1}| = |a\mathbf{I_C} + b\mathbf{J_C}\mathbf{J_C'}| = a^{C-1}(a+Cb)$ and

$$\begin{aligned}|\mathbf{K_4} - \mathbf{K_3}\mathbf{K_1^{-1}}\mathbf{K_2}| &= det\left(d\mathbf{I_S} + \left(e - \frac{Cf^2}{(a+Cb)}\right)\mathbf{J_S}\mathbf{J_S'}\right) \\ &= d^{S-1}\left(d + S\left(e - \frac{Cf^2}{(a+Cb)}\right)\right).\end{aligned}$$

Thus, the determinant of $\mathbf{K_Q}$ is given by

$$\begin{aligned}|\mathbf{K_Q}| &= |\mathbf{K_1}||\mathbf{K_4} - \mathbf{K_3}\mathbf{K_1^{-1}}\mathbf{K_2}| \\ &= a^{C-1}d^{S-1}(a+Cb)\left(d + S\left(e - \frac{Cf^2}{a+Cb}\right)\right).\end{aligned}$$

By substituting the values for a, b, d, e, and f, we find that

$$\begin{aligned}|\mathbf{K_Q}| &= 2^{C-1}(2\alpha^4)^{S-1}(2 + Ca_2)\left(2\alpha^4 + S\left(a_4 - \frac{Ca_5^2}{2 + Ca_2}\right)\right) \\ &= 2^{C+S-2}\alpha^{4S-4}\left(4\alpha^4 + 2C\alpha^4 a_2 + 2Sa_4 + CSa_2a_4 - CSa_5^2\right) \\ &= 2^{C+S-2}\alpha^{4S-4}\left[4\alpha^4 + 2C\alpha^4 a_2 + 2Sa_4 + CS(a_2a_4 - a_5^2)\right] \qquad (2.9)\end{aligned}$$

Next, by applying equations 2.1, 2.2, 2.3, 2.4, and 2.5 to equation 2.9, and upon simplification, we have

$$\begin{aligned}|\mathbf{K_Q}| = 2^{C+S-1}\alpha^{4S-4} \cdot &\left[\frac{2N\alpha^4 + C\alpha^4\left[NF - (F+2)^2\right]}{N}\right. \\ &\left.+\frac{S\left[NF - (F + 2\alpha^2)^2\right] - 2CSF\left(1-\alpha^2\right)^2}{N}\right] \qquad (2.10)\end{aligned}$$

Now that we have $|\mathbf{K_Q}|$ we arrive at a closed form for the determinant of $\mathbf{X_\Delta'}\mathbf{X_\Delta}$ which in turn gives us the determinant of $\mathbf{X'X}$. We state the result in the following theorem.

Theorem 2.1 *For a cylindrical design with C cuboidal factors and S spherical factors, the determinant of* $\mathbf{X'X}$ *is given by:*

$$\begin{aligned} |\mathbf{X'X}| &= |\mathbf{X}'_{\mathbf{\Delta}}\mathbf{X}_{\mathbf{\Delta}}| \\ &= N(F+2)^C(F+2\alpha^2)^S F^{\binom{C}{2}+\binom{S}{2}+CS} \cdot |\mathbf{K_Q}| \\ &= 2^{C+S-1}\alpha^{4S-4}(F+2)^C(F+2\alpha^2)^S F^{\binom{C}{2}+\binom{S}{2}+CS} \times \\ &\quad \left\{2N\alpha^4 + C\alpha^4\left[NF-(F+2)^2\right] + S\left[NF-(F+2\alpha^2)^2\right] \right. \\ &\quad \left. -2CSF\left(1-\alpha^2\right)^2\right\} \end{aligned} \tag{2.11}$$

D-efficiencies for Cylindrical Designs

Now that we have a closed form solution for the determinant of the $\mathbf{X'X}$ matrix, we can study the D-efficiency of cylindrical designs. Recall that from Equation 1.1, the D-efficiency is defined as $D_{eff} = \frac{|X'X|^{\frac{1}{p}}}{N}$ where $p = 1 + 2(C+S) + \binom{C}{2} + \binom{S}{2} + CS = \binom{C+S+2}{2}$ is the number of second order model parameters for a cylindrical design. Using the statistical software package R, we have calculated exact D-efficiencies for cylindrical designs with between 3 and 10 factors which are given in Table 2.1.

First note that in Table 2.1, for a given number of factors D-efficiencies are given when there are all spherical factors and 0 cuboidal factors or all cuboidal factors and 0 spherical factors. These values are in fact the D-efficiencies for Central Composite Designs with spherical and cuboidal regions, respectively. When C and S are both positive, the D-efficiency given is that for a Cylindrical Design. For a given number of total factors, the D-efficiency increases as the number of spherical factors increases. This phenomenon can also be seen in Figure 2.3 shown on page 25 which shows D-efficiencies for between 3 and 10 factors and compares the utilization of 1 center point versus 5 center points. For five or more factors, the D-efficiencies plotted in Figure 2.3

are those for which a fractional factorial is used because fractional factorials would typically be used in practice for cost effectiveness. The horizontal axis represents the number of spherical factors. Hence, for the graph showing D-efficiencies for 6 factors, when the number of spherical factors is 4 the resulting number of cuboidal factors is 2. For this combination of factors, when one center point is used, the D-efficiency is 64.13% while it is 60.26% with 5 center points. These values from Table 2.1 agree with what is seen in Figure 2.3.

The results shown here indicate that the cylindrical design is an excellent alternative, according to the D-criterion, to the Central Composite Design when some but not all factors have strict ranges on their levels. For example, consider the case of 5 factors and suppose the experimenter uses a fractional factorial design for the factorial portion of the design. Suppose further that only one factor has strict bounds on its levels and the experimenter decides to use 3 center points. From Table 2.1, the D-efficiency for a cylindrical design with 4 spherical factors, 1 cuboidal factor, and 3 center points is 65.34%. A CCD with a cuboidal region and 3 center points has a D-efficiency of 40.21% while a CCD with a spherical region and 3 center points has a D-efficiency of 78.50%. Thus, by using a CCD with a cuboidal region, the D-efficiency drops by 38.29% from a CCD with a spherical region. If a cylindrical design is used, the D-efficiency drop from the CCD with a spherical region is only 13.16%. Therefore, using a cylindrical design instead of a CCD with cuboidal region greatly improves estimation of the model parameters.

Table 2.1: D-efficiencies for between 3 and 10 factors with between 1 and 5 center points

$N_0 = 1$						
Factors	C	S	D-eff (Full)	D-eff (Frac)	N (Full)	N (Frac)
3	0	3	71.13		15	
	1	2	54.83			
	3	0	44.72			
4	0	4	76.73		25	
	1	3	63.55			
	2	2	51.73			
	4	0	44.52			
5	0	5	80.16	80.02	43	27
	1	4	69.90	68.22		
	2	3	58.69	56.61		
	3	2	50.13	47.96		
	5	0	44.84	42.69		
6	0	6	81.43	83.84	77	45
	1	5	73.45	74.67		
	2	4	63.51	64.13		
	3	3	55.17	55.43		
	4	2	48.87	48.91		
	6	0	44.84	44.80		
7	0	7	80.82	85.47	143	79
	1	6	74.53	78.30		
	2	5	65.98	69.06		
	3	4	58.41	60.95		
	4	3	52.19	54.34		
	5	2	47.41	49.29		
	7	0	44.29	46.01		
8	0	8	78.90	87.87	273	81
	1	7	73.87	81.50		
	2	6	66.60	73.09		
	3	5	59.93	65.48		
	4	4	54.19	59.00		
	5	3	49.45	53.69		
	6	2	45.75	49.57		
	8	0	43.29	46.86		
9	0	9	76.26	87.94	531	147
	1	8	72.16	82.83		
	2	7	66.01	75.56		
	3	6	60.21	68.76		
	4	5	55.07	62.77		
	5	4	50.64	57.63		
	6	3	46.94	53.35		
	7	2	44.02	49.99		
	9	0	42.05	47.73		
10	0	10	73.35	89.99	1045	149
	1	9	69.97	85.40		
	2	8	64.73	78.77		
	3	7	59.72	72.48		
	4	6	55.17	66.81		
	5	5	51.15	61.81		
	6	4	47.65	57.50		
	7	3	44.70	53.88		
	8	2	42.35	51.01		
	10	0	40.75	49.06		

Table 2.1 Continued

$N_0 = 2$						
Factors	C	S	D-eff (Full)	D-eff (Frac)	N (Full)	N (Frac)
3	0	3	71.47		16	
	1	2	53.41			
	3	0	43.00			
4	0	4	77.26		26	
	1	3	62.56			
	2	2	50.48			
	4	0	43.30			
5	0	5	80.97	79.75	44	28
	1	4	69.41	66.86		
	2	3	57.93	55.14		
	3	2	49.35	46.59		
	5	0	44.09	41.42		
6	0	6	82.40	84.07	78	46
	1	5	73.34	73.91		
	2	4	63.14	63.20		
	3	3	54.75	54.51		
	4	2	48.44	48.05		
	6	0	44.43	43.98		
7	0	7	81.82	86.04	144	80
	1	6	74.67	78.00		
	2	5	65.88	68.57		
	3	4	58.23	60.43		
	4	3	51.99	53.83		
	5	2	47.21	48.80		
	7	0	44.09	45.54		
8	0	8	79.83	88.14	274	82
	1	7	74.11	81.07		
	2	6	66.64	72.52		
	3	5	59.90	64.89		
	4	4	54.13	58.42		
	5	3	49.37	53.14		
	6	2	45.66	49.06		
	8	0	43.20	46.36		
9	0	9	77.08	88.46	532	148
	1	8	72.43	82.73		
	2	7	66.11	75.31		
	3	6	60.25	68.47		
	4	5	55.08	62.47		
	5	4	50.63	57.33		
	6	3	46.92	53.07		
	7	2	43.99	49.71		
	9	0	42.02	47.47		
10	0	10	74.05	90.33	1046	150
	1	9	70.22	85.22		
	2	8	64.86	78.48		
	3	7	59.79	72.15		
	4	6	55.21	66.47		
	5	5	51.17	61.49		
	6	4	47.66	57.18		
	7	3	44.71	53.58		
	8	2	42.35	50.71		
	10	0	40.75	48.77		

Table 2.1 Continued

$N_0 = 3$						
Factors	C	S	D-eff (Full)	D-eff (Frac)	N (Full)	N (Frac)
3	0	3	70.05		17	
	1	2	51.67			
	3	0	41.30			
4	0	4	76.44		27	
	1	3	61.29			
	2	2	49.20			
	4	0	42.11			
5	0	5	80.71	78.50	45	29
	1	4	68.68	65.34		
	2	3	57.10	53.68		
	3	2	48.56	45.27		
	5	0	43.34	40.21		
6	0	6	82.54	83.48	79	47
	1	5	73.05	72.97		
	2	4	62.72	62.22		
	3	3	54.31	53.59		
	4	2	48.01	47.20		
	6	0	44.02	43.19		
7	0	7	82.17	85.94	145	81
	1	6	74.65	77.56		
	2	5	65.72	68.04		
	3	4	58.03	59.89		
	4	3	51.78	53.32		
	5	2	46.99	48.32		
	7	0	43.88	45.08		
8	0	8	80.26	87.87	275	83
	1	7	74.23	80.52		
	2	6	66.64	71.90		
	3	5	59.85	64.28		
	4	4	54.05	57.85		
	5	3	49.28	52.60		
	6	2	45.57	48.54		
	8	0	43.11	45.88		
9	0	9	77.51	88.51	533	149
	1	8	72.61	82.53		
	2	7	66.18	75.02		
	3	6	60.27	68.17		
	4	5	55.08	62.16		
	5	4	50.61	57.04		
	6	3	46.89	52.78		
	7	2	43.96	49.44		
	9	0	41.99	47.20		
10	0	10	74.44	90.29	1047	151
	1	9	70.41	84.96		
	2	8	64.95	78.15		
	3	7	59.84	71.81		
	4	6	55.24	66.13		
	5	5	51.18	61.15		
	6	4	47.67	56.87		
	7	3	44.71	53.27		
	8	2	42.35	50.42		
	10	0	40.74	48.49		

Table 2.1 Continued

$N_0 = 4$						
Factors	C	S	D-eff (Full)	D-eff (Frac)	N (Full)	N (Frac)
3	0	3	68.09		18	
	1	2	49.87			
	3	0	39.66			
4	0	4	75.14		28	
	1	3	59.92			
	2	2	47.93			
	4	0	40.95			
5	0	5	80.04	76.93	46	30
	1	4	67.83	63.77		
	2	3	56.25	52.26		
	3	2	47.77	44.01		
	5	0	42.60	39.06		
6	0	6	82.35	82.59	80	48
	1	5	72.64	71.96		
	2	4	62.25	61.24		
	3	3	53.84	52.69		
	4	2	47.57	46.38		
	6	0	43.60	42.42		
7	0	7	82.26	85.57	146	82
	1	6	74.53	77.03		
	2	5	65.53	67.47		
	3	4	57.81	59.35		
	4	3	51.55	52.80		
	5	2	46.78	47.83		
	7	0	43.67	44.62		
8	0	8	80.48	87.38	276	84
	1	7	74.27	79.90		
	2	6	66.60	71.27		
	3	5	59.77	63.68		
	4	4	53.97	57.28		
	5	3	49.19	52.06		
	6	2	45.48	48.04		
	8	0	43.01	45.39		
9	0	9	77.77	88.38	534	150
	1	8	72.72	82.27		
	2	7	66.23	74.71		
	3	6	60.28	67.85		
	4	5	55.06	61.85		
	5	4	50.59	56.74		
	6	3	46.86	52.49		
	7	2	43.93	49.16		
	9	0	41.95	46.93		
10	0	10	74.69	90.08	1048	152
	1	9	70.54	84.65		
	2	8	65.03	77.79		
	3	7	59.88	71.45		
	4	6	55.26	65.79		
	5	5	51.19	60.82		
	6	4	47.67	56.55		
	7	3	44.70	52.97		
	8	2	42.34	50.13		
	10	0	40.73	48.21		

Table 2.1 Continued

$N_0 = 5$						
Factors	C	S	D-eff (Full)	D-eff (Frac)	N (Full)	N (Frac)
3	0	3	65.96		19	
	1	2	48.09			
	3	0	38.12			
4	0	4	73.64		29	
	1	3	58.52			
	2	2	46.48			
	4	0	39.83			
5	0	5	79.18	75.25	49	31
	1	4	66.91	62.21		
	2	3	55.39	50.89		
	3	2	46.99	42.80		
	5	0	41.88	37.97		
6	0	6	81.99	81.55	81	49
	1	5	72.17	70.91		
	2	4	61.76	60.26		
	3	3	53.37	51.80		
	4	2	47.13	45.57		
	6	0	43.18	41.67		
7	0	7	82.21	85.07	147	83
	1	6	74.36	76.44		
	2	5	65.31	66.89		
	3	4	57.58	58.80		
	4	3	51.32	52.29		
	5	2	46.55	47.35		
	7	0	43.45	44.16		
8	0	8	80.59	86.78	277	85
	1	7	74.27	79.25		
	2	6	66.55	70.62		
	3	5	59.69	63.07		
	4	4	53.87	56.71		
	5	3	49.09	51.53		
	6	2	45.38	47.54		
	8	0	42.92	44.92		
9	0	9	77.94	88.16	535	151
	1	8	72.80	81.96		
	2	7	66.25	74.38		
	3	6	60.28	67.52		
	4	5	55.04	61.53		
	5	4	50.56	56.43		
	6	3	46.83	52.21		
	7	2	43.89	48.89		
	9	0	41.91	46.67		
10	0	10	74.88	89.80	1049	153
	1	9	70.64	84.30		
	2	8	65.09	77.43		
	3	7	59.92	71.09		
	4	6	55.28	65.44		
	5	5	51.20	60.49		
	6	4	47.67	56.23		
	7	3	44.70	52.67		
	8	2	42.33	49.84		
	10	0	40.72	47.93		

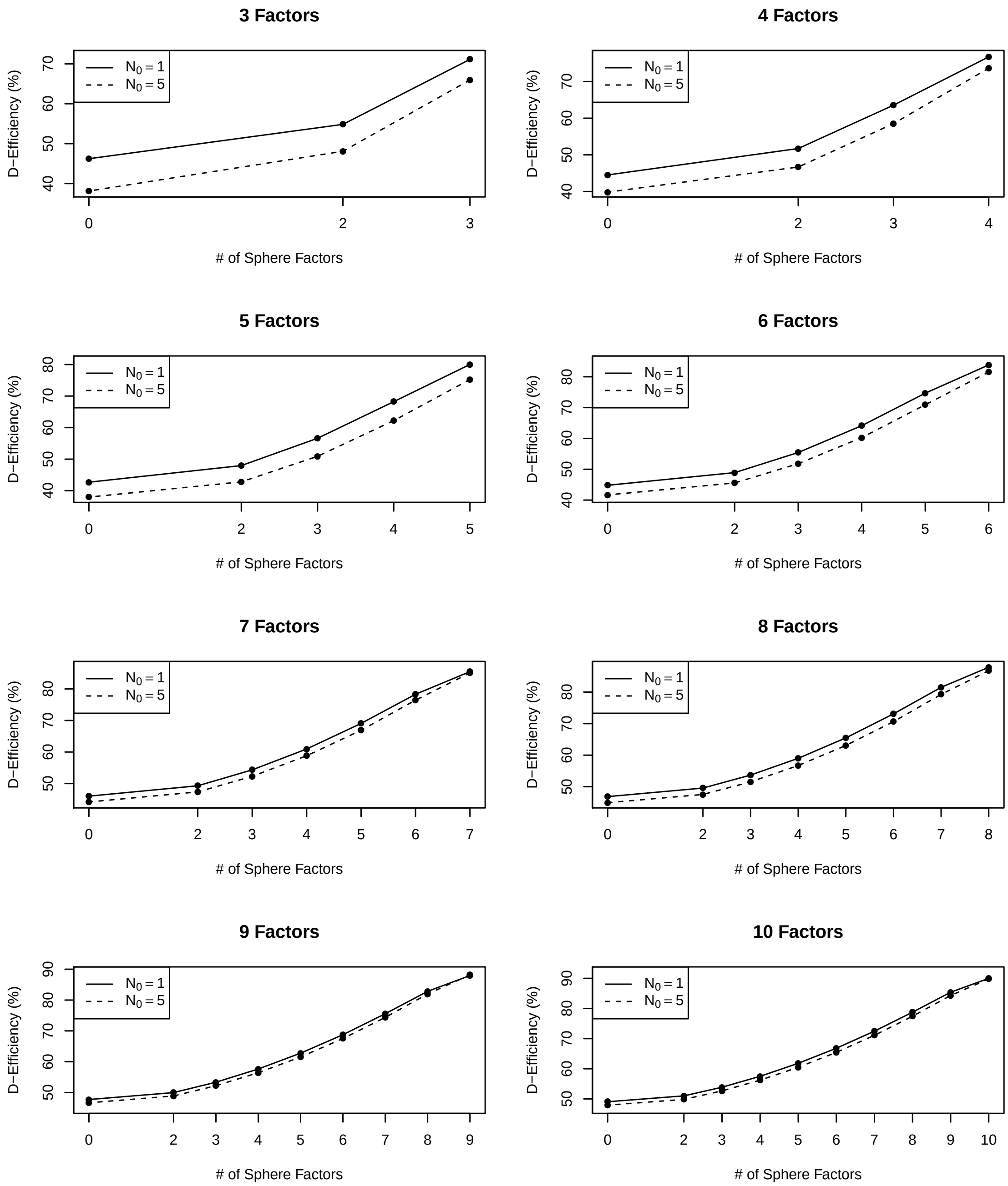

Figure 2.3: D-efficiencies for between 3 and 10 factors comparing use of 1 and 5 center points. For 5 or more factors, it is assumed that the appropriate fractional factorial design is used.

THE INVERSE OF $\mathbf{X'X}$ AND THE A-CRITERION

Finding $(\mathbf{X'X})^{-1}$

For the A-efficiency, G-efficiency, and IV-efficiency, it is necessary to derive a closed form for the $\mathbf{X'X}$ matrix. In this chapter, we will derive the general form of $(\mathbf{X'X})^{-1}$ and calculate the trace to study A-efficiencies of cylindrical designs. We will also give a closed form for the scaled prediction variance which will be used in later chapters to study G- and IV-efficiencies. The general form of the $\mathbf{X'X}$ matrix for any two cuboidal and any two spherical factors was shown in Figure 1.5 on page 11. In order to find $(\mathbf{X'X})^{-1}$ for a cylindrical design, it is necessary to write $\mathbf{X'X}$ in the block form shown in Figure 3.1.

$$\mathbf{X'X} = \left[\begin{array}{cc|cc} N & \phi_1' & (F+2)\mathbf{J_C'} & (F+2\alpha^2)\mathbf{J_S'} \\ \phi_1 & \mathbf{diag}(d_i) & \phi_2' & \phi_3' \\ \hline (F+2)\mathbf{J_C} & \phi_2 & F\mathbf{J_C}\mathbf{J_C'} + 2\mathbf{I_C} & F\mathbf{J_C}\mathbf{J_S'} \\ (F+2\alpha^2)\mathbf{J_S} & \phi_3 & F\mathbf{J_S}\mathbf{J_C'} & F\mathbf{J_S}\mathbf{J_S'} + 2\alpha^4\mathbf{I_S} \end{array}\right]$$

Figure 3.1: General Block Form of the $\mathbf{X'X}$ Matrix

- ϕ_1, ϕ_2, ϕ_3 are zero matrices of dimensions $K^* \times 1$, $C \times K^*$, and $S \times K^*$
- $\mathbf{diag}(d_i)$ is a $K^* \times K^*$ diagonal matrix with diagonal entries

$$d_i = \begin{cases} F+2 & 1 \le i \le C \\ F+2\alpha^2 & C+1 \le i \le C+S \\ F & C+S+1 \le i \le K^* \end{cases}$$

- $\mathbf{J_C}$ and $\mathbf{J_S}$ are $C \times 1$ and $S \times 1$ unit column vectors.
- $\mathbf{I_C}$ and $\mathbf{I_S}$ are $C \times C$ and $S \times S$ identity matrices.

- $K^* = C + S + \binom{C}{2} + \binom{S}{2} + CS$

From Hocking [7] we have that for a matrix of the block form

$$\left[\begin{array}{c|c} \mathbf{A_{11}} & \mathbf{A_{12}} \\ \hline \mathbf{A_{21}} & \mathbf{A_{22}} \end{array}\right]$$

the general form of the inverse is given by:

$$\left[\begin{array}{c|c} \mathbf{A^{11}} & \mathbf{A^{12}} \\ \hline \mathbf{A^{21}} & \mathbf{A^{22}} \end{array}\right]$$

where

$$\begin{aligned} \mathbf{A^{11}} &= \left(\mathbf{A_{11}} - \mathbf{A_{12}}\mathbf{A_{22}^{-1}}\mathbf{A_{21}}\right)^{-1} \\ \mathbf{A^{12}} &= -\mathbf{A_{11}^{-1}}\mathbf{A_{12}}\mathbf{A^{22}} \\ \mathbf{A^{22}} &= \left(\mathbf{A_{22}} - \mathbf{A_{21}}\mathbf{A_{11}^{-1}}\mathbf{A_{12}}\right)^{-1} \\ \mathbf{A^{21}} &= -\mathbf{A_{22}^{-1}}\mathbf{A_{21}}\mathbf{A^{11}} \end{aligned}$$

Thus to compute $(\mathbf{X}'\mathbf{X})^{-1}$, we find each of the components $\mathbf{A^{11}}$, $\mathbf{A^{12}}$, $\mathbf{A^{22}}$, and $\mathbf{A^{21}}$.

We first find the components of $\mathbf{A^{11}}$ which first requires finding $\mathbf{A_{22}^{-1}}$. Because

$$\mathbf{A_{22}} = \left[\begin{array}{c|c} F\mathbf{J_C}\mathbf{J_C'} + 2\mathbf{I_C} & F\mathbf{J_C}\mathbf{J_S'} \\ \hline F\mathbf{J_S}\mathbf{J_C'} & F\mathbf{J_S}\mathbf{J_S'} + 2\alpha^4\mathbf{I_S} \end{array}\right] = \left[\begin{array}{c|c} \mathbf{B_{11}} & \mathbf{B_{12}} \\ \hline \mathbf{B_{21}} & \mathbf{B_{22}} \end{array}\right],$$

$\mathbf{A_{22}^{-1}}$ is found in the same fashion we intend to find $(\mathbf{X}'\mathbf{X})^{-1}$. That is,

$$\mathbf{A_{22}^{-1}} = \left[\begin{array}{c|c} \mathbf{B^{11}} & \mathbf{B^{12}} \\ \hline \mathbf{B^{21}} & \mathbf{B^{22}} \end{array}\right]$$

where

$$\begin{aligned} \mathbf{B^{11}} &= \left(\mathbf{B_{11}} - \mathbf{B_{12}}\mathbf{B_{22}^{-1}}\mathbf{B_{21}}\right)^{-1} \\ \mathbf{B^{12}} &= -\mathbf{B_{11}^{-1}}\mathbf{B_{12}}\mathbf{B^{22}} \\ \mathbf{B^{22}} &= \left(\mathbf{B_{22}} - \mathbf{B_{21}}\mathbf{B_{11}^{-1}}\mathbf{B_{12}}\right)^{-1} \\ \mathbf{B^{21}} &= -\mathbf{B_{22}^{-1}}\mathbf{B_{21}}\mathbf{B^{11}} \end{aligned}$$

The components of $\mathbf{B^{11}}$

Using (2.7), we have

$$\begin{aligned}
\mathbf{B_{22}^{-1}} &= \left(F\mathbf{J_S}\mathbf{J_S'} + 2\alpha^4\mathbf{I_S}\right)^{-1} \\
&= \frac{1}{2\alpha^4}\left(\mathbf{I_S} - \frac{F}{2\alpha^4+SF}\mathbf{J_S}\mathbf{J_S'}\right)
\end{aligned}$$

Pre-multiplying by $\mathbf{B_{12}}$ and post-multiplying by $\mathbf{B_{21}}$ we obtain

$$\begin{aligned}
\mathbf{B_{12}}\mathbf{B_{22}^{-1}}\mathbf{B_{21}} &= F\mathbf{J_C}\mathbf{J_S'}\cdot\frac{1}{2\alpha^4}\left(\mathbf{I_S} - \frac{F}{2\alpha^4+SF}\mathbf{J_S}\mathbf{J_S'}\right)\mathbf{B_{21}} \\
&= \frac{F}{2\alpha^4}\left(\mathbf{J_C}\mathbf{J_S'} - \frac{F}{2\alpha^4+SF}\mathbf{J_C}\mathbf{J_S'}\mathbf{J_S}\mathbf{J_S'}\right)\mathbf{B_{21}} \\
&= \frac{F}{2\alpha^4}\left(\mathbf{J_C}\mathbf{J_S'} - \frac{SF}{2\alpha^4+SF}\mathbf{J_C}\mathbf{J_S'}\right)\mathbf{B_{21}} \\
&= \frac{F}{2\alpha^4}\left(\mathbf{J_C}\mathbf{J_S'} - \frac{SF}{2\alpha^4+SF}\mathbf{J_C}\mathbf{J_S'}\right)\cdot F\mathbf{J_S}\mathbf{J_C'} \\
&= \frac{F^2}{2\alpha^4}\left(\mathbf{J_C}\mathbf{J_S'}\mathbf{J_S}\mathbf{J_C'} - \frac{SF}{2\alpha^4+SF}\mathbf{J_C}\mathbf{J_S'}\mathbf{J_S}\mathbf{J_C'}\right) \\
&= \frac{F^2}{2\alpha^4}\left(S - \frac{S^2F}{2\alpha^4+SF}\right)\mathbf{J_C}\mathbf{J_C'} \\
&= \frac{SF^2}{2\alpha^4+SF}\mathbf{J_C}\mathbf{J_C'}
\end{aligned}$$

Next we subtract from $\mathbf{B_{11}}$ and we have

$$\begin{aligned}
\mathbf{B_{11}} - \mathbf{B_{12}}\mathbf{B_{22}^{-1}}\mathbf{B_{21}} &= (2\mathbf{I_C} + F\mathbf{J_C}\mathbf{J_C'}) - \frac{SF^2}{2\alpha^4+SF}\mathbf{J_C}\mathbf{J_C'} \\
&= 2\mathbf{I_C} + \left(F - \frac{SF^2}{2\alpha^4+SF}\right)\mathbf{J_C}\mathbf{J_C'} \\
&= 2\mathbf{I_C} + \frac{2F\alpha^4}{2\alpha^4+SF}\mathbf{J_C}\mathbf{J_C'}
\end{aligned}$$

Now that we have the components of $\mathbf{B^{11}}$ we simply need to find the inverse.

$$\begin{aligned}
\mathbf{B^{11}} &= \left(\mathbf{B_{11}} - \mathbf{B_{12}}\mathbf{B_{22}^{-1}}\mathbf{B_{21}}\right)^{-1} \\
&= \left(2\mathbf{I_C} + \frac{2F\alpha^4}{2\alpha^4+SF}\mathbf{J_C}\mathbf{J_C'}\right)^{-1}
\end{aligned}$$

$$
\begin{aligned}
&= \frac{1}{2}\left(\mathbf{I_C} - \frac{2F\alpha^4}{2\alpha^4+SF}\cdot\frac{1}{2+C\left(\frac{2F\alpha^4}{2\alpha^4+SF}\right)}\mathbf{J_C J'_C}\right)\\
&= \frac{1}{2}\left(\mathbf{I_C} - \frac{2F\alpha^4}{2(2\alpha^4+SF)+2CF\alpha^4}\mathbf{J_C J'_C}\right)\\
&= \frac{1}{2}\left(\mathbf{I_C} - \frac{F\alpha^4}{2\alpha^4+SF+CF\alpha^4}\mathbf{J_C J'_C}\right) \qquad (3.1)
\end{aligned}
$$

The Components of $\mathbf{B^{22}}$

First note that $\mathbf{B_{11}^{-1}} = \frac{1}{2}\left(\mathbf{I_C} - \frac{F}{2+CF}\mathbf{J_C J'_C}\right)$. Pre-multiplying by $\mathbf{B_{21}}$ and post-multiplying by $\mathbf{B_{12}}$, we find

$$
\begin{aligned}
\mathbf{B_{21}B_{11}^{-1}B_{12}} &= (F\mathbf{J_S J'_C})\cdot\frac{1}{2}\left(\mathbf{I_C} - \frac{F}{2+CF}\mathbf{J_C J'_C}\right)\cdot F\mathbf{J_C J'_S}\\
&= \frac{F^2}{2}\left(\mathbf{J_S J'_C J_C J'_S} - \frac{F}{2+CF}\mathbf{J_S J'_C J_C J'_C J_C J'_S}\right)\\
&= \frac{F^2}{2}\left(C\mathbf{J_S J'_S} - \frac{C^2F}{2+CF}\mathbf{J_S J'_S}\right)\\
&= \frac{CF^2}{2+CF}\mathbf{J_S J'_S}
\end{aligned}
$$

Then

$$
\begin{aligned}
\mathbf{B^{22}} &= \left(\mathbf{B_{22}} - \mathbf{B_{21}B_{11}^{-1}B_{12}}\right)^{-1}\\
&= \left(\left[F\mathbf{J_S J'_S} + 2\alpha^4\mathbf{I_S}\right] - \frac{CF^2}{2+CF}\mathbf{J_S J'_S}\right)^{-1}\\
&= \left(2\alpha^4\mathbf{I_S} + \left(F - \frac{CF^2}{2+CF}\right)\mathbf{J_S J'_S}\right)^{-1}\\
&= \left(2\alpha^4\mathbf{I_S} + \frac{2F}{2+CF}\mathbf{J_S J'_S}\right)^{-1}\\
&= \frac{1}{2\alpha^4}\left(\mathbf{I_S} - \frac{2F}{2+CF}\cdot\frac{1}{2\alpha^4+S\left(\frac{2F}{2+CF}\right)}\mathbf{J_S J'_S}\right)\\
&= \frac{1}{2\alpha^4}\left(\mathbf{I_S} - \frac{2F}{2\alpha^4(2+CF)+2SF}\mathbf{J_S J'_S}\right)\\
&= \frac{1}{2\alpha^4}\left(\mathbf{I_S} - \frac{F}{2\alpha^4+SF+CF\alpha^4}\mathbf{J_S J'_S}\right) \qquad (3.2)
\end{aligned}
$$

The components of $\mathbf{B^{12}}$

$$\begin{aligned}
\mathbf{B^{12}} &= -\mathbf{B_{11}^{-1}B_{12}B^{22}} \\
&= -\frac{1}{2}\left(\mathbf{I_C} - \frac{F}{2+CF}\mathbf{J_C J_C'}\right)\cdot F\mathbf{J_C J_S'}\cdot\frac{1}{2\alpha^4}\left(\mathbf{I_S} - \frac{F}{2\alpha^4+SF+CF\alpha^4}\mathbf{J_S J_S'}\right) \\
&= -\frac{F}{4\alpha^4}\left(\mathbf{J_C J_S'} - \frac{F}{2+CF}\mathbf{J_C J_C' J_C J_S'}\right)\left(\mathbf{I_S} - \frac{F}{2\alpha^4+SF+CF\alpha^4}\mathbf{J_S J_S'}\right) \\
&= -\frac{F}{4\alpha^4}\left(\frac{2}{2+CF}\mathbf{J_C J_S'}\right)\left(\mathbf{I_S} - \frac{F}{2\alpha^4+SF+CF\alpha^4}\mathbf{J_S J_S'}\right) \\
&= -\frac{F}{2\alpha^4(2+CF)}\left(\mathbf{J_C J_S'} - \frac{F}{2\alpha^4+SF+CF\alpha^4}\mathbf{J_C J_S' J_S J_S'}\right) \\
&= -\frac{F}{2\alpha^4(2+CF)}\left(\frac{2\alpha^4+CF\alpha^4}{2\alpha^4+SF+CF\alpha^4}\mathbf{J_C J_S'}\right) \\
&= -\frac{F}{2(2\alpha^4+SF+CF\alpha^4)}\mathbf{J_C J_S'} \qquad (3.3)
\end{aligned}$$

The components of $\mathbf{B^{21}}$

$$\begin{aligned}
\mathbf{B^{21}} &= -\mathbf{B_{22}^{-1}B_{21}B^{11}} \\
&= -\frac{1}{2\alpha^4}\left(\mathbf{I_S} - \frac{F}{2\alpha^4+SF}\mathbf{J_S J_S'}\right)\cdot F\mathbf{J_S J_C'}\cdot\frac{1}{2}\left(\mathbf{I_C} - \frac{F\alpha^4}{2\alpha^4+SF+CF\alpha^4}\mathbf{J_C J_C'}\right) \\
&= -\frac{F}{4\alpha^4}\left(\mathbf{J_S J_C'} - \frac{SF}{2\alpha^4+SF}\mathbf{J_S J_C'}\right)\left(\mathbf{I_C} - \frac{F\alpha^4}{2\alpha^4+SF+CF\alpha^4}\mathbf{J_C J_C'}\right) \\
&= -\frac{F}{2}\left(\frac{1}{2\alpha^4+SF}\mathbf{J_S J_C'}\right)\left(\mathbf{I_C} - \frac{F\alpha^4}{2\alpha^4+SF+CF\alpha^4}\mathbf{J_C J_C'}\right) \\
&= -\frac{F}{2(2\alpha^4+SF)}\left(\mathbf{J_S J_C'} - \frac{CF\alpha^4}{2\alpha^4+SF+CF\alpha^4}\mathbf{J_S J_C'}\right) \\
&= -\frac{F}{2(2\alpha^4+SF+CF\alpha^4)}\mathbf{J_S J_C'} \qquad (3.4)
\end{aligned}$$

Now, combining the pieces from equations 3.1, 3.2, 3.3, and 3.4 we have

$$\mathbf{A_{22}^{-1}} = \frac{1}{2}\left[\begin{array}{c|c} \mathbf{I_C} - \gamma\alpha^4\mathbf{J_C J_C'} & -\gamma\mathbf{J_C J_S'} \\ \hline -\gamma\mathbf{J_S J_C'} & \frac{1}{\alpha^4}\left(\mathbf{I_S} - \gamma\mathbf{J_S J_S'}\right) \end{array}\right] \qquad (3.5)$$

where

$$\gamma = \frac{F}{2\alpha^4 + SF + CF\alpha^4} \tag{3.6}$$

The Components of $\mathbf{A^{11}}$

Recall that the purpose of obtaining $\mathbf{A_{22}^{-1}}$ was to find $\mathbf{A^{11}} = \left(\mathbf{A_{11}} - \mathbf{A_{12}}\mathbf{A_{22}^{-1}}\mathbf{A_{21}}\right)^{-1}$. Pre-multiplying $\mathbf{A_{22}^{-1}}$ by $\mathbf{A_{12}}$ and post-multiplying by $\mathbf{A_{21}}$, we have

$$\begin{aligned}
\mathbf{A_{12}}\mathbf{A_{22}^{-1}}\mathbf{A_{21}} &= \left[\begin{array}{c|c} (F+2)\mathbf{J'_C} & (F+2\alpha^2)\mathbf{J'_S} \\ \hline \phi'_2 & \phi'_3 \end{array}\right] \times \\
&\quad \frac{1}{2}\left[\begin{array}{c|c} \mathbf{I_C} - \gamma\alpha^4\mathbf{J_C}\mathbf{J'_C} & -\gamma\mathbf{J_C}\mathbf{J'_S} \\ \hline -\gamma\mathbf{J_S}\mathbf{J'_C} & \frac{1}{\alpha^4}\left(\mathbf{I_S} - \gamma\mathbf{J_S}\mathbf{J'_S}\right) \end{array}\right] \cdot \left[\begin{array}{c|c} (F+2)\mathbf{J_C} & \phi_2 \\ \hline (F+2\alpha^2)\mathbf{J_S} & \phi_3 \end{array}\right] \\
&= \left[\begin{array}{c|c} \psi & \phi'_1 \\ \hline \phi_1 & \phi'_2\phi_2 \end{array}\right]
\end{aligned} \tag{3.7}$$

where

$$\psi = \frac{C\alpha^4(F+2)\big[(F+2) - C\gamma\alpha^4(F+2) - S\gamma(F+2\alpha^2)\big] + S(F+2\alpha^2)\big[(F+2\alpha^2) - C\gamma\alpha^4(F+2) - S\gamma(F+2\alpha^2)\big]}{2\alpha^4}$$

Next, we subtract the matrix in (3.7) from $\mathbf{A_{11}}$ to obtain

$$\begin{aligned}
\mathbf{A_{11}} - \mathbf{A_{12}}\mathbf{A_{22}^{-1}}\mathbf{A_{21}} &= \left[\begin{array}{c|c} N & \phi'_1 \\ \hline \phi_1 & \mathbf{diag}(d_i) \end{array}\right] - \left[\begin{array}{c|c} \psi & \phi'_1 \\ \hline \phi_1 & \phi'_2\phi_2 \end{array}\right] \\
&= \left[\begin{array}{c|c} N - \psi & \phi'_1 \\ \hline \phi_1 & \mathbf{diag}(d_i) \end{array}\right]
\end{aligned} \tag{3.8}$$

Note that because the matrix in (3.8) is diagonal, the inverse is readily found so that

$$\begin{aligned}
\mathbf{A^{11}} &= \left(\mathbf{A_{11}} - \mathbf{A_{12}}\mathbf{A_{22}^{-1}}\mathbf{A_{21}}\right)^{-1} \\
&= \left[\begin{array}{c|c} \frac{1}{N-\psi} & \phi'_1 \\ \hline \phi_1 & \mathbf{diag}(\frac{1}{d_i}) \end{array}\right]
\end{aligned}$$

$$= \left[\begin{array}{c|c} \gamma_1 & \phi_1' \\ \hline \phi_1 & \mathbf{diag}(\frac{1}{d_i}) \end{array}\right] \tag{3.9}$$

where

$$\begin{aligned} \gamma_1 &= \frac{1}{N-\psi} \\ &= 2\alpha^4 \div \Big\{2N\alpha^4 - C\alpha^4(F+2)\Big[(F+2) - C\gamma\alpha^4(F+2) - S\gamma(F+2\alpha^2)\Big] \\ &\quad -S(F+2\alpha^2)\Big[(F+2\alpha^2) - C\gamma\alpha^4(F+2) - S\gamma(F+2\alpha^2)\Big]\Big\} \end{aligned}$$

Substituting $\frac{F}{2\alpha^4+SF+CF\alpha^4}$ for γ and after algebraic simplification we have

$$\gamma_1 = \frac{2\alpha^4 + SF + CF\alpha^4}{N(2\alpha^4+SF+CF\alpha^4) - C\alpha^4(F+2)^2 - S(F+2\alpha^2)^2 - 2CSF(\alpha^2-1)^2} \tag{3.10}$$

The components of $\mathbf{A^{22}}$

$$\begin{aligned} \mathbf{A_{21}A_{11}^{-1}A_{12}} &= \begin{bmatrix} (F+2)\mathbf{J_C} & \phi_2 \\ (F+2\alpha^2)\mathbf{J_S} & \phi_3 \end{bmatrix} \cdot \begin{bmatrix} \frac{1}{N} & \phi_1' \\ \phi_1 & \mathbf{diag}\left(\frac{1}{d_i}\right) \end{bmatrix} \times \\ &\quad \begin{bmatrix} (F+2)\mathbf{J_C'} & (F+2\alpha^2)\mathbf{J_S'} \\ \phi_2' & \phi_3' \end{bmatrix} \\ &= \frac{1}{N}\left[\begin{array}{c|c} (F+2)^2\mathbf{J_C J_C'} & (F+2)(F+2\alpha^2)\mathbf{J_C J_S'} \\ \hline (F+2)(F+2\alpha^2)\mathbf{J_S J_C'} & (F+2\alpha^2)^2\mathbf{J_S J_S'} \end{array}\right] \end{aligned}$$

Then $\mathbf{A_{22}} - \mathbf{A_{21}A_{11}^{-1}A_{12}} =$

$$\left[\begin{array}{c|c} F\mathbf{J_C J_C'} + 2\mathbf{I_C} & F\mathbf{J_C J_S'} \\ \hline F\mathbf{J_S J_C'} & F\mathbf{J_S J_S'} + 2\alpha^4\mathbf{I_S} \end{array}\right]$$

$$-\frac{1}{N}\left[\begin{array}{c|c} (F+2)^2\mathbf{J_C J_C'} & (F+2)(F+2\alpha^2)\mathbf{J_C J_S'} \\ \hline (F+2)(F+2\alpha^2)\mathbf{J_S J_C'} & (F+2\alpha^2)^2\mathbf{J_S J_S'} \end{array}\right]$$

$$= \left[\begin{array}{c|c} 2\mathbf{I_C} + \left(F - \frac{(F+2)^2}{N}\right)\mathbf{J_C J_C'} & \left(F - \frac{(F+2)(F+2\alpha^2)}{N}\right)\mathbf{J_C J_S'} \\ \hline \left(F - \frac{(F+2)(F+2\alpha^2)}{N}\right)\mathbf{J_S J_C'} & 2\alpha^4 I_S + \left(F - \frac{(F+2\alpha^2)^2}{N}\right)\mathbf{J_S J_S'} \end{array}\right]$$

$$= \left[\begin{array}{c|c} 2\mathbf{I_C} + \left(\frac{NF-(F+2)^2}{N}\right)\mathbf{J_C J_C'} & \left(\frac{NF-(F+2)(F+2\alpha^2)}{N}\right)\mathbf{J_C J_S'} \\ \hline \left(\frac{NF-(F+2)(F+2\alpha^2)}{N}\right)\mathbf{J_S J_C'} & 2\alpha^4\mathbf{I_S} + \left(\frac{NF-(F+2\alpha^2)^2}{N}\right)\mathbf{J_S J_S'} \end{array}\right]$$

$$= \left[\begin{array}{c|c} \mathbf{D_{11}} & \mathbf{D_{12}} \\ \hline \mathbf{D_{21}} & \mathbf{D_{22}} \end{array}\right]$$

In order to compute $\mathbf{A^{22}} = (\mathbf{A_{22}} - \mathbf{A_{21}}\mathbf{A_{11}^{-1}}\mathbf{A_{12}})^{-1}$ we must again employ the matrix inversion technique used for the general block form found above. This involves finding

$$\left[\begin{array}{c|c} \mathbf{D^{11}} & \mathbf{D^{12}} \\ \hline \mathbf{D^{21}} & \mathbf{D^{22}} \end{array}\right]$$

where

$$\begin{aligned} \mathbf{D^{11}} &= \left(\mathbf{D_{11}} - \mathbf{D_{12}}\mathbf{D_{22}^{-1}}\mathbf{D_{21}}\right)^{-1} \\ \mathbf{D^{12}} &= -\mathbf{D_{11}^{-1}}\mathbf{D_{12}}\mathbf{D^{22}} \\ \mathbf{D^{22}} &= \left(\mathbf{D_{22}} - \mathbf{D_{21}}\mathbf{D_{11}^{-1}}\mathbf{D_{12}}\right)^{-1} \\ \mathbf{D^{21}} &= -\mathbf{D_{22}^{-1}}\mathbf{D_{21}}\mathbf{D^{11}} \end{aligned}$$

The Components of $\mathbf{D^{11}}$

First note that $\mathbf{D_{22}^{-1}}$ can be written as

$$\mathbf{D_{22}^{-1}} = \frac{1}{2\alpha^4}\left(\mathbf{I_S} - \frac{NF-(F+2\alpha^2)^2}{2N\alpha^4 + S\left[NF-(F+2\alpha^2)^2\right]}\mathbf{J_S J_S'}\right)$$

Pre-multiplying by $\mathbf{D_{12}}$, we find

$$\mathbf{D_{12}}\mathbf{D_{22}^{-1}} = \left(\frac{NF-(F+2)(F+2\alpha^2)}{N}\mathbf{J_C J_S'}\right) \times$$

$$
\begin{aligned}
& \left[\frac{1}{2\alpha^4}\left(\mathbf{I_S} - \frac{NF-(F+2\alpha^2)^2}{2N\alpha^4 + S\left[NF-(F+2\alpha^2)^2\right]}\mathbf{J_S}\mathbf{J_S'}\right)\right] \\
= & \frac{NF-(F+2)(F+2\alpha^2)}{2N\alpha^4}\left(\mathbf{J_C}\mathbf{J_S'} - S\frac{NF-(F+2\alpha^2)^2}{2N\alpha^4 + S\left[NF-(F+2\alpha^2)^2\right]}\mathbf{J_C}\mathbf{J_S'}\right) \\
= & \frac{NF-(F+2)(F+2\alpha^2)}{2N\alpha^4 + S\left[NF-(F+2\alpha^2)^2\right]}\mathbf{J_C}\mathbf{J_S'}
\end{aligned}
$$

Post-multiplying by $\mathbf{D_{21}}$,

$$
\begin{aligned}
\mathbf{D_{12}}\mathbf{D_{22}^{-1}}\mathbf{D_{21}} &= \left(\frac{NF-(F+2)(F+2\alpha^2)}{2N\alpha^4 + S\left[NF-(F+2\alpha^2)^2\right]}\mathbf{J_C}\mathbf{J_S'}\right) \times \\
&\quad \left(\frac{NF-(F+2)(F+2\alpha^2)}{N}\mathbf{J_S}\mathbf{J_C'}\right) \\
&= \frac{S\left[NF-(F+2)(F+2\alpha^2)\right]^2}{N\left[2N\alpha^4 + SNF - S(F+2\alpha^2)^2\right]}\mathbf{J_C}\mathbf{J_C'}
\end{aligned}
$$

Next, we subtract the above quantity from $\mathbf{D_{11}}$ to obtain

$$
\begin{aligned}
\mathbf{D_{11}} - \mathbf{D_{12}}\mathbf{D_{22}^{-1}}\mathbf{D_{21}} &= \left(2\mathbf{I_C} + \frac{NF-(F+2)^2}{N}\mathbf{J_C}\mathbf{J_C'}\right) - \\
&\quad \frac{S\left[NF-(F+2)(F+2\alpha^2)\right]^2}{N\left[2N\alpha^4 + SNF - S(F+2\alpha^2)^2\right]}\mathbf{J_C}\mathbf{J_C'} \\
&= 2\mathbf{I_C} + \frac{2\alpha^4\left[NF-(F+2)^2\right] - 4SF(\alpha^2-1)^2}{2N\alpha^4 + SNF - S(F+2\alpha^2)^2}\mathbf{J_C}\mathbf{J_C'} \\
&= 2\mathbf{I_C} + \gamma_2\mathbf{J_C}\mathbf{J_C'}
\end{aligned}
$$

where

$$
\gamma_2 = \frac{2\alpha^4\left[NF-(F+2)^2\right] - 4SF(\alpha^2-1)^2}{2N\alpha^4 + SNF - S(F+2\alpha^2)^2} \tag{3.11}
$$

Thus $\mathbf{D^{11}} = \left(\mathbf{D_{11}} - \mathbf{D_{12}}\mathbf{D_{22}^{-1}}\mathbf{D_{21}}\right)^{-1}$ is given by

$$
\mathbf{D^{11}} = \frac{1}{2}\left(\mathbf{I_C} - \frac{\gamma_2}{2 + C\gamma_2}\mathbf{J_C}\mathbf{J_C'}\right) \tag{3.12}
$$

The Components of $\mathbf{D^{22}}$

$$
\mathbf{D_{11}^{-1}} = \frac{1}{2}\left(\mathbf{I_C} - \frac{NF-(F+2)^2}{2N + C\left[NF-(F+2)^2\right]}\mathbf{J_C}\mathbf{J_C'}\right)
$$

Then, pre-multiplying by $\mathbf{D_{21}}$ and post-multiplying by $\mathbf{D_{12}}$, we have

$$\begin{aligned}
\mathbf{D_{21}D_{11}^{-1}D_{12}} &= \left(\frac{NF-(F+2)(F+2\alpha^2)}{N}\mathbf{J_S J_C'}\right)\times \\
&\quad \left[\frac{1}{2}\left(\mathbf{I_C}-\frac{NF-(F+2)^2}{2N+C\left[NF-(F+2)^2\right]}\mathbf{J_C J_C'}\right)\right]\cdot\mathbf{D_{12}} \\
&= \left[\frac{NF-(F+2)(F+2\alpha^2)}{2N+CNF-C(F+2)^2}\mathbf{J_S J_C'}\right]\cdot\mathbf{D_{12}} \\
&= \left[\frac{NF-(F+2)(F+2\alpha^2)}{2N+CNF-C(F+2)^2}\mathbf{J_S J_C'}\right]\cdot\left[\frac{NF-(F+2)(F+2\alpha^2)}{N}\mathbf{J_C J_S'}\right] \\
&= \frac{C\left[NF-(F+2)(F+2\alpha^2)\right]^2}{N\left[2N+CNF-C(F+2)^2\right]}\mathbf{J_S J_S'}
\end{aligned}$$

Then,

$$\begin{aligned}
\mathbf{D_{22}}-\mathbf{D_{21}D_{11}^{-1}D_{12}} &= \left(2\alpha^4\mathbf{I_S}+\frac{NF-(F+2\alpha^2)^2}{N}\mathbf{J_S J_S'}\right)- \\
&\quad \frac{C\left[NF-(F+2)(F+2\alpha^2)\right]^2}{N\left[2N+CNF-C(F+2)^2\right]}\mathbf{J_S J_S'} \\
&= 2\alpha^4\mathbf{I_S}+\frac{2\left[NF-(F+2\alpha^2)^2\right]-4CF(\alpha^2-1)^2}{\left[2N+CNF-C(F+2)^2\right]}\mathbf{J_S J_S'} \\
&= 2\alpha^4\mathbf{I_S}+\gamma_3\mathbf{J_S J_S'} \qquad (3.13)
\end{aligned}$$

where

$$\gamma_3=\frac{2\left[NF-(F+2\alpha^2)^2\right]-4CF(\alpha^2-1)^2}{2N+CNF-C(F+2)^2} \qquad (3.14)$$

Thus, by taking the inverse of (3.13), we find that

$$\mathbf{D^{22}}=\frac{1}{2\alpha^4}\left(\mathbf{I_S}-\frac{\gamma_3}{2\alpha^4+S\gamma_3}\mathbf{J_S J_S'}\right) \qquad (3.15)$$

The Components of $\mathbf{D^{12}}$

$$\mathbf{D_{11}^{-1}D_{12}} = \left[\frac{1}{2}\left(\mathbf{I_C}-\frac{NF-(F+2)^2}{2N+C\left[NF-(F+2)^2\right]}\mathbf{J_C J_C'}\right)\right]\times$$

$$
\begin{aligned}
& \left[\frac{NF-(F+2)(F+2\alpha^2)}{N}\mathbf{J_C J_S'}\right] \\
= & \frac{NF-(F+2)(F+2\alpha^2)}{2N}\left(\mathbf{J_C J_S'}-\frac{C\left[NF-(F+2)^2\right]}{2N+C\left[NF-(F+2)^2\right]}\mathbf{J_C J_S'}\right) \\
= & \frac{NF-(F+2)(F+2\alpha^2)}{2N+C\left[NF-(F+2)^2\right]}\mathbf{J_C J_S'}
\end{aligned}
$$

Then by post-multiplying by $\mathbf{D^{22}}$ given in (3.15), we have

$$
\begin{aligned}
\mathbf{D^{12}} &= -\mathbf{D_{11}^{-1}D_{12}D^{22}} \\
&= -\left[\frac{NF-(F+2)(F+2\alpha^2)}{2N+C\left[NF-(F+2)^2\right]}\mathbf{J_C J_S'}\right]\cdot\left[\frac{1}{2\alpha^4}\left(\mathbf{I_S}-\frac{\gamma_3}{2\alpha^4+S\gamma_3}\mathbf{J_S J_S'}\right)\right] \\
&= -\frac{NF-(F+2)(F+2\alpha^2)}{2\alpha^4\left\{2N+C\left[NF-(F+2)^2\right]\right\}}\cdot\left(\mathbf{J_C J_S'}-\frac{S\gamma_3}{2\alpha^4+S\gamma_3}\mathbf{J_C J_S'}\right) \\
&= -\frac{NF-(F+2)(F+2\alpha^2)}{\left[2\alpha^4+S\gamma_3\right]\left[2N+CNF-C(F+2)^2\right]}\mathbf{J_C J_S'} \qquad (3.16)
\end{aligned}
$$

The Components of $\mathbf{D^{21}}$

First,

$$
\mathbf{D_{22}^{-1}} = \frac{1}{2\alpha^4}\left(\mathbf{I_S}-\frac{NF-(F+2\alpha^2)^2}{2N\alpha^4+S\left[NF-(F+2\alpha^2)^2\right]}\mathbf{J_S J_S'}\right)
$$

Next, we post-multiply by $\mathbf{D_{21}}$ to obtain

$$
\begin{aligned}
\mathbf{D_{22}^{-1}D_{21}} &= \left[\frac{1}{2\alpha^4}\left(\mathbf{I_S}-\frac{NF-(F+2\alpha^2)^2}{2N\alpha^4+S\left[NF-(F+2\alpha^2)^2\right]}\mathbf{J_S J_S'}\right)\right]\times \\
&\quad \left[\frac{NF-(F+2)(F+2\alpha^2)}{N}\mathbf{J_S J_C'}\right] \\
&= \frac{NF-(F+2)(F+2\alpha^2)}{2N\alpha^4}\left(\mathbf{J_S J_C'}-\frac{S\left[NF-(F+2\alpha^2)^2\right]}{2N\alpha^4+S\left[NF-(F+2\alpha^2)^2\right]}\mathbf{J_S J_C'}\right) \\
&= \frac{NF-(F+2)(F+2\alpha^2)}{2N\alpha^4+S\left[NF-(F+2\alpha^2)^2\right]}\mathbf{J_S J_C'}
\end{aligned}
$$

Then,

$$
\mathbf{D^{21}} = -\mathbf{D_{22}^{-1}D_{21}D^{11}}
$$

$$
\begin{aligned}
&= -\left[\frac{NF-(F+2)(F+2\alpha^2)}{2N\alpha^4+S\left[NF-(F+2\alpha^2)^2\right]}\mathbf{J_S J_C'}\right]\cdot\left[\frac{1}{2}\left(\mathbf{I_C}-\frac{\gamma_2}{2+C\gamma_2}\mathbf{J_C J_C'}\right)\right] \\
&= -\frac{NF-(F+2)(F+2\alpha^2)}{2\left\{2N\alpha^4+S\left[NF-(F+2\alpha^2)^2\right]\right\}}\left(\mathbf{J_S J_C'}-\frac{C\gamma_2}{2+C\gamma_2}\mathbf{J_S J_C'}\right) \\
&= -\frac{NF-(F+2)(F+2\alpha^2)}{(2+C\gamma_2)\left\{2N\alpha^4+S\left[NF-(F+2\alpha^2)^2\right]\right\}}\mathbf{J_S J_C'} \qquad (3.17)
\end{aligned}
$$

It can be shown algebraically that the scalars in (3.16) and (3.17) are equal to the quantity $\frac{1}{2}\gamma_4$ where

$$
\gamma_4 = -\frac{NF-(F+2)(F+2\alpha^2)}{S\left[NF-(F+2\alpha^2)^2\right]+C\alpha^4\left[NF-(F+2)^2\right]+2\left[N\alpha^4-CSF(\alpha^2-1)^2\right]} \qquad (3.18)
$$

Therefore, combining the matrix forms from (3.12), (3.15), (3.16), and (3.17), we now have $\mathbf{A^{22}}$.

$$
\mathbf{A^{22}} = \frac{1}{2}\left[\begin{array}{c|c} \mathbf{I_C}-\frac{\gamma_2}{2+C\gamma_2}\mathbf{J_C J_C'} & \gamma_4\mathbf{J_C J_S'} \\ \hline \gamma_4\mathbf{J_S J_C'} & \frac{1}{\alpha^4}\left(\mathbf{I_S}-\frac{\gamma_3}{2\alpha^4+S\gamma_3}\mathbf{J_S J_S'}\right) \end{array}\right] \qquad (3.19)
$$

The Components of $\mathbf{A^{21}}$

$$
\begin{aligned}
\mathbf{A^{21}} &= -\mathbf{A_{22}^{-1}A_{21}A^{11}} \\
&= -\frac{1}{2}\left[\begin{array}{c|c} \mathbf{I_C}-\gamma\alpha^4\mathbf{J_C J_C'} & -\gamma\mathbf{J_C J_S'} \\ \hline -\gamma\mathbf{J_S J_C'} & \frac{1}{\alpha^4}\left(\mathbf{I_S}-\gamma\mathbf{J_S J_S'}\right) \end{array}\right]\cdot\left[\begin{array}{cc} (F+2)\mathbf{J_C} & \phi_2 \\ (F+2\alpha^2)\mathbf{J_S} & \phi_3 \end{array}\right]\cdot\mathbf{A^{11}} \\
&= -\frac{1}{2}\left[\begin{array}{cc} \left[(F+2)-C\gamma\alpha^4(F+2)-S\gamma(F+2\alpha^2)\right]\mathbf{J_C} & \phi_2 \\ \frac{1}{\alpha^4}\left[(F+2\alpha^2)-C\gamma\alpha^4(F+2)-S\gamma(F+2\alpha^2)\right]\mathbf{J_S} & \phi_3 \end{array}\right]\cdot\mathbf{A^{11}} \\
&= -\frac{1}{2}\left[\begin{array}{cc} \left[(F+2)-C\gamma\alpha^4(F+2)-S\gamma(F+2\alpha^2)\right]\mathbf{J_C} & \phi_2 \\ \frac{1}{\alpha^4}\left[(F+2\alpha^2)-C\gamma\alpha^4(F+2)-S\gamma(F+2\alpha^2)\right]\mathbf{J_S} & \phi_3 \end{array}\right]\times \\
&\quad \left[\begin{array}{c|c} \gamma_1 & \phi_1' \\ \hline \phi_1 & \mathbf{diag}(\frac{1}{d_i}) \end{array}\right]
\end{aligned}
$$

$$= -\frac{\gamma_1}{2}\begin{bmatrix} [(F+2) - C\gamma\alpha^4(F+2) - S\gamma(F+2\alpha^2)]\,\mathbf{J_C} & \phi_2 \\ \frac{1}{\alpha^4}\,[(F+2\alpha^2) - C\gamma\alpha^4(F+2) - S\gamma(F+2\alpha^2)]\,\mathbf{J_S} & \phi_3 \end{bmatrix}$$

$$= \begin{bmatrix} \gamma_5\mathbf{J_C} & \phi_2 \\ \gamma_6\mathbf{J_S} & \phi_3 \end{bmatrix} \tag{3.20}$$

where, after algebraic simplification

$$\gamma_5 = -\frac{2(F+2) + S\gamma_4(F+2\alpha^2)(2+C\gamma_2)}{2N(2+C\gamma_2)} \tag{3.21}$$

$$\gamma_6 = -\frac{2(F+2\alpha^2) + C\gamma_4(F+2)(2\alpha^4+S\gamma_3)}{2N(2\alpha^4+S\gamma_3)} \tag{3.22}$$

The Components of $\mathbf{A^{12}}$

$$\begin{aligned}
\mathbf{A^{12}} &= -\mathbf{A_{11}^{-1}A_{12}A^{22}} \\
&= -\begin{bmatrix} \frac{1}{N} & \phi_1' \\ \phi_1 & \mathbf{diag}\left(\frac{1}{d_i}\right) \end{bmatrix} \cdot \begin{bmatrix} (F+2)\mathbf{J_C'} & (F+2\alpha^2)\mathbf{J_S'} \\ \phi_2' & \phi_3' \end{bmatrix} \cdot \mathbf{A^{22}} \\
&= -\frac{1}{N}\begin{bmatrix} (F+2)\mathbf{J_C'} & (F+2\alpha^2)\mathbf{J_S'} \\ \phi_2' & \phi_3' \end{bmatrix} \cdot \mathbf{A^{22}} \\
&= -\frac{1}{2N}\begin{bmatrix} (F+2)\mathbf{J_C'} & (F+2\alpha^2)\mathbf{J_S'} \\ \phi_2' & \phi_3' \end{bmatrix} \times \\
&\quad \left[\begin{array}{c|c} \mathbf{I_C} - \frac{\gamma_2}{2+C\gamma_2}\mathbf{J_C J_C'} & \gamma_4\mathbf{J_C J_S'} \\ \hline \gamma_4\mathbf{J_S J_C'} & \frac{1}{\alpha^4}\left(\mathbf{I_S} - \frac{\gamma_3}{2\alpha^4+S\gamma_3}\mathbf{J_S J_S'}\right) \end{array}\right] \\
&= -\frac{1}{2N}\left[\begin{array}{c|c} \mathbf{E_1} & \mathbf{E_2} \\ \hline \phi_2' & \phi_3' \end{array}\right]
\end{aligned}$$

where

$$\mathbf{E_1} = (F+2)\left[\mathbf{J_C'} - \frac{C\gamma_2}{2+C\gamma_2}\mathbf{J_C'}\right] + S\gamma_4(F+2\alpha^2)\mathbf{J_C'} \tag{3.23}$$

$$\mathbf{E_2} = C\gamma_4(F+2)\mathbf{J_S'} + \frac{(F+2\alpha^2)}{\alpha^4}\left[\mathbf{J_S'} - \frac{S\gamma_3}{2\alpha^4+S\gamma_3}\mathbf{J_S'}\right] \tag{3.24}$$

Then,

$$\mathbf{A^{12}} = \begin{bmatrix} \gamma_5 \mathbf{J_C'} & \gamma_6 \mathbf{J_S'} \\ \phi_2' & \phi_3' \end{bmatrix} \tag{3.25}$$

where, after simplifying (3.23) and (3.24), γ_5 and γ_6 are the same quantities found in equations 3.21 and 3.22.

Therefore, by combining the forms for $\mathbf{A^{11}}, \mathbf{A^{12}}, \mathbf{A^{21}}$, and $\mathbf{A^{22}}$, we now have the closed form for the $(\mathbf{X'X})^{-1}$ matrix for a cylindrical design. The block form for the $(\mathbf{X'X})^{-1}$ matrix is given in Figure 3.2. For convenience, the values for $\gamma_1, \gamma_2, \ldots, \gamma_6$ are displayed again below.

$$\left[\begin{array}{cc|cc} \gamma_1 & \phi_1' & \gamma_5 \mathbf{J_C'} & \gamma_6 \mathbf{J_S'} \\ \phi_1 & \mathbf{diag}\left(\frac{1}{d_i}\right) & \phi_2' & \phi_3' \\ \hline \gamma_5 \mathbf{J_C} & \phi_2 & \multicolumn{2}{l}{\frac{1}{2}\left[\begin{array}{c|c} \mathbf{I_C} - \frac{\gamma_2}{2+C\gamma_2}\mathbf{J_C}\mathbf{J_C'} & \gamma_4 \mathbf{J_C}\mathbf{J_S'} \\ \hline \gamma_4 \mathbf{J_S}\mathbf{J_C'} & \frac{1}{\alpha^4}\left(\mathbf{I_S} - \frac{\gamma_3}{2\alpha^4 + S\gamma_3}\mathbf{J_S}\mathbf{J_S'}\right) \end{array}\right]} \\ \gamma_6 J_S & \phi_3 & & \end{array}\right]$$

Figure 3.2: The $(\mathbf{X'X})^{-1}$ Matrix for a Cylindrical Design

$$\gamma_1 = \frac{2\alpha^4 + SF + CF\alpha^4}{N(2\alpha^4 + SF + CF\alpha^4) - C\alpha^4(F+2)^2 - S(F+2\alpha^2)^2 - 2CSF(\alpha^2-1)^2}$$

$$\gamma_2 = \frac{2\alpha^4\left[NF - (F+2)^2\right] - 4SF(\alpha^2-1)^2}{2N\alpha^4 + SNF - S(F+2\alpha^2)^2}$$

$$\gamma_3 = \frac{2\left[NF - (F+2\alpha^2)^2\right] - 4CF(\alpha^2-1)^2}{2N + CNF - C(F+2)^2}$$

$$\gamma_4 = -\frac{NF - (F+2)(F+2\alpha^2)}{S\left[NF - (F+2\alpha^2)^2\right] + C\alpha^4\left[NF - (F+2)^2\right] + 2\left[N\alpha^4 - CSF(\alpha^2-1)^2\right]}$$

$$\gamma_5 = -\frac{2(F+2) + S\gamma_4(F+2\alpha^2)(2+C\gamma_2)}{2N(2+C\gamma_2)}$$

$$\gamma_6 = -\frac{2(F+2\alpha^2)+C\gamma_4(F+2)(2\alpha^4+S\gamma_3)}{2N(2\alpha^4+S\gamma_3)}$$

Now that we have the closed form for the inverse of the $\mathbf{X}'\mathbf{X}$ matrix, we can easily find a closed form for the trace which will allow study of A-efficiencies. However, we first desire to find a closed form for the scaled prediction function in order to study G-efficiencies and IV-efficiencies.

Scaled Prediction Variance Function

In order to study G- and IV-efficiencies, we need a closed form for the scaled prediction variance $Nf(x,z)'(\mathbf{X}'\mathbf{X})^{-1}f(x,z)$ where $f(x,z)$ is the vector of polynomial terms from the second order model for a cylindrical design.

$$f(x,z)' = \left[\begin{array}{c|c|c|c|c|c|c|c} 1 & x_L & z_L & x_\times & z_\times & (xz)_\times & x_Q & z_Q \end{array}\right] \tag{3.26}$$

$$\begin{aligned} x_L &= [x_1,\ldots,x_C] \\ z_L &= [z_1,\ldots,z_S] \\ x_\times &= [x_1x_2,\ldots,x_{C-1}x_C] \\ z_\times &= [z_1z_2,\ldots,z_{S-1}z_S] \\ (xz)_\times &= [x_1z_1,\ldots,x_Cz_S] \\ x_Q &= \left[x_1^2,\ldots,x_C^2\right] \\ z_Q &= \left[z_1^2,\ldots,z_S^2\right] \end{aligned}$$

Using Equation 3.26 we begin by post-multiplying $(\mathbf{X}'\mathbf{X})^{-1}$ by $f(x,z)$ and get:

$$(\mathbf{X}'\mathbf{X})^{-1}f(x,z) = \begin{bmatrix} \gamma_1 + \gamma_5 \sum_{i=1}^{C} x_i^2 + \gamma_6 \sum_{k=1}^{S} z_k^2 \\ \frac{1}{F+2} x_L \\ \frac{1}{F+2\alpha^2} z_L \\ \frac{1}{F} x_\times \\ \frac{1}{F} z_\times \\ \frac{1}{F}(xz)_\times \\ \gamma_5 + \frac{1}{2}\left(x_1^2 - \frac{\gamma_2}{2+C\gamma_2}\sum_{i=1}^{C} x_i^2 + \gamma_4 \sum_{k=1}^{S} z_k^2\right) \\ \gamma_5 + \frac{1}{2}\left(x_2^2 - \frac{\gamma_2}{2+C\gamma_2}\sum_{i=1}^{C} x_i^2 + \gamma_4 \sum_{k=1}^{S} z_k^2\right) \\ \vdots \\ \gamma_5 + \frac{1}{2}\left(x_C^2 - \frac{\gamma_2}{2+C\gamma_2}\sum_{i=1}^{C} x_i^2 + \gamma_4 \sum_{k=1}^{S} z_k^2\right) \\ \gamma_6 + \frac{1}{2}\left(\gamma_4 \sum_{i=1}^{C} x_i^2 + \frac{1}{\alpha^4}\left[z_1^2 - \frac{\gamma_3}{2\alpha^4+S\gamma_3}\sum_{k=1}^{S} z_k^2\right]\right) \\ \gamma_6 + \frac{1}{2}\left(\gamma_4 \sum_{i=1}^{C} x_i^2 + \frac{1}{\alpha^4}\left[z_2^2 - \frac{\gamma_3}{2\alpha^4+S\gamma_3}\sum_{k=1}^{S} z_k^2\right]\right) \\ \vdots \\ \gamma_6 + \frac{1}{2}\left(\gamma_4 \sum_{i=1}^{C} x_i^2 + \frac{1}{\alpha^4}\left[z_S^2 - \frac{\gamma_3}{2\alpha^4+S\gamma_3}\sum_{k=1}^{S} z_k^2\right]\right) \end{bmatrix}$$

Next, pre-multiplying by $Nf(x,z)'$ yields

$$\begin{aligned} V(\mathbf{x},\mathbf{z}) &= Nf(x,z)'(\mathbf{X}'\mathbf{X})^{-1}f(x,z) \\ &= N\Bigg[\gamma_1 + \gamma_5 \sum_{i=1}^{C} x_i^2 + \gamma_6 \sum_{k=1}^{S} z_k^2 + \frac{1}{F+2}\sum_{i=1}^{C} x_i^2 + \frac{1}{F+2\alpha^2}\sum_{k=1}^{S} z_k^2 \\ &\quad + \frac{1}{F}\left(\sum_{i=1}^{C-1}\sum_{j=i+1}^{C} x_i^2 x_j^2 + \sum_{k=1}^{S-1}\sum_{l=k+1}^{S} z_k^2 z_l^2 + \sum_{i=1}^{C}\sum_{k=1}^{S} x_i^2 z_k^2\right) + \gamma_5 \sum_{i=1}^{C} x_i^2 \\ &\quad + \frac{1}{2}\sum_{i=1}^{C} x_i^4 - \frac{1}{2}\left(\frac{\gamma_2}{2+C\gamma_2}\right)\left(\sum_{i=1}^{C} x_i^2\right)^2 + \gamma_6 \sum_{k=1}^{S} z_k^2 + \frac{1}{2\alpha^4}\sum_{k=1}^{S} z_k^4 \\ &\quad - \frac{1}{2\alpha^4}\left(\frac{\gamma_3}{2\alpha^4+S\gamma_3}\right)\left(\sum_{k=1}^{S} z_k^2\right)^2 + \gamma_4\left(\sum_{i=1}^{C} x_i^2\right)\left(\sum_{k=1}^{S} z_k^2\right)\Bigg] \end{aligned}$$

After simplification, we have the closed form for the scaled prediction variance of a second order model for a cylindrical design.

Theorem 3.1 *For a cylindrical design with C cuboidal factors and S spherical factors, the scaled prediction variance for the second order model is given by*

$$\begin{aligned} V(\mathbf{x},\mathbf{z}) &= Nf(x,z)'(\mathbf{X}'\mathbf{X})^{-1}f(x,z) \\ &= N\Bigg[\gamma_1 + \left(2\gamma_5 + \frac{1}{F+2}\right)\sum_{i=1}^{C} x_i^2 + \left(2\gamma_6 + \frac{1}{F+2\alpha^2}\right)\sum_{k=1}^{S} z_k^2 \\ &\quad + \frac{1}{F}\left(\sum_{i=1}^{C-1}\sum_{j=i+1}^{C} x_i^2 x_j^2 + \sum_{k=1}^{S-1}\sum_{l=k+1}^{S} z_k^2 z_l^2\right) + \left(\frac{1}{F} + \gamma_4\right)\sum_{i=1}^{C}\sum_{k=1}^{S} x_i^2 z_k^2 \\ &\quad + \frac{1}{2}\sum_{i=1}^{C} x_i^4 + \frac{1}{2\alpha^4}\sum_{k=1}^{S} z_k^4 - \frac{1}{2}\left(\frac{\gamma_2}{2+C\gamma_2}\right)\left(\sum_{i=1}^{C} x_i^2\right)^2 \\ &\quad - \frac{1}{2\alpha^4}\left(\frac{\gamma_3}{2\alpha^4 + S\gamma_3}\right)\left(\sum_{k=1}^{S} z_k^2\right)^2\Bigg] \end{aligned} \qquad (3.27)$$

Equation 3.27 will be used in later chapters as we study the maximum and average prediction variance of cylindrical designs. However, we now turn our attention to the trace of the $(\mathbf{X}'\mathbf{X})^{-1}$ matrix, so that we can study the A-criterion.

A-efficiencies for Cylindrical Designs

Recall that A-efficiencies are based on the trace of the $(\mathbf{X}'\mathbf{X})^{-1}$ matrix. Because the trace is just the sum of the diagonal elements, we easily find the closed form for the trace of $(\mathbf{X}'\mathbf{X})^{-1}$ for a cylindrical design.

Theorem 3.2 *For a cylindrical design with C cuboidal factors and S spherical factors, the closed form for the trace of the $(\mathbf{X}'\mathbf{X})^{-1}$ matrix is given by:*

$$\begin{aligned} tr\left[(\mathbf{X}'\mathbf{X})^{-1}\right] &= \gamma_1 + \frac{C}{F+2} + \frac{S}{F+2\alpha^2} + \frac{\binom{C}{2} + \binom{S}{2} + CS}{F} \\ &\quad + \frac{C}{2}\left(\frac{2+(C-1)\gamma_2}{2+C\gamma_2}\right) + \frac{S}{2\alpha^4}\left(\frac{2\alpha^4 + (S-1)\gamma_3}{2\alpha^4 + S\gamma_3}\right) \end{aligned} \qquad (3.28)$$

Using the statistical software package R, exact A-efficiencies have been found by applying Equation 3.28 to the formula given in Equation 1.2.

From Table 3.1, it can be seen that the cylindrical design with 1 cuboidal factor has the highest A-efficiency when 1 center point is used among other designs with the same number of factors. The pattern of A-efficiencies can be seen in Figure 3.3. The CCD with cuboidal region has the lowest A-efficiency, and as the number of spherical factors increases, the A-efficiency increases until all factors are spherical in which case the A-efficiency drops. Therefore if one center point is utilized and there are restrictions on one or more of the factors, it is advantageous to use the cylindrical design. Even if there are no restrictions on any factors, a cylindrical design with 1 cuboidal factor would be better than a CCD with a spherical region according to the A-criterion.

When a second center point is added, the A-efficiency increases significantly for the CCD with a spherical region. However, the cylindrical design with 1 cuboidal factor still has the highest A-efficiency except for the case of when there are 3 factors. As the number of center points increases, the CCD with a spherical region becomes the most A-efficient design. This can be seen in Figure 3.3 for the case of using 5 center points. Interestingly, the A-efficiency for a cylindrical design with 1 cuboidal factor increases as more center points are added. Note that in Figure 3.3, the A-efficiencies for the cylindrical design with 1 factor and the CCD with a spherical region are quite similar for larger numbers of factors.

The results shown here indicate that if an experiment requires restrictions on 1 or more of the factors and the experimenter uses at least 1 center point, the best design to choose according to A-efficiency is a cylindrical design where the factors with restrictions should be the cuboidal factors and all other factors spherical. This advice is the same as what was implied by the D-efficiency.

Table 3.1: A-efficiencies for between 3 and 10 factors with between 1 and 5 center points

$N_0 = 1$						
Factors	C	S	A-eff (Full)	A-eff (Frac)	N (Full)	N (Frac)
3	0	3	32.40		15	
	1	2	38.28			
	3	0	31.29			
4	0	4	31.65		25	
	1	3	42.10			
	2	2	34.21			
	4	0	25.49			
5	0	5	28.45	36.95	43	27
	1	4	41.97	48.35		
	2	3	33.11	40.55		
	3	2	24.75	32.11		
	5	0	18.55	25.20		
6	0	6	23.44	33.72	77	45
	1	5	38.05	48.74		
	2	4	28.73	39.29		
	3	3	21.06	30.40		
	4	2	16.02	24.01		
	6	0	12.31	18.98		
7	0	7	17.75	28.06	143	79
	1	6	31.50	44.79		
	2	5	22.63	34.31		
	3	4	16.15	25.67		
	4	3	12.21	20.00		
	5	2	9.60	16.05		
	7	0	7.58	12.88		
8	0	8	12.50	32.32	273	81
	1	7	24.02	50.25		
	2	6	16.42	39.15		
	3	5	11.41	29.87		
	4	4	8.54	23.67		
	5	3	6.73	19.37		
	6	2	5.46	16.16		
	8	0	4.42	13.40		
9	0	9	8.30	24.87	531	147
	1	8	17.06	42.88		
	2	7	11.15	31.41		
	3	6	7.58	22.98		
	4	5	5.62	17.77		
	5	4	4.42	14.35		
	6	3	3.61	11.93		
	7	2	3.01	10.08		
	9	0	2.49	8.46		
10	0	10	5.27	28.31	1045	149
	1	9	11.43	47.65		
	2	8	7.20	35.41		
	3	7	4.81	26.27		
	4	6	3.54	20.51		
	5	5	2.77	16.69		
	6	4	2.26	14.00		
	7	3	1.90	11.98		
	8	2	1.62	10.36		
	10	0	1.37	8.87		

Table 3.1 Continued

$N_0 = 2$						
Factors	C	S	A-eff (Full)	A-eff (Frac)	N (Full)	N (Frac)
3	0	3	44.94		15	
	1	2	40.90			
	3	0	30.68			
4	0	4	45.40		25	
	1	3	45.69			
	2	2	34.14			
	4	0	24.91			
5	0	5	42.75	49.83	43	27
	1	4	46.50	51.29		
	2	3	33.57	40.28		
	3	2	24.55	31.36		
	5	0	18.27	24.47		
6	0	6	37.07	48.24	77	45
	1	5	43.14	53.00		
	2	4	29.47	39.66		
	3	3	21.10	30.12		
	4	2	15.93	23.64		
	6	0	12.20	18.64		
7	0	7	29.52	42.76	143	79
	1	6	36.56	50.01		
	2	5	23.41	35.07		
	3	4	16.28	25.70		
	4	3	12.22	19.88		
	5	2	9.58	15.91		
	7	0	7.55	12.75		
8	0	8	21.71	47.46	273	81
	1	7	28.50	55.30		
	2	6	17.08	39.90		
	3	5	11.55	29.88		
	4	4	8.57	23.53		
	5	3	6.73	19.20		
	6	2	5.46	16.00		
	8	0	4.41	13.25		
9	0	9	14.93	39.18	531	147
	1	8	20.64	48.60		
	2	7	11.65	32.33		
	3	6	7.69	23.14		
	4	5	5.65	17.76		
	5	4	4.43	14.30		
	6	3	3.61	11.88		
	7	2	3.00	10.03		
	9	0	2.49	8.41		
10	0	10	9.73	43.36	1045	149
	1	9	14.05	53.38		
	2	8	7.54	36.36		
	3	7	4.88	26.43		
	4	6	3.56	20.50		
	5	5	2.78	16.64		
	6	4	2.27	13.93		
	7	3	1.90	11.92		
	8	2	1.62	10.30		
	10	0	1.37	8.82		

Table 3.1 Continued

$N_0 = 3$						
Factors	C	S	A-eff (Full)	A-eff (Frac)	N (Full)	N (Frac)
3	0	3	50.33		15	
	1	2	41.50			
	3	0	29.74			
4	0	4	52.29		25	
	1	3	47.29			
	2	2	33.73			
	4	0	24.28			
5	0	5	50.93	55.49	43	27
	1	4	49.13	52.41		
	2	3	33.68	39.70		
	3	2	24.28	30.57		
	5	0	17.97	23.75		
6	0	6	45.80	55.82	77	45
	1	5	46.52	55.34		
	2	4	29.90	39.69		
	3	3	21.08	29.78		
	4	2	15.83	23.26		
	6	0	12.09	18.30		
7	0	7	37.82	51.57	143	79
	1	6	40.21	53.37		
	2	5	23.94	35.51		
	3	4	16.37	25.65		
	4	3	12.20	19.75		
	5	2	9.54	15.76		
	7	0	7.51	12.61		
8	0	8	28.76	55.97	273	81
	1	7	31.92	58.46		
	2	6	17.57	40.30		
	3	5	11.66	29.81		
	4	4	8.59	23.36		
	5	3	6.73	19.03		
	6	2	5.45	15.84		
	8	0	4.40	13.11		
9	0	9	20.34	48.35	531	147
	1	8	23.50	52.57		
	2	7	12.02	32.95		
	3	6	7.78	23.23		
	4	5	5.67	17.74		
	5	4	4.43	14.25		
	6	3	3.61	11.82		
	7	2	3.00	9.98		
	9	0	2.48	8.36		
10	0	10	13.55	52.57	1045	149
	1	9	16.22	57.28		
	2	8	7.79	36.99		
	3	7	4.94	26.52		
	4	6	3.58	20.47		
	5	5	2.79	16.58		
	6	4	2.27	13.87		
	7	3	1.90	11.85		
	8	2	1.62	10.25		
	10	0	1.37	8.76		

Table 3.1 Continued

$N_0 = 4$						
Factors	C	S	A-eff (Full)	A-eff (Frac)	N (Full)	N (Frac)
3	0	3	52.53		15	
	1	2	41.15			
	3	0	28.68			
4	0	4	55.90		25	
	1	3	47.85			
	2	2	33.14			
	4	0	23.63			
5	0	5	55.93	58.09	43	27
	1	4	50.67	52.61		
	2	3	33.59	38.96		
	3	2	23.97	29.77		
	5	0	17.67	23.06		
6	0	6	51.73	60.14	77	45
	1	5	48.83	56.62		
	2	4	30.15	39.51		
	3	3	21.00	29.38		
	4	2	15.70	22.87		
	6	0	11.97	17.96		
7	0	7	43.93	57.27	143	79
	1	6	42.92	55.63		
	2	5	24.32	35.74		
	3	4	16.41	25.55		
	4	3	12.18	19.59		
	5	2	9.50	15.61		
	7	0	7.47	12.48		
8	0	8	34.31	61.22	273	81
	1	7	34.60	60.52		
	2	6	17.93	40.50		
	3	5	11.73	29.68		
	4	4	8.61	23.18		
	5	3	6.73	18.85		
	6	2	5.44	15.67		
	8	0	4.39	12.97		
9	0	9	24.84	54.66	531	147
	1	8	25.83	55.43		
	2	7	12.31	33.38		
	3	6	7.84	23.28		
	4	5	5.69	17.70		
	5	4	4.44	14.19		
	6	3	3.61	11.76		
	7	2	3.00	9.92		
	9	0	2.48	8.31		
10	0	10	16.86	58.69	1045	149
	1	9	18.04	60.05		
	2	8	7.99	37.42		
	3	7	4.99	26.56		
	4	6	3.59	20.42		
	5	5	2.79	16.51		
	6	4	2.27	13.80		
	7	3	1.90	11.79		
	8	2	1.62	10.19		
	10	0	1.37	8.71		

Table 3.1 Continued

$N_0 = 5$						
Factors	C	S	A-eff (Full)	A-eff (Frac)	N (Full)	N (Frac)
3	0	3	53.12		15	
	1	2	40.35			
	3	0	27.60			
4	0	4	57.74		25	
	1	3	47.82			
	2	2	32.46			
	4	0	22.98			
5	0	5	59.08	59.16	43	27
	1	4	51.53	52.30		
	2	3	33.37	38.15		
	3	2	23.62	28.98		
	5	0	17.36	22.39		
6	0	6	55.91	62.68	77	45
	1	5	50.45	57.26		
	2	4	30.26	39.21		
	3	3	20.90	28.97		
	4	2	15.57	22.49		
	6	0	11.85	17.64		
7	0	7	48.58	61.13	143	79
	1	6	44.98	57.16		
	2	5	24.58	35.83		
	3	4	16.43	25.42		
	4	3	12.15	19.43		
	5	2	9.46	15.46		
	7	0	7.43	12.35		
8	0	8	38.78	64.66	273	81
	1	7	36.75	61.87		
	2	6	18.20	40.55		
	3	5	11.78	29.52		
	4	4	8.61	22.99		
	5	3	6.72	18.67		
	6	2	5.43	15.51		
	8	0	4.38	12.83		
9	0	9	28.63	59.20	531	147
	1	8	27.76	57.56		
	2	7	12.53	33.67		
	3	6	7.89	23.28		
	4	5	5.71	17.65		
	5	4	4.44	14.13		
	6	3	3.61	11.70		
	7	2	3.00	9.87		
	9	0	2.48	8.26		
10	0	10	19.75	62.99	1045	149
	1	9	19.59	62.08		
	2	8	8.15	37.71		
	3	7	5.03	26.56		
	4	6	3.60	20.36		
	5	5	2.80	16.44		
	6	4	2.27	13.73		
	7	3	1.90	11.72		
	8	2	1.62	10.13		
	10	0	1.37	8.66		

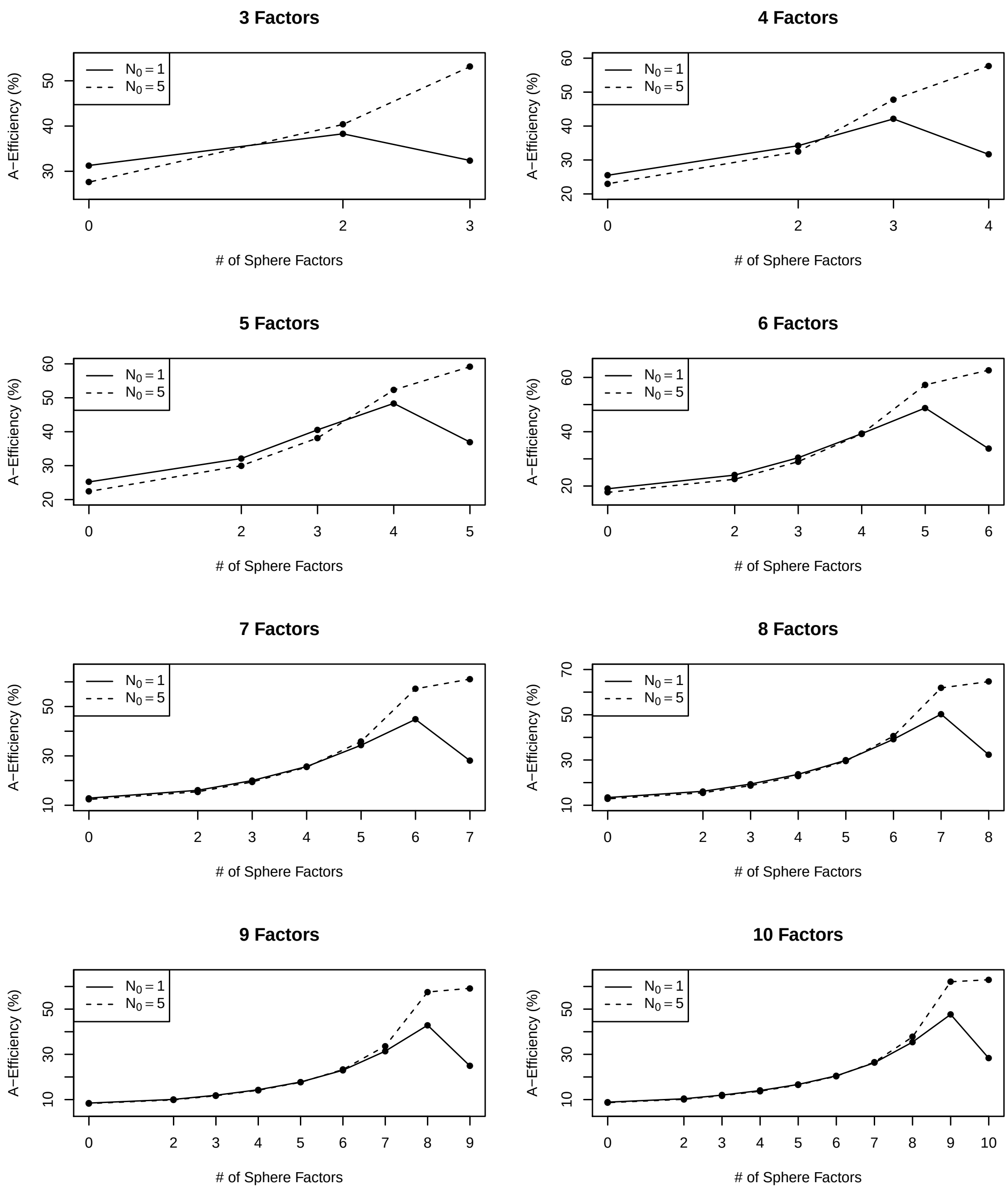

Figure 3.3: A-efficiencies for between 3 and 10 factors comparing use of 1 and 5 center points. For 5 or more factors, it is assumed that the appropriate fractional factorial design is used.

SPHERICAL PREDICTION VARIANCE AND THE G-CRITERION

The Maximum Spherical Prediction Variance

In choosing a design based on the G-criterion, the goal is to select the design that has the smallest maximum prediction variance. In order to find G-efficiencies, it simplifies calculations to consider an alternate form of the prediction variance. First, note that by rearranging terms in the scaled prediction variance function given in (3.27), we can rewrite the scaled prediction variance function as:

$$\begin{aligned} V(\mathbf{x},\mathbf{z}) &= Nf(x,z)'(\mathbf{X}'\mathbf{X})^{-1}f(x,z) \\ &= N\Bigg[\gamma_1 + \left(2\gamma_5 + \frac{1}{F+2}\right)\sum_{i=1}^{C} x_i^2 + \left(2\gamma_6 + \frac{1}{F+2\alpha^2}\right)\sum_{k=1}^{S} z_k^2 \\ &+ \frac{1}{2}\left(\frac{1}{F} - \frac{\gamma_2}{2+C\gamma_2}\right)\left(\sum_{i=1}^{C} x_i^2\right)^2 + \frac{1}{2}\left(\frac{1}{F} - \frac{\gamma_3}{\alpha^4(2\alpha^4+S\gamma_3)}\right)\left(\sum_{k=1}^{S} z_k^2\right)^2 \\ &+ \left(\frac{1}{F}+\gamma_4\right)\left(\sum_{i=1}^{C} x_i^2\right)\left(\sum_{k=1}^{S} z_k^2\right) + \frac{1}{2}\left(1-\frac{1}{F}\right)\sum_{i=1}^{C} x_i^4 \\ &+ \frac{1}{2}\left(\frac{1}{\alpha^4} - \frac{1}{F}\right)\sum_{k=1}^{S} z_k^4\Bigg] \end{aligned} \tag{4.1}$$

In their paper that introduced the concept of rotatable designs, Box and Hunter [3] wrote the scaled prediction variance function in terms of a radius from the center of the design space. Since then, writing the prediction variance function in terms of a spherical radius has been used in studying the properties of the prediction variance throughout the design space. Because cylindrical designs have two sets of variables, cuboidal and spherical, it is natural to consider writing the scaled prediction variance in terms of two radii, one for each set of factors. For example, the scaled prediction variance function given in (4.1) can be written as:

$$V(\mathbf{x},\mathbf{z}) = N\left[A + B\rho_x^2 + D\rho_z^2 + E\rho_x^4 + G\rho_z^4 + H\rho_x^2\rho_z^2 + I\sum_{i=1}^{C} x_i^4 + J\sum_{k=1}^{S} z_k^4\right] \tag{4.2}$$

where

$$\rho_x^2 = \sum_{i=1}^{C} x_i^2 \text{ where } 0 \le \rho_x \le \sqrt{C}$$

$$\rho_z^2 = \sum_{k=1}^{S} z_k^2 \text{ where } 0 \le \rho_z \le \sqrt{S}$$

and

$$\begin{array}{ll} A = \gamma_1 & G = \frac{1}{2}\left(\frac{1}{F} - \frac{\gamma_3}{\alpha^4(2\alpha^4+S\gamma_3)}\right) \\ B = 2\gamma_5 + \frac{1}{F+2} & H = \frac{1}{F} + \gamma_4 \\ D = 2\gamma_6 + \frac{1}{F+2\alpha^2} & I = \frac{1}{2}\left(1 - \frac{1}{F}\right) \\ E = \frac{1}{2}\left(\frac{1}{F} - \frac{\gamma_2}{2+C\gamma_2}\right) & J = \frac{1}{2}\left(\frac{1}{\alpha^4} - \frac{1}{F}\right) \end{array}$$

Our goal is to write the maximum spherical prediction variance in terms of the two radii and then find the maximum of the maximum spherical prediction variances over the entire hypercylindrical space. Borkowski [2] gave closed forms for the average, maximum, and minimum spherical prediction variance for CCDs in both a hypersphere and a hypercube. Because our interest is in finding G-efficiencies, we will focus on finding a closed form for the maximum spherical prediction variance for a cylindrical design. By following and slightly modifying Borkowski's proof, we derive this closed form.

First note from (4.2) that the maximum spherical prediction variance depends only on ρ_x, ρ_z, and the sums of quartic terms. Let

$$C_{\rho_x,\rho_z} = \left\{\mathbf{x},\mathbf{z} : \sum_{i=1}^{C} x_i^2 = \rho_x^2, \; -1 \le x_i \le 1, \; \sum_{k=1}^{S} z_k^2 = \rho_z^2, \; -\sqrt{S} \le z_k \le \sqrt{S}\right\}$$

be the set of points that make up the hypercylindrical design space. We seek to maximize $V(\mathbf{x},\mathbf{z})$ in (4.2) by considering all possible combinations of the radii ρ_x and ρ_z. Let $\mathbf{x}$ be fixed and let λ_z be the Lagrange multiplier associated with the constraint

$$\sum_{k=1}^{S} z_k^2 = \rho_z^2$$

and consider the function

$$w_z(\mathbf{x}, \mathbf{z}, \lambda_z) = V(\mathbf{x}, \mathbf{z}) + \lambda_z \left(\sum_{k=1}^{S} z_k^2 - \rho_z^2 \right)$$

The corresponding system of partial derivatives is

$$\begin{aligned} \frac{\partial w_z}{\partial z_k} &= 2z_k(2Jz_k^2 + \lambda_z) \quad \text{for} \quad 1 \leq k \leq S \\ \frac{\partial w_z}{\partial \lambda_z} &= \sum_{k=1}^{S} z_k^2 - \rho_z^2 \end{aligned}$$

Equating these partial derivatives to zero yields $z_k = 0$ or $\lambda_z = -2Jz_k^2$. Let

$$\begin{aligned} n_z &= \text{the number of occurrences where } z_k = 0 \text{ and} \\ S - n_z &= \text{the number of occurrences where } \lambda_z = -2Jz_k^2 \end{aligned}$$

Because of permutation invariance of the z_ks in $\sum_{k=1}^{S} z_k^4$, we can, without loss of generality, let $z_k = 0$ for $1 \leq k \leq n_z$ and let $\lambda_z = -2Jz_k^2$ for $n_z + 1 \leq k \leq S$. Then

$$z_1 = z_2 = \ldots = z_{n_z} = 0$$

and

$$|z_{n_z+1}| = |z_{n_z+2}| = \ldots = |z_S|$$

This implies that

$$\rho_z^2 = \sum_{k=1}^{S} z_k^2 = (S - n_z) z_k^2$$

which in turn implies that

$$z_k = \begin{cases} 0 & \text{for } 1 \leq k \leq n_z \\ \frac{\pm \rho_z}{\sqrt{S - n_z}} & \text{for } n_z + 1 \leq k \leq S \end{cases}$$

Substitution yields

$$\sum_{k=1}^{S} z_k^4 = (S - n_z) \left(\frac{\rho_z^4}{(S - n_z)^2} \right) = \frac{\rho_z^4}{S - n_z}$$

which is an increasing function of n_z. Thus to maximize $\sum_{k=1}^{S} z_k^4$, set $n_z = S-1$ and to minimize $\sum_{k=1}^{S} z_k^4$, set $n_z = 0$. Then using sign and permutation invariance, we have

$$\begin{aligned} \min_{z \in \mathcal{Z}} \sum_{k=1}^{S} z_k^4 &= \frac{\rho_z^4}{S} \text{ which occurs at any } \mathbf{z} = \left(\frac{\pm\rho_z}{\sqrt{S}}, \ldots, \frac{\pm\rho_z}{\sqrt{S}} \right) \\ \max_{z \in \mathcal{Z}} \sum_{k=1}^{S} z_k^4 &= \rho_z^4 \text{ which occurs at any } \mathbf{z} = (0, \ldots, 0, \pm\rho_z, 0, \ldots, 0) \end{aligned}$$

By substituting the above values into (4.2) and considering $\mathbf{x}$ fixed, the spherical prediction variance function maximized with respect to ρ_z can be written as

$$VMAX_{\mathbf{x},\rho_z} = N \left[A + B\rho_x^2 + D\rho_z^2 + E\rho_x^4 + G\rho_z^4 + H\rho_x^2\rho_z^2 + I \sum_{i=1}^{C} x_i^4 + J_0\rho_z^4 \right] \quad (4.3)$$

with

$$J_0 = \begin{cases} \frac{J}{S} & J \leq 0 \\ J & J > 0 \end{cases}$$

Now to maximize $VMAX_{\mathbf{x},\rho_z}$ with respect to ρ_x, we fix ρ_z and maximize $I \sum_{i=1}^{C} x_i^4$ subject to the constraint $\rho_x^2 = \sum_{i=1}^{C} x_i^2$.

<u>Case I</u>: $0 \leq \rho_x \leq 1$

Fix ρ_z and let λ_x be the Lagrange multiplier associated with $\rho_x^2 = \sum_{i=1}^{C} x_i^2$. Consider the following function.

$$w_x(\mathbf{x}, \rho_x, \rho_z, \lambda_x) = A + B\rho_x^2 + D\rho_z^2 + E\rho_x^4 + G\rho_z^4 + H\rho_x^2\rho_z^2 + I \sum_{i=1}^{C} x_i^4 + J_0\rho_z^4 + \lambda_x \left(\sum_{i=1}^{C} x_i^2 - \rho_x^2 \right)$$

Taking partial derivatives and equating to zero yields results similar to the case of maximizing $\sum_{k=1}^{S} z_k^4$ subject to $\rho_z^2 = \sum_{k=1}^{S} z_k^2$. Note that $I = \frac{1}{2}\left(1 - \frac{1}{F}\right)$ is always positive because $F > 1$. Thus, to maximize $V(\mathbf{x}, \mathbf{z})$ we need only maximize $\sum_{i=1}^{C} x_i^4$. Therefore, for fixed ρ_z and for $0 \le \rho_x \le 1$, we substitute ρ_x^4 for $\sum_{i=1}^{C} x_i^4$ in (4.3) and obtain

$$VMAX_{\rho_x,\rho_z} = N\left[A + B\rho_x^2 + D\rho_z^2 + E\rho_x^4 + G\rho_z^4 + H\rho_x^2\rho_z^2 + I\rho_x^4 + J_0\rho_z^4\right] \qquad (4.4)$$

and the maximum occurs at any $(\mathbf{x}) = (0, \ldots, 0, \pm\rho_x, 0, \ldots, 0)$.

<u>*Case II*</u>: $1 < \rho_x \le \sqrt{C}$

Define r and t as $r = \sum_{i=1}^{C} x_i^2$ and $t = \sum_{i=1}^{C} x_i^4$. Since $\rho_x > 1$ and $-1 \le x_i \le 1$ for each i, we know $1 < r \le C$. Also, there exists an integer $i \in \{1, 2, \ldots, C\}$ and a $\delta \in [0, 1)$ such that $r = i + \delta^2$. Because of sign and permutation invariance of $r = \sum_{i=1}^{C} x_i^2$ with respect to $\mathbf{x}$ we can suppose without loss of generality that

$$1 \ge x_1 \ge x_2 \ge \ldots \ge x_C \ge 0$$

Let u be the largest integer such that $x_u > 0$ and $x_{u+1} = 0$. By fixing $r, x_2, \ldots x_{u-1}$ we can consider x_u and t as functions of x_1:

$$\begin{aligned} x_u^2 &= r - \sum_{i=2}^{u-1} x_i^2 - x_1^2 \\ t &= \sum_{i=2}^{u-1} x_i^4 + x_1^4 + x_u^4 \end{aligned}$$

Taking partial derivatives with respect to x_1 yields

$$2x_u\left(\frac{\partial x_u}{\partial x_1}\right) = -2x_1 \;\Rightarrow\; \frac{\partial x_u}{\partial x_1} = -\frac{x_1}{x_u}$$

and

$$\begin{aligned} \frac{\partial t}{\partial x_1} &= 4x_1^3 + 4x_u^3\left(\frac{\partial x_u}{\partial x_1}\right) \\ &= 4x_1^3 + 4x_u^3\left(-\frac{x_1}{x_u}\right) \\ &= 4x_1\left(x_1^2 - x_u^2\right) \end{aligned}$$

Because $x_1 \geq x_u > 0$, increasing x_1 will simultaneously decrease x_u and increase t while preserving the ordering of $x_1 \geq x_2 \geq \ldots \geq x_u > 0$. The process is iterated until t is maximized. Thus, for a fixed $r = i + \delta^2$ (and using sign invariance), t is maximized at

$$\mathbf{x}_{max} = \begin{cases} |x_1| = |x_2| = \ldots = |x_i| = 1 \\ |x_{i+1}| = \delta \\ x_{i+2} = x_{i+3} = \ldots = x_C = 0 \end{cases}$$

or at any permutation of these coordinates. Evaluated at $\mathbf{x}_{max}$ we have

$$t = i + \delta^4 = i + (r - i)^2$$

Let the floor function $\lfloor r \rfloor$ represent the greatest integer $\leq r$. When $1 < \rho_x \leq \sqrt{C}$ we have $r = \rho_x^2$ and $i = \lfloor \rho_x^2 \rfloor$. Therefore,

$$\max_{1 \leq \rho_x \leq \sqrt{C}} \sum_{i=1}^{C} x_i^4 \;=\; \lfloor \rho_x^2 \rfloor + \left(\rho_x^2 - \lfloor \rho_x^2 \rfloor \right)^2 \tag{4.5}$$

Then, for $1 < \rho_x \leq \sqrt{C}$ and for a fixed ρ_z we substitute the value in (4.5) for $\sum_{i=1}^{C} x_i^4$ in (4.3) and obtain

$$\begin{aligned} VMAX_{\rho_x,\rho_z} \;=\; & N \Big\{ A + B\rho_x^2 + D\rho_z^2 + E\rho_x^4 + G\rho_z^4 + H\rho_x^2\rho_z^2 \\ & + I \left[\lfloor \rho_x^2 \rfloor + \left(\rho_x^2 - \lfloor \rho_x^2 \rfloor \right)^2 \right] + J_0\rho_z^4 \Big\} \end{aligned} \tag{4.6}$$

Next, note that for $0 \leq \rho_x \leq 1$, we have that $\rho_x^4 = \lfloor \rho_x^2 \rfloor + (\rho_x^2 - \lfloor \rho_x^2 \rfloor)^2$. Therefore, the maximum spherical prediction variance given in (4.6) holds true for all values of ρ_x. The equation for the maximum spherical prediction variance is stated formally in the following theorem.

Theorem 4.1 *For a cylindrical design with C cuboidal factors and S spherical factors, the maximum spherical prediction variance function is given by*

$$\begin{aligned} VMAX_{\rho_x,\rho_z} &= N\Big\{A + B\rho_x^2 + D\rho_z^2 + E\rho_x^4 + G\rho_z^4 + H\rho_x^2\rho_z^2 \\ &\quad + I\left[\lfloor\rho_x^2\rfloor + \left(\rho_x^2 - \lfloor\rho_x^2\rfloor\right)^2\right] + J_0\rho_z^4\Big\} \end{aligned}$$

with

$$J_0 = \begin{cases} \frac{J}{S} & J \leq 0 \\ J & J > 0 \end{cases}$$

and for any $\mathbf{x}, \mathbf{z} \in C_{\rho_x,\rho_z}$ the maximum occurs at any permutation of the following coordinates:

$$\begin{aligned} \mathbf{x}_{max} &= \begin{cases} (0,\ldots,0,\pm\rho_x,0,\ldots,0) & 0 \leq \rho_x \leq 1 \\ (\pm 1,\pm 1,\ldots,\pm 1,\delta,0,\ldots,0) & 1 < \rho_x \leq \sqrt{C},\ \delta \in [0,1) \end{cases} \\ \mathbf{z}_{max} &= \begin{cases} \left(\frac{\pm\rho_z}{\sqrt{S}},\ldots,\frac{\pm\rho_z}{\sqrt{S}}\right) & J \leq 0 \\ (0,\ldots,0,\pm\rho_z,0,\ldots,0) & J > 0 \end{cases} \end{aligned}$$

G-efficiencies for Cylindrical Designs

From Theorem 4.1, the coordinates of the point(s) of maximum prediction variance can be ascertained from knowing where the maximum prediction variance occurs in terms of the radii. Using the statistical software package R, we used a fine grid of ρ_x and ρ_z values to search for the maximum spherical prediction variance. The maximum occurred at a radius $\rho_z = 0$ or $\rho_z = \alpha$ for the spherical variables and at $\rho_x = \sqrt{i}$ for $i = 1, 2, \ldots, C$ for the cuboidal variables. Because only a grid search was used, we have not proven that the proposed G-efficiencies are exact. These results, however, are consistent with the results for CCDs in cuboidal and spherical regions in Borkowski [2]. A proof of the exactness of the efficiencies is left for future research.

As an example, consider the case of an experiment with 7 factors where 4 are cuboidal and 3 are spherical. Further assume that a 2_{VII}^{7-1} fractional factorial is used for the factorial points and that there is 1 center point. According to Table 4.1, the maximum occurs at the radii $(\rho_x, \rho_z) = (\sqrt{2},\ \sqrt{3})$. Because $\rho_x > 1$, the maximum prediction variance over $\mathbf{x}$ occurs at $(\pm 1, \pm 1, 0, 0)$ or at any permutation of these coordinates. The coordinates for $\mathbf{z}$ depend on whether J in (4.6) is positive or negative. Because

$$
\begin{aligned}
J &= \frac{1}{2}\left(\frac{1}{\alpha^4} - \frac{1}{F}\right) \\
&= \frac{1}{2}\left(\frac{1}{\left(\sqrt{3}\right)^4} - \frac{1}{64}\right) \\
&= \frac{55}{1152} \\
&> 0,
\end{aligned}
$$

the maximum prediction variance over $\mathbf{z}$ occurs at $(0, \ldots, 0, \pm\sqrt{3}, 0, \ldots, 0)$ or any permutation of these coordinates. Thus, the maximum prediction variance occurs at $(\pm 1, \pm 1, 0, 0|0, \ldots, 0, \pm\sqrt{3}, 0, \ldots, 0)$ or any permutation of the $x-$ and $z-$coordinates where the $|$ notation indicates the location of the separation between the cuboidal and spherical factors.

We now discuss the G-efficiencies in Table 4.1, and we use the definitions of CCD(c) and CCD(s) as defined on page 6. If a response surface study involves 3 or 4 factors and the experimenter decides to use just one center point, then the CCD(c) has higher G-efficiency than the CCD(s) or a cylindrical design. However, for 5 or more factors and the same scenario, the cylindrical design with one cuboidal factor and the rest spherical is the most efficient design by the G-criterion. When 2 or more center points are used, the G-efficiency for the CCD(s) increases dramatically and the CCD(s) is more G-efficient than the CCD(c) or a cylindrical design. In the class of cylindrical designs, the G-efficiency increases as the number of spherical factors increases, regardless of the number of center points.

Cylindrical designs with fewer number of spherical factors tend to have lower G-efficiency than the CCD(c). For example, consider an experiment in 8 factors where a 2_V^{8-2} fractional factorial is used and further suppose that 4 center points are used. Then, according to Table 4.1, a CCD(c) has a G-efficiency of 45.27% while a cylindrical design with 6 cuboidal and 2 spherical factors has a G-efficiency of 41.83%. A cylindrical design with 5 cuboidal and 3 spherical factors has a G-efficiency of 43.17%, but a cylindrical design with 4 cuboidal and 4 spherical factors is 47.15% G-efficient. Thus, as long as there is at least one but not more than 4 factors with strict ranges on the levels, a cylindrical design is more G-efficient than the CCD(c). For a graphical summary of G-efficiencies for cylindrical designs and CCDs, see Figure 4.1 on 64.

In general, if the experiment consists of 3 or 4 factors, and some but not all factors have strict ranges on the levels, a CCD(c) is the more efficient design by the G-criterion. For 5 or more factors, determining patterns in G-efficiencies when using a cylindrical design or a CCD(c) depends on how many factors have strict ranges. Consulting Table 4.1 or Figure 4.1 will help in coming to a decision.

Table 4.1: G-efficiencies for between 3 and 10 factors with between 1 and 5 center points

$N_0 = 1$								
Factors	C	S	G-eff (Full)	G-eff (Frac)	N (Full)	N (Frac)	max $(\rho_x, \rho_z)_{full}$	max $(\rho_x, \rho_z)_{frac}$
3	0	3	66.67		15		$(NA, 0)$	
	1	2	75.47				$(1, 0)$	
	3	0	83.62				$(\sqrt{3}, NA)$	
4	0	4	60.00		25		$(NA, 0)$	
	1	3	77.62				$(1, \sqrt{3})$	
	2	2	70.01				$(1, \sqrt{2})$	
	4	0	77.98				$(\sqrt{3}, NA)$	
5	0	5	48.84	77.78	43	27	$(NA, 0)$	$(NA, 0)$
	1	4	73.99	85.71			$(1, 2)$	$(1, 2)$
	2	3	58.56	72.01			$(1, \sqrt{3})$	$(\sqrt{2}, \sqrt{3})$
	3	2	54.55	66.91			$(\sqrt{2}, \sqrt{2})$	$(\sqrt{2}, \sqrt{2})$
	5	0	60.16	74.91			$(\sqrt{3}, NA)$	$(2, 0)$
6	0	6	36.36	62.22	77	45	$(NA, 0)$	$(NA, 0)$
	1	5	63.10	84.61			$(1, \sqrt{5})$	$(1, \sqrt{5})$
	2	4	45.87	67.78			$(1, 2)$	$(1, 2)$
	3	3	41.58	58.95			$(\sqrt{2}, \sqrt{3})$	$(\sqrt{2}, \sqrt{3})$
	4	2	38.14	57.07			$(\sqrt{2}, \sqrt{2})$	$(\sqrt{2}, \sqrt{2})$
	6	0	41.71	62.52			$(\sqrt{3}, NA)$	$(2, NA)$
7	0	7	25.17	45.57	143	79	$(NA, 0)$	$(NA, 0)$
	1	6	46.75	73.50			$(0, \sqrt{6})$	$(1, \sqrt{6})$
	2	5	33.15	54.29			$(1, \sqrt{5})$	$(1, \sqrt{5})$
	3	4	29.95	47.69			$(\sqrt{2}, 2)$	$(\sqrt{2}, 2)$
	4	3	25.98	42.94			$(\sqrt{2}, \sqrt{3})$	$(\sqrt{2}, \sqrt{3})$
	5	2	24.92	41.02			$(\sqrt{2}, \sqrt{2})$	$(\sqrt{3}, \sqrt{2})$
	7	0	26.41	44.17			$(2, NA)$	$(2, NA)$
8	0	8	16.48	55.56	273	81	$(NA, 0)$	$(NA, 0)$
	1	7	31.54	84.39			$(0, \sqrt{7})$	$(1, \sqrt{7})$
	2	6	22.34	63.20			$(1, \sqrt{6})$	$(1, \sqrt{6})$
	3	5	20.10	54.41			$(1, \sqrt{5})$	$(\sqrt{2}, \sqrt{5})$
	4	4	17.08	48.88			$(\sqrt{2}, 2)$	$(\sqrt{2}, 2)$
	5	3	15.85	44.76			$(\sqrt{2}, \sqrt{3})$	$(\sqrt{3}, \sqrt{3})$
	6	2	14.75	43.35			$(\sqrt{3}, \sqrt{2})$	$(\sqrt{3}, \sqrt{2})$
	8	0	15.57	47.23			$(2, NA)$	$(2, NA)$
9	0	9	10.36	37.41	531	147	$(NA, 0)$	$(NA, 0)$
	1	8	20.20	65.52			$(0, \sqrt{8})$	$(1, \sqrt{8})$
	2	7	14.27	46.20			$(1, \sqrt{7})$	$(1, \sqrt{7})$
	3	6	12.75	40.56			$(1, \sqrt{6})$	$(\sqrt{2}, \sqrt{6})$
	4	5	10.79	35.15			$(\sqrt{2}, \sqrt{5})$	$(\sqrt{2}, \sqrt{5})$
	5	4	9.87	32.05			$(\sqrt{2}, 2)$	$(\sqrt{3}, 2)$
	6	3	8.93	29.55			$(\sqrt{3}, \sqrt{3})$	$(\sqrt{3}, \sqrt{3})$
	7	2	8.52	28.55			$(\sqrt{3}, \sqrt{2})$	$(2, \sqrt{2})$
	9	0	9.00	30.11			$(2, NA)$	$(\sqrt{5}, NA)$
10	0	10	6.32	44.30	1045	149	$(NA, 0)$	$(NA, 0)$
	1	9	12.47	74.84			$(0, 3)$	$(1, 3)$
	2	8	8.78	53.32			$(1, \sqrt{8})$	$(1, \sqrt{8})$
	3	7	7.82	46.38			$(1, \sqrt{7})$	$(\sqrt{2}, \sqrt{7})$
	4	6	6.59	40.30			$(\sqrt{2}, \sqrt{6})$	$(\sqrt{2}, \sqrt{6})$
	5	5	5.99	36.35			$(\sqrt{2}, \sqrt{5})$	$(\sqrt{3}, \sqrt{5})$
	6	4	5.36	33.36			$(\sqrt{3}, 2)$	$(\sqrt{3}, 2)$
	7	3	5.00	31.25			$(\sqrt{3}, \sqrt{3})$	$(2, \sqrt{3})$
	8	2	4.74	30.14			$(2, \sqrt{2})$	$(2, \sqrt{2})$
	10	0	4.94	32.04			$(\sqrt{5}, NA)$	$(\sqrt{5}, NA)$

Table 4.1 Continued

$N_0 = 2$								
Factors	C	S	G-eff (Full)	G-eff (Frac)	N (Full)	N (Frac)	max $(\rho_x, \rho_z)_{full}$	max $(\rho_x, \rho_z)_{frac}$
3	0	3	94.59		16		$(NA, \sqrt{3})$	
	1	2	71.00				$(1, \sqrt{2})$	
	3	0	78.55				$(\sqrt{3}, NA)$	
4	0	4	98.90		26		$(NA, 2)$	
	1	3	74.72				$(1, \sqrt{3})$	
	2	2	67.40				$(1, \sqrt{2})$	
	4	0	75.08				$(\sqrt{3}, NA)$	
5	0	5	87.92	87.64	44	28	$(NA, \sqrt{5})$	$(NA, \sqrt{5})$
	1	4	72.33	82.74			$(1, 2)$	$(1, 2)$
	2	3	57.26	69.47			$(1, \sqrt{3})$	$(\sqrt{2}, \sqrt{3})$
	3	2	53.33	64.53			$(\sqrt{2}, \sqrt{2})$	$(\sqrt{2}, \sqrt{2})$
	5	0	58.95	72.25			$(\sqrt{3}, NA)$	$(2, 0)$
6	0	6	70.56	96.95	78	46	$(NA, \sqrt{6})$	$(NA, \sqrt{6})$
	1	5	62.29	82.80			$(1, \sqrt{5})$	$(1, \sqrt{5})$
	2	4	45.30	66.32			$(1, 2)$	$(1, 2)$
	3	3	41.06	57.67			$(\sqrt{2}, \sqrt{3})$	$(\sqrt{2}, \sqrt{3})$
	4	2	37.67	55.86			$(\sqrt{2}, \sqrt{2})$	$(\sqrt{2}, \sqrt{2})$
	6	0	41.30	61.22			$(\sqrt{3}, NA)$	$(2, NA)$
7	0	7	50.00	84.72	144	80	$(NA, 0)$	$(NA, \sqrt{7})$
	1	6	46.60	72.59			$(0, \sqrt{6})$	$(1, \sqrt{6})$
	2	5	32.93	53.62			$(1, \sqrt{5})$	$(1, \sqrt{5})$
	3	4	29.74	47.10			$(\sqrt{2}, 2)$	$(\sqrt{2}, 2)$
	4	3	25.81	42.42			$(\sqrt{2}, \sqrt{3})$	$(\sqrt{2}, \sqrt{3})$
	5	2	24.77	40.52			$(\sqrt{2}, \sqrt{2})$	$(\sqrt{3}, \sqrt{2})$
	7	0	26.27	43.67			$(2, NA)$	$(2, NA)$
8	0	8	32.85	99.78	274	82	$(NA, 0)$	$(NA, 0)$
	1	7	31.51	83.37			$(0, \sqrt{7})$	$(1, \sqrt{7})$
	2	6	22.26	62.44			$(1, \sqrt{6})$	$(1, \sqrt{6})$
	3	5	20.04	53.75			$(1, \sqrt{5})$	$(\sqrt{2}, \sqrt{5})$
	4	4	17.02	48.29			$(\sqrt{2}, 2)$	$(\sqrt{2}, 2)$
	5	3	15.79	44.21			$(\sqrt{2}, \sqrt{3})$	$(\sqrt{3}, \sqrt{3})$
	6	2	14.70	42.83			$(\sqrt{3}, \sqrt{2})$	$(\sqrt{3}, \sqrt{2})$
	8	0	15.53	46.33			$(2, NA)$	$(\sqrt{5}, NA)$
9	0	9	20.68	72.45	532	148	$(NA, 0)$	$(NA, 3)$
	1	8	20.21	65.08			$(0, \sqrt{8})$	$(1, \sqrt{8})$
	2	7	14.25	45.89			$(1, \sqrt{7})$	$(1, \sqrt{7})$
	3	6	12.73	40.29			$(1, \sqrt{6})$	$(\sqrt{2}, \sqrt{6})$
	4	5	10.77	34.92			$(\sqrt{2}, \sqrt{5})$	$(\sqrt{2}, \sqrt{5})$
	5	4	9.85	31.83			$(\sqrt{2}, 2)$	$(\sqrt{3}, 2)$
	6	3	8.91	29.36			$(\sqrt{3}, \sqrt{3})$	$(\sqrt{3}, \sqrt{3})$
	7	2	8.50	28.36			$(\sqrt{3}, \sqrt{2})$	$(2, \sqrt{2})$
	9	0	8.97	29.92			$(\sqrt{5}, NA)$	$(\sqrt{5}, NA)$
10	0	10	12.62	83.92	1046	150	$(NA, 0)$	$(NA, \sqrt{10})$
	1	9	12.48	74.34			$(0, 3)$	$(1, 3)$
	2	8	8.77	52.97			$(1, \sqrt{8})$	$(1, \sqrt{8})$
	3	7	7.81	46.07			$(1, \sqrt{7})$	$(\sqrt{2}, \sqrt{7})$
	4	6	6.59	40.03			$(\sqrt{2}, \sqrt{6})$	$(\sqrt{2}, \sqrt{6})$
	5	5	5.99	36.11			$(\sqrt{2}, \sqrt{5})$	$(\sqrt{3}, \sqrt{5})$
	6	4	5.36	33.14			$(\sqrt{3}, 2)$	$(\sqrt{3}, 2)$
	7	3	5.00	31.05			$(\sqrt{3}, \sqrt{3})$	$(2, \sqrt{3})$
	8	2	4.74	29.95			$(2, \sqrt{2})$	$(2, \sqrt{2})$
	10	0	4.93	31.84			$(\sqrt{5}, NA)$	$(\sqrt{5}, NA)$

Table 4.1 Continued

$N_0 = 3$								
Factors	C	S	G-eff (Full)	G-eff (Frac)	N (Full)	N (Frac)	max $(\rho_x, \rho_z)_{full}$	max $(\rho_x, \rho_z)_{frac}$
3	0	3	89.03		17		$(NA, \sqrt{3})$	
	1	2	66.94				$(1, \sqrt{2})$	
	3	0	74.02				$(\sqrt{3}, NA)$	
4	0	4	95.24		27		$(NA, 2)$	
	1	3	72.00				$(1, \sqrt{3})$	
	2	2	64.95				$(1, \sqrt{2})$	
	4	0	72.36				$(\sqrt{3}, NA)$	
5	0	5	85.96	84.62	45	29	$(NA, \sqrt{5})$	$(NA, \sqrt{5})$
	1	4	70.74	79.94			$(1, 2)$	$(1, 2)$
	2	3	56.01	67.09			$(1, \sqrt{3})$	$(\sqrt{2}, \sqrt{3})$
	3	2	52.15	62.31			$(\sqrt{2}, \sqrt{2})$	$(\sqrt{2}, \sqrt{2})$
	5	0	57.77	69.77			$(\sqrt{3}, NA)$	$(2, 0)$
6	0	6	69.66	94.89	79	47	$(NA, \sqrt{6})$	$(NA, \sqrt{6})$
	1	5	61.51	81.06			$(1, \sqrt{5})$	$(1, \sqrt{5})$
	2	4	44.74	64.92			$(1, 2)$	$(1, 2)$
	3	3	40.54	56.45			$(\sqrt{2}, \sqrt{3})$	$(\sqrt{2}, \sqrt{3})$
	4	2	37.21	54.69			$(\sqrt{2}, \sqrt{2})$	$(\sqrt{2}, \sqrt{2})$
	6	0	40.87	59.96			$(\sqrt{3}, NA)$	$(2, NA)$
7	0	7	51.20	83.68	145	81	$(NA, \sqrt{7})$	$(NA, \sqrt{7})$
	1	6	46.38	71.70			$(0, \sqrt{6})$	$(1, \sqrt{6})$
	2	5	32.71	52.97			$(1, \sqrt{5})$	$(1, \sqrt{5})$
	3	4	29.54	46.52			$(\sqrt{2}, 2)$	$(\sqrt{2}, 2)$
	4	3	25.63	41.90			$(\sqrt{2}, \sqrt{3})$	$(\sqrt{2}, \sqrt{3})$
	5	2	24.61	40.03			$(\sqrt{2}, \sqrt{2})$	$(\sqrt{3}, \sqrt{2})$
	7	0	26.12	43.17			$(2, NA)$	$(2, NA)$
8	0	8	34.77	98.58	275	83	$(NA, \sqrt{8})$	$(NA, \sqrt{8})$
	1	7	31.45	82.37			$(0, \sqrt{7})$	$(1, \sqrt{7})$
	2	6	22.19	61.70			$(1, \sqrt{6})$	$(1, \sqrt{6})$
	3	5	19.97	53.10			$(1, \sqrt{5})$	$(\sqrt{2}, \sqrt{5})$
	4	4	16.96	47.72			$(\sqrt{2}, 2)$	$(\sqrt{2}, 2)$
	5	3	15.74	43.68			$(\sqrt{2}, \sqrt{3})$	$(\sqrt{3}, \sqrt{3})$
	6	2	14.65	42.32			$(\sqrt{3}, \sqrt{2})$	$(\sqrt{3}, \sqrt{2})$
	8	0	15.49	45.79			$(2, NA)$	$(\sqrt{5}, NA)$
9	0	9	22.27	71.96	533	149	$(NA, 3)$	$(NA, 3)$
	1	8	20.20	64.65			$(0, \sqrt{8})$	$(1, \sqrt{8})$
	2	7	14.23	45.59			$(1, \sqrt{7})$	$(1, \sqrt{7})$
	3	6	12.71	40.02			$(1, \sqrt{6})$	$(\sqrt{2}, \sqrt{6})$
	4	5	10.75	34.69			$(\sqrt{2}, \sqrt{5})$	$(\sqrt{2}, \sqrt{5})$
	5	4	9.84	31.62			$(\sqrt{2}, 2)$	$(\sqrt{3}, 2)$
	6	3	8.89	29.16			$(\sqrt{3}, \sqrt{3})$	$(\sqrt{3}, \sqrt{3})$
	7	2	8.49	28.17			$(\sqrt{3}, \sqrt{2})$	$(2, \sqrt{2})$
	9	0	8.95	29.74			$(\sqrt{5}, NA)$	$(\sqrt{5}, NA)$
10	0	10	13.69	83.36	1047	151	$(NA, \sqrt{10})$	$(NA, \sqrt{10})$
	1	9	12.48	73.85			$(0, 3)$	$(1, 3)$
	2	8	8.76	52.63			$(1, \sqrt{8})$	$(1, \sqrt{8})$
	3	7	7.80	45.76			$(1, \sqrt{7})$	$(\sqrt{2}, \sqrt{7})$
	4	6	6.58	39.77			$(\sqrt{2}, \sqrt{6})$	$(\sqrt{2}, \sqrt{6})$
	5	5	5.98	35.87			$(\sqrt{2}, \sqrt{5})$	$(\sqrt{3}, \sqrt{5})$
	6	4	5.35	32.92			$(\sqrt{3}, 2)$	$(\sqrt{3}, 2)$
	7	3	4.99	30.84			$(\sqrt{3}, \sqrt{3})$	$(2, \sqrt{3})$
	8	2	4.73	29.75			$(2, \sqrt{2})$	$(2, \sqrt{2})$
	10	0	4.93	31.65			$(\sqrt{5}, NA)$	$(\sqrt{5}, NA)$

Table 4.1 Continued

$N_0 = 4$								
Factors	C	S	G-eff (Full)	G-eff (Frac)	N (Full)	N (Frac)	max $(\rho_x, \rho_z)_{full}$	max $(\rho_x, \rho_z)_{frac}$
3	0	3	84.08		18		$(NA, \sqrt{3})$	
	1	2	63.29				$(1, \sqrt{2})$	
	3	0	69.97				$(\sqrt{3}, NA)$	
4	0	4	91.84		28		$(NA, 2)$	
	1	3	69.46				$(1, \sqrt{3})$	
	2	2	62.67				$(1, \sqrt{2})$	
	4	0	69.83				$(\sqrt{3}, NA)$	
5	0	5	84.10	81.80	46	30	$(NA, \sqrt{5})$	$(NA, \sqrt{5})$
	1	4	69.21	77.30			$(1, 2)$	$(1, 2)$
	2	3	54.82	64.87			$(1, \sqrt{3})$	$(\sqrt{2}, \sqrt{3})$
	3	2	51.03	60.24			$(\sqrt{2}, \sqrt{2})$	$(\sqrt{2}, \sqrt{2})$
	5	0	56.61	67.46			$(\sqrt{3}, NA)$	$(2, 0)$
6	0	6	68.79	92.91	80	48	$(NA, \sqrt{6})$	$(NA, \sqrt{6})$
	1	5	60.74	79.38			$(1, \sqrt{5})$	$(1, \sqrt{5})$
	2	4	44.19	63.58			$(1, 2)$	$(1, 2)$
	3	3	40.04	55.28			$(\sqrt{2}, \sqrt{3})$	$(\sqrt{2}, \sqrt{3})$
	4	2	36.76	53.56			$(\sqrt{2}, \sqrt{2})$	$(\sqrt{2}, \sqrt{2})$
	6	0	40.44	58.75			$(\sqrt{3}, NA)$	$(2, NA)$
7	0	7	50.85	82.66	146	82	$(NA, \sqrt{7})$	$(NA, \sqrt{7})$
	1	6	46.12	70.83			$(0, \sqrt{6})$	$(1, \sqrt{6})$
	2	5	32.49	52.33			$(1, \sqrt{5})$	$(1, \sqrt{5})$
	3	4	29.34	45.95			$(\sqrt{2}, 2)$	$(\sqrt{2}, 2)$
	4	3	25.46	41.40			$(\sqrt{2}, \sqrt{3})$	$(\sqrt{2}, \sqrt{3})$
	5	2	24.45	39.54			$(\sqrt{2}, \sqrt{2})$	$(\sqrt{3}, \sqrt{2})$
	7	0	25.96	42.68			$(2, NA)$	$(2, NA)$
8	0	8	34.65	97.40	276	84	$(NA, \sqrt{8})$	$(NA, \sqrt{8})$
	1	7	31.37	81.39			$(0, \sqrt{7})$	$(1, \sqrt{7})$
	2	6	22.11	60.97			$(1, \sqrt{6})$	$(1, \sqrt{6})$
	3	5	19.90	52.47			$(1, \sqrt{5})$	$(\sqrt{2}, \sqrt{5})$
	4	4	16.90	47.15			$(\sqrt{2}, 2)$	$(\sqrt{2}, 2)$
	5	3	15.69	43.17			$(\sqrt{2}, \sqrt{3})$	$(\sqrt{3}, \sqrt{3})$
	6	2	14.60	41.83			$(\sqrt{3}, \sqrt{2})$	$(\sqrt{3}, \sqrt{2})$
	8	0	15.45	45.27			$(2, NA)$	$(\sqrt{5}, NA)$
9	0	9	22.23	71.48	534	150	$(NA, 3)$	$(NA, 3)$
	1	8	20.18	64.22			$(0, \sqrt{8})$	$(1, \sqrt{8})$
	2	7	14.20	45.29			$(1, \sqrt{7})$	$(1, \sqrt{7})$
	3	6	12.69	39.75			$(1, \sqrt{6})$	$(\sqrt{2}, \sqrt{6})$
	4	5	10.73	34.46			$(\sqrt{2}, \sqrt{5})$	$(\sqrt{2}, \sqrt{5})$
	5	4	9.82	31.41			$(\sqrt{2}, 2)$	$(\sqrt{3}, 2)$
	6	3	8.88	28.97			$(\sqrt{3}, \sqrt{3})$	$(\sqrt{3}, \sqrt{3})$
	7	2	8.48	27.98			$(\sqrt{3}, \sqrt{2})$	$(2, \sqrt{2})$
	9	0	8.94	29.56			$(\sqrt{5}, NA)$	$(\sqrt{5}, NA)$
10	0	10	13.67	82.81	1048	152	$(NA, \sqrt{10})$	$(NA, \sqrt{10})$
	1	9	12.48	73.37			$(0, 3)$	$(1, 3)$
	2	8	8.75	52.29			$(1, \sqrt{8})$	$(1, \sqrt{8})$
	3	7	7.80	45.46			$(1, \sqrt{7})$	$(\sqrt{2}, \sqrt{7})$
	4	6	6.57	39.51			$(\sqrt{2}, \sqrt{6})$	$(\sqrt{2}, \sqrt{6})$
	5	5	5.98	35.63			$(\sqrt{2}, \sqrt{5})$	$(\sqrt{3}, \sqrt{5})$
	6	4	5.35	32.71			$(\sqrt{3}, 2)$	$(\sqrt{3}, 2)$
	7	3	4.99	30.64			$(\sqrt{3}, \sqrt{3})$	$(2, \sqrt{3})$
	8	2	4.73	29.56			$(2, \sqrt{2})$	$(2, \sqrt{2})$
	10	0	4.93	31.45			$(\sqrt{5}, NA)$	$(\sqrt{5}, NA)$

Table 4.1 Continued

$N_0 = 5$								
Factors	C	S	G-eff (Full)	G-eff (Frac)	N (Full)	N (Frac)	max $(\rho_x, \rho_z)_{full}$	max $(\rho_x, \rho_z)_{frac}$
3	0	3	79.66		16		$(NA, \sqrt{3})$	
	1	2	60.00				$(1, \sqrt{2})$	
	3	0	66.32				$(\sqrt{3}, NA)$	
4	0	4	88.67		26		$(NA, 2)$	
	1	3	67.08				$(1, \sqrt{3})$	
	2	2	60.53				$(1, \sqrt{2})$	
	4	0	67.46				$(\sqrt{3}, NA)$	
5	0	5	82.31	79.16	44	28	$(NA, \sqrt{5})$	$(NA, \sqrt{5})$
	1	4	67.75	74.83			$(1, 2)$	$(1, 2)$
	2	3	53.66	62.79			$(1, \sqrt{3})$	$(\sqrt{2}, \sqrt{3})$
	3	2	49.95	58.30			$(\sqrt{2}, \sqrt{2})$	$(\sqrt{2}, \sqrt{2})$
	5	0	55.49	65.29			$(\sqrt{3}, NA)$	$(2, 0)$
6	0	6	67.94	91.01	78	46	$(NA, \sqrt{6})$	$(NA, \sqrt{6})$
	1	5	60.00	77.77			$(1, \sqrt{5})$	$(1, \sqrt{5})$
	2	4	43.66	62.29			$(1, 2)$	$(1, 2)$
	3	3	39.55	54.15			$(\sqrt{2}, \sqrt{3})$	$(\sqrt{2}, \sqrt{3})$
	4	2	36.32	52.48			$(\sqrt{2}, \sqrt{2})$	$(\sqrt{2}, \sqrt{2})$
	6	0	40.01	57.59			$(\sqrt{3}, NA)$	$(2, NA)$
7	0	7	50.50	81.66	144	80	$(NA, \sqrt{7})$	$(NA, \sqrt{7})$
	1	6	45.85	69.98			$(0, \sqrt{6})$	$(1, \sqrt{6})$
	2	5	32.27	51.71			$(1, \sqrt{5})$	$(1, \sqrt{5})$
	3	4	29.14	45.40			$(\sqrt{2}, 2)$	$(\sqrt{2}, 2)$
	4	3	25.29	40.90			$(\sqrt{2}, \sqrt{3})$	$(\sqrt{2}, \sqrt{3})$
	5	2	24.29	39.07			$(\sqrt{2}, \sqrt{2})$	$(\sqrt{3}, \sqrt{2})$
	7	0	25.81	42.20			$(2, NA)$	$(2, NA)$
8	0	8	34.52	96.26	274	82	$(NA, \sqrt{8})$	$(NA, \sqrt{8})$
	1	7	31.28	80.44			$(0, \sqrt{7})$	$(1, \sqrt{7})$
	2	6	22.03	60.25			$(1, \sqrt{6})$	$(1, \sqrt{6})$
	3	5	19.83	51.85			$(1, \sqrt{5})$	$(\sqrt{2}, \sqrt{5})$
	4	4	16.84	46.60			$(\sqrt{2}, 2)$	$(\sqrt{2}, 2)$
	5	3	15.63	42.66			$(\sqrt{2}, \sqrt{3})$	$(\sqrt{3}, \sqrt{3})$
	6	2	14.55	41.34			$(\sqrt{3}, \sqrt{2})$	$(\sqrt{3}, \sqrt{2})$
	8	0	15.41	44.75			$(2, NA)$	$(\sqrt{5}, NA)$
9	0	9	22.19	71.01	532	148	$(NA, 3)$	$(NA, 3)$
	1	8	20.16	63.79			$(0, \sqrt{8})$	$(1, \sqrt{8})$
	2	7	14.18	44.99			$(1, \sqrt{7})$	$(1, \sqrt{7})$
	3	6	12.67	39.49			$(1, \sqrt{6})$	$(\sqrt{2}, \sqrt{6})$
	4	5	10.71	34.23			$(\sqrt{2}, \sqrt{5})$	$(\sqrt{2}, \sqrt{5})$
	5	4	9.80	31.21			$(\sqrt{2}, 2)$	$(\sqrt{3}, 2)$
	6	3	8.86	28.78			$(\sqrt{3}, \sqrt{3})$	$(\sqrt{3}, \sqrt{3})$
	7	2	8.46	27.80			$(\sqrt{3}, \sqrt{2})$	$(2, \sqrt{2})$
	9	0	8.93	29.37			$(\sqrt{5}, NA)$	$(\sqrt{5}, NA)$
10	0	10	13.66	82.27	1046	150	$(NA, \sqrt{10})$	$(NA, \sqrt{10})$
	1	9	12.47	72.89			$(0, 3)$	$(1, 3)$
	2	8	8.75	51.95			$(1, \sqrt{8})$	$(1, \sqrt{8})$
	3	7	7.79	45.17			$(1, \sqrt{7})$	$(\sqrt{2}, \sqrt{7})$
	4	6	6.57	39.25			$(\sqrt{2}, \sqrt{6})$	$(\sqrt{2}, \sqrt{6})$
	5	5	5.97	35.40			$(\sqrt{2}, \sqrt{5})$	$(\sqrt{3}, \sqrt{5})$
	6	4	5.34	32.49			$(\sqrt{3}, 2)$	$(\sqrt{3}, 2)$
	7	3	4.99	30.44			$(\sqrt{3}, \sqrt{3})$	$(2, \sqrt{3})$
	8	2	4.73	29.37			$(2, \sqrt{2})$	$(2, \sqrt{2})$
	10	0	4.93	31.26			$(\sqrt{5}, NA)$	$(\sqrt{5}, NA)$

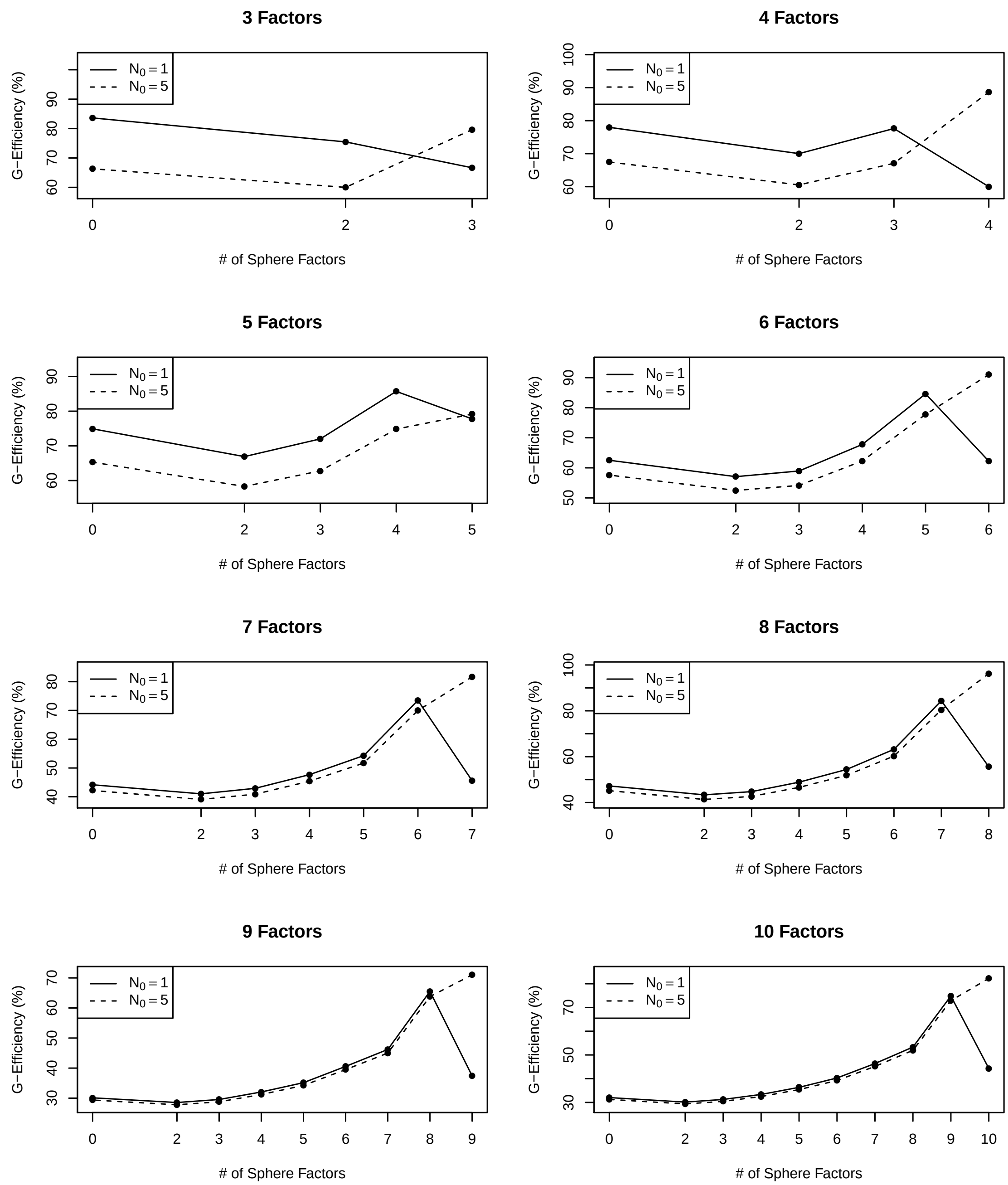

Figure 4.1: G-efficiencies for between 3 and 10 factors comparing use of 1 and 5 center points. For 5 or more factors, it is assumed that the appropriate fractional factorial design is used.

Graphical Assessment of Maximum Spherical Prediction Variance

So far, we have discussed selecting designs based on single-number design efficiencies. While design efficiencies provide excellent information and can assist in choosing a design, the design efficiencies do not give information about all aspects of design performance. In particular, the G-efficiency only focuses on the maximum prediction variance, so it can be misleading in regards to a design's performance throughout the entire design space [11]. In order to study prediction variance throughout a design's entire space, Giovanitti-Jensen and Myers [5] and Myers et al. [12] developed variance dispersion graphs. A variance dispersion graph plots average, maximum and minimum spherical prediction variance against a radius where the radius ranges from the center to the outermost surface of the design space.

Because we derived a closed form for the *maximum* prediction variance, the plots we examine will deal only with maximum prediction variance. Figure 4.2 shows

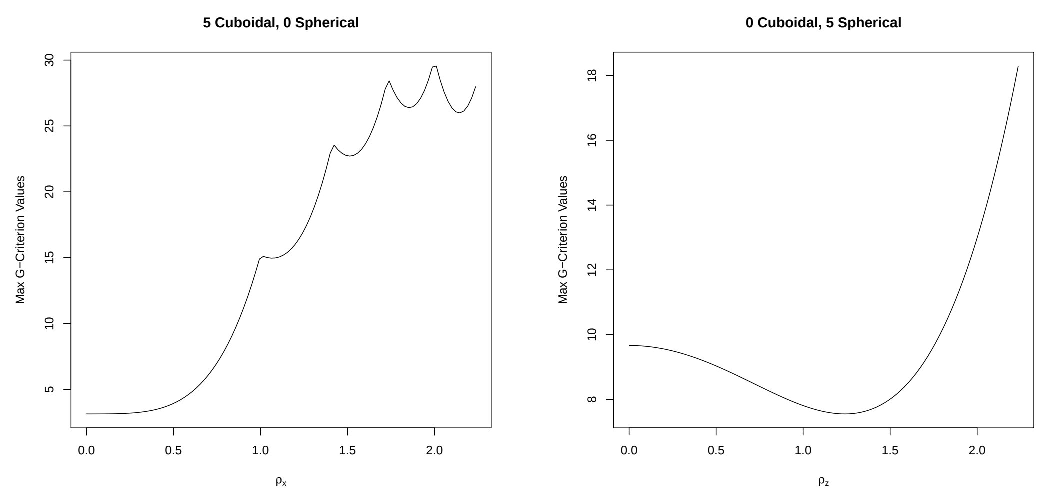

Figure 4.2: Variance dispersion graphs for CCDs with cuboidal region (left) and spherical region (right). $N_0 = 3$ for both.

the maximum spherical prediction variance plotted against the radius for a 5-factor CCD(c) and a 5-factor CCD(s). Notice how both designs have smaller maximum prediction variance near the center of the design space, but larger maximum prediction variance near the boundary of the design space. The largest maximum prediction variance for both designs occurs on the boundary of the space, and note how the maximum prediction variance for the CCD(c) is larger on the boundary than it is for the CCD(s). This fact is confirmed by the G-efficiencies given for these designs in Table 4.1. The local extrema on the CCD(c) occur where the spherical radius (ρ_x) is the square root of an integer [2].

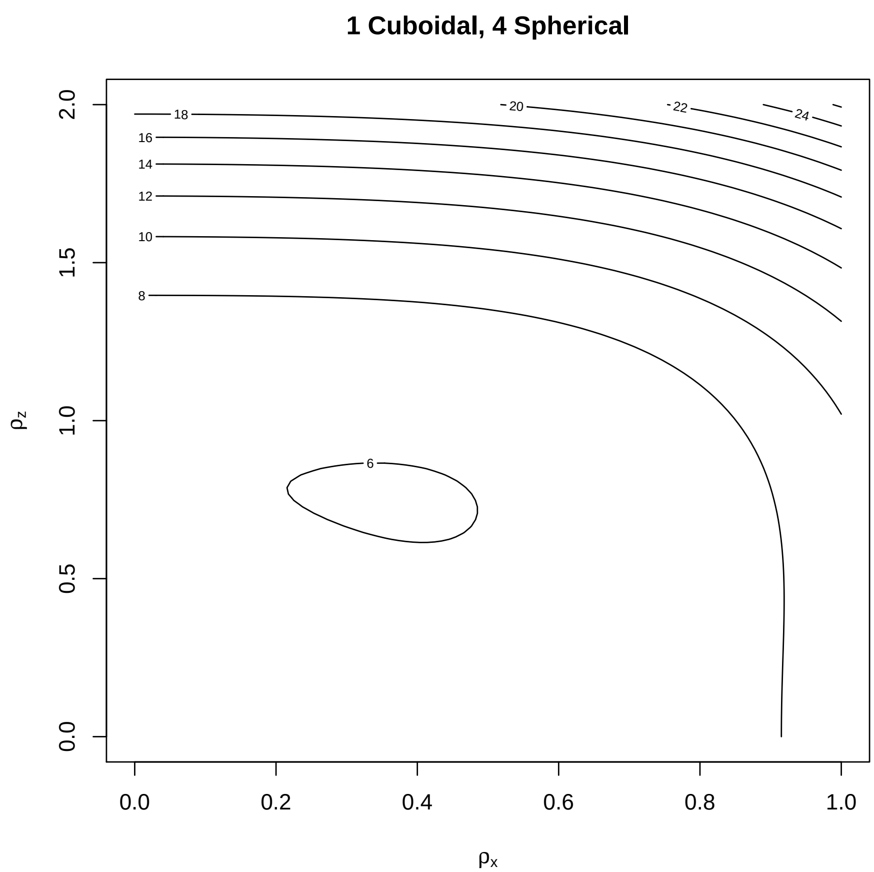

Figure 4.3: Contour Plot of $VMAX_{\rho_x,\rho_z}$ for a Cyl(1,4) Design. $N_0 = 3$.

Recall that the maximum spherical prediction variance for a cylindrical design in (4.6) was written in terms of two radii, one for the spherical factors and one for the cuboidal factors. Since there are two radii, it was natural to consider plotting the maximum spherical prediction variance for cylindrical designs using contour plots where each radius is assigned to one axis. Let Cyl(a, b) be defined as a cylindrical design where a is the number of cuboidal factors and b is the number of spherical factors. Figures 4.3, 4.4, and 4.5 show contour plots of maximum spherical prediction variance for Cyl(1,4), Cyl(2,3) and Cyl(3,2) designs, each having 3 center points and using a 2_V^{5-1} fractional factorial design.

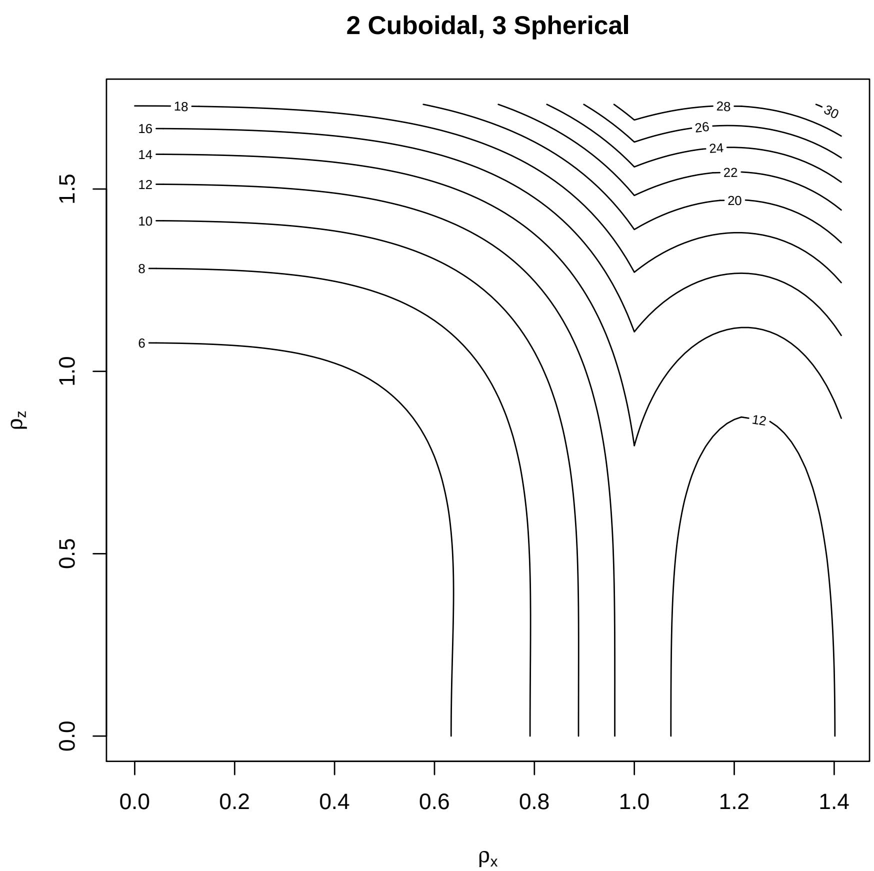

Figure 4.4: Contour Plot of $VMAX_{\rho_x,\rho_z}$ for a Cyl(2,3) Design. $N_0 = 3$.

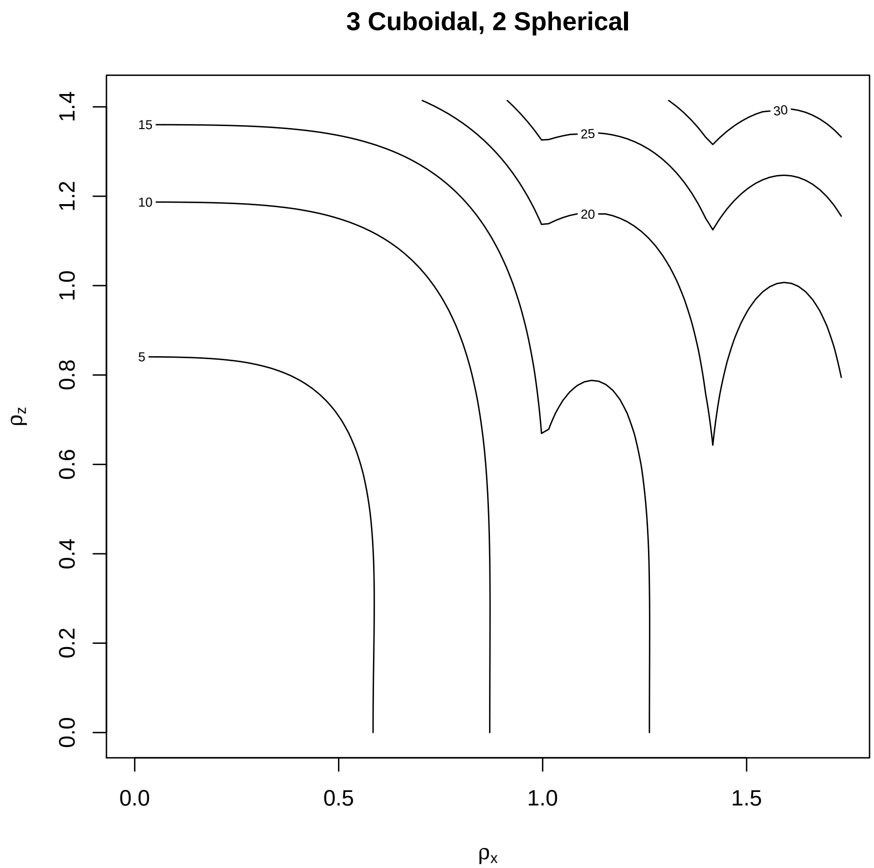

Figure 4.5: Contour Plot of $VMAX_{\rho_x,\rho_z}$ for a Cyl(3,2) Design. $N_0 = 3$.

First, note how the largest maximum spherical prediction variance appears to occur at the greatest distance for each radius. This fact gives evidence to the G-efficiencies being correct in Table 4.1. Also, note the behavior in the contours for the Cyl(2,3) and Cyl(3,2) designs. As ρ_z decreases and as ρ_x simultaneously approaches the square roots of integers, the maximum spherical prediction variance increases. Next, note how the maximum spherical prediction variance tends to be lower in a greater portion of the space for the Cyl(1,4) design than the other two cylindrical designs. For example, consider the maximum spherical prediction variance value of 10, which is displayed in each of the contour plots. In the Cyl(1,4) design, it appears that about 2/3 of the design space has maximum spherical prediction variance less than 10. It is not surprising that it is the central area of the design that has lower maximum spherical prediction variance since 3 center points were used. The proportion of maximum spherical prediction variance that is less than 10 for the Cyl(2,3) design is considerably less than that of the Cyl(1,4) design. The Cyl(3,2) design has an even smaller proportion of the its space with maximum spherical prediction variance less than 10. For a cylindrical design with 5 factors and 3 center points, these contour plots show that the maximum spherical prediction variance is lower throughout a greater fraction of the space when more spherical factors are used.

THE IV-CRITERION

Deriving the Average Prediction Variance

While the G-criterion deals with maximum prediction variance, the IV-criterion assesses a design's average prediction variance. The fact that the IV-criterion is calculated by averaging the prediction variance over the entire design space is appealing. On this note, Myers et al. [11] say, "The [IV]-optimality is conceptually a very reasonable device to use for choosing experimental designs, since selecting a design with good average prediction variance should produce satisfactory results throughout the design space."

In order to find IV-efficiencies, one must integrate the scaled prediction variance function over the design space and divide by the volume of the design space. In order to integrate over the hypercylinder, it simplifies calculations to rewrite the scaled prediction variance function. By rearranging terms, we find that $V(\mathbf{x}, \mathbf{z})$ as given in (3.27) can be written as

$$\begin{aligned} V(\mathbf{x}, \mathbf{z}) \;=\; N\Bigg[\gamma_1 \;&+\; \left(2\gamma_5 + \frac{1}{F+2}\right)\sum_{i=1}^{C} x_i^2 \;+\; \left(\frac{1}{F} - \frac{\gamma_2}{2+C\gamma_2}\right)\sum_{i=1}^{C-1}\sum_{j=i+1}^{C} x_i^2 x_j^2 \\ &+ \frac{1}{2}\left(1 - \frac{\gamma_2}{2+C\gamma_2}\right)\sum_{i=1}^{C} x_i^4 \;+\; \left(\frac{1}{F} + \gamma_4\right)\sum_{i=1}^{C}\sum_{k=1}^{S} x_i^2 z_k^2 \\ &+ \left(2\gamma_6 + \frac{1}{F+2\alpha^2}\right)\sum_{k=1}^{S} z_k^2 \;+\; \frac{1}{2}\left(\frac{1}{F} - \frac{\gamma_3}{\alpha^4(2\alpha^4 + S\gamma_3)}\right)\left(\sum_{k=1}^{S} z_k^2\right)^2 \\ &+ \frac{1}{2}\left(\frac{1}{\alpha^4} - \frac{1}{F}\right)\sum_{k=1}^{S} z_k^4\Bigg] \end{aligned}$$

For simplicity we rewrite $V(\mathbf{x}, \mathbf{z})$ as

$$\begin{aligned} V(\mathbf{x}, \mathbf{z}) \;=\; N\Bigg[K \;+\; L\sum_{i=1}^{C} x_i^2 \;&+\; M\sum_{i=1}^{C-1}\sum_{j=i+1}^{C} x_i^2 x_j^2 \;+\; P\sum_{i=1}^{C} x_i^4 \;+\; Q\sum_{i=1}^{C}\sum_{k=1}^{S} x_i^2 z_k^2 \\ &+ R\sum_{k=1}^{S} z_k^2 \;+\; T\left(\sum_{k=1}^{S} z_k^2\right)^2 \;+\; U\sum_{k=1}^{S} z_k^4\Bigg] \end{aligned} \tag{5.1}$$

where

$$
\begin{array}{ll}
K = \gamma_1 & Q = \frac{1}{F} + \gamma_4 \\
L = 2\gamma_5 + \frac{1}{F+2} & R = 2\gamma_6 + \frac{1}{F+2\alpha^2} \\
M = \frac{1}{F} - \frac{\gamma_2}{2+C\gamma_2} & T = \frac{1}{2}\left(\frac{1}{F} - \frac{\gamma_3}{\alpha^4(2\alpha^4+S\gamma_3)}\right) \\
P = \frac{1}{2}\left(1 - \frac{\gamma_2}{2+C\gamma_2}\right) & U = \frac{1}{2}\left(\frac{1}{\alpha^4} - \frac{1}{F}\right)
\end{array}
$$

We define C^* to be the set of points that make up the design space for a cylindrical design where

$$C^* = \left\{\mathbf{x}, \mathbf{z} : -1 \leq x_i \leq 1, i = 1, 2, \ldots, C, \sum_{k=1}^{S} z_k^2 \leq \alpha^2, \alpha = \sqrt{S}\right\}$$

Furthermore, we define the subspace made up by the cuboidal factors as H^* and the subspace made up by the spherical factors as S^* where

$$
\begin{aligned}
H^* &= \{\mathbf{x} : -1 \leq x_i \leq 1 \text{ for } i = 1, \ldots, C\} \\
S^* &= \left\{\mathbf{z} : \sum_{k=1}^{S} z_k^2 \leq \alpha^2,\ \alpha = \sqrt{S}\right\}
\end{aligned}
$$

Let Vol denote the volume of a region. Then the volume of C^* is

$$
\begin{aligned}
Vol(C^*) &= Vol(H^*) \cdot Vol(S^*) \\
&= \left(\int_{H^*} d\mathbf{x}\right)\left(\int_{S^*} d\mathbf{z}\right) \\
&= \left[2^C\right] \cdot \left[\frac{\alpha^S \pi^{\frac{S}{2}}}{\Gamma\left(\frac{S}{2}+1\right)}\right]
\end{aligned}
$$

The volume of the hypercube is 2^C because the corners of the hypercube are at combinations of ± 1 which means that each of the C sides of the hypercube has length 2. The formula for the volume of a hypersphere can be found in Gradshteyn and Ryzhik [6]. The average prediction variance, APV, is then found by calculating the following integral:

$$APV = \frac{1}{Vol(C^*)} \int_{C^*} V(\mathbf{x}, \mathbf{z}) \mathbf{dxdz} \tag{5.2}$$

By substituting (5.1) into (5.2), we have

$$\begin{aligned}
APV &= \frac{N}{Vol(C^*)}\int_{C^*}\left[K \;+\; L\sum_{i=1}^{C} x_i^2 \;+\; M\sum_{i=1}^{C-1}\sum_{j=i+1}^{C} x_i^2x_j^2 \;+\; P\sum_{i=1}^{C} x_i^4\right. \\
&\quad \left. + Q\sum_{i=1}^{C}\sum_{k=1}^{S} x_i^2z_k^2 \;+\; R\sum_{k=1}^{S} z_k^2 + \; T\left(\sum_{k=1}^{S} z_k^2\right)^2 \;+\; U\sum_{k=1}^{S} z_k^4\right] d\mathbf{x}d\mathbf{z} \\
&= \frac{N}{Vol(C^*)}\int_{S^*}\int_{H^*}\left[K \;+\; L\sum_{i=1}^{C} x_i^2 \;+\; M\sum_{i=1}^{C}\sum_{j=i+1}^{C-1} x_i^2x_j^2 \;+\; P\sum_{i=1}^{C} x_i^4\right. \\
&\quad \left. + Q\sum_{i=1}^{C}\sum_{k=1}^{S} x_i^2z_k^2 \;+\; R\sum_{k=1}^{S} z_k^2 + \; T\left(\sum_{k=1}^{S} z_k^2\right)^2 \;+\; U\sum_{k=1}^{S} z_k^4\right] d\mathbf{x}d\mathbf{z}
\end{aligned}$$

We begin by integrating over H^*. Note that the limits of integration for each x_i are -1 and 1. Then

$$\begin{aligned}
APV &= \frac{N}{Vol(C^*)}\int_{S^*}\left\{K\cdot 2^C + L\cdot 2^{C-1}\left(C\cdot\frac{2}{3}\right) + M\cdot 2^{C-2}\cdot\binom{C}{2}\cdot\frac{2}{3}\cdot\frac{2}{3}\right. \\
&\quad + P\cdot 2^{C-1}\left(C\cdot\frac{2}{5}\right) + Q\cdot 2^{C-1}\cdot\left(C\cdot\frac{2}{3}\right)\sum_{k=1}^{S} z_k^2 \\
&\quad \left. + 2^C\left[R\sum_{k=1}^{S} z_k^2 + T\left(\sum_{k=1}^{S} z_k^2\right)^2 + U\sum_{k=1}^{S} z_k^4\right]\right\} d\mathbf{z} \\
&= \frac{N}{Vol(C^*)}\int_{S^*} 2^C\left[K + \frac{LC}{3} + \frac{M\binom{C}{2}}{9} + \frac{PC}{5} + \frac{QC}{3}\sum_{k=1}^{S} z_k^2 + R\sum_{k=1}^{S} z_k^2\right. \\
&\quad \left. + T\left(\sum_{k=1}^{S} z_k^2\right)^2 + U\sum_{k=1}^{4} z_k^4\right] d\mathbf{z} \\
&= \frac{2^C N}{2^C\int_{S^*} d\mathbf{z}}\left[K + \frac{LC}{3} + \frac{M\binom{C}{2}}{9} + \frac{PC}{3}\right]\int_{S^*} d\mathbf{z} \\
&\quad + \frac{2^C N}{2^C\int_{S^*} d\mathbf{z}}\int_{S^*}\left[\left(\frac{QC}{3} + R\right)\sum_{k=1}^{S} z_k^2 + T\left(\sum_{k=1}^{S} z_k^2\right)^2 + U\sum_{k=1}^{S} z_k^4\right] d\mathbf{z} \\
&= N\left[K + \frac{LC}{3} + \frac{M\binom{C}{2}}{9} + \frac{PC}{3}\right] \\
&\quad + \frac{N}{Vol(S^*)}\int_{S^*}\left[\left(\frac{QC}{3} + R\right)\sum_{k=1}^{S} z_k^2 + T\left(\sum_{k=1}^{S} z_k^2\right)^2 + U\sum_{k=1}^{S} z_k^4\right] d\mathbf{z} \qquad (5.3)
\end{aligned}$$

In order to compute the integral in (5.3), conversion to hyperspherical coordinates is necessary. Define the parametric representation of $\mathbf{z} = (z_1, \ldots, z_k)$ as:

$$\begin{aligned}
z_1(\underset{\sim}{\theta}) &= \rho_z cos(\theta_1) \\
z_2(\underset{\sim}{\theta}) &= \rho_z sin(\theta_1) cos(\theta_2) \\
z_3(\underset{\sim}{\theta}) &= \rho_z sin(\theta_1) sin(\theta_2) cos(\theta_3) \\
\vdots \;\; &\vdots \;\; \vdots \\
z_{S-2}(\underset{\sim}{\theta}) &= \rho_z sin(\theta_1) \ldots sin(\theta_{S-3}) cos(\theta_{S-2}) \\
z_{S-1}(\underset{\sim}{\theta}) &= \rho_z sin(\theta_1) \ldots sin(\theta_{S-3}) sin(\theta_{S-2}) cos(\theta_{S-1}) \\
z_S(\underset{\sim}{\theta}) &= \rho_z sin(\theta_1) \ldots sin(\theta_{S-3}) sin(\theta_{S-2}) sin(\theta_{S-1})
\end{aligned}$$

where $\underset{\sim}{\theta} = (\rho_z, \theta_1, \ldots, \theta_{S-1})$ such that $\rho_z \geq 0$, $0 \leq \theta_i \leq \pi$ for $i = 1, \ldots, S-2$ and $0 \leq \theta_{S-1} \leq 2\pi$.

Then (5.3) can be written as

$$APV = K + \frac{LC}{3} + \frac{M\binom{C}{2}}{9} + \frac{PC}{3} + \frac{\mathcal{I}}{Vol(S^*)} \tag{5.4}$$

where

$$\begin{aligned}
\mathcal{I} &= \int_{S^*} \left[\left(\frac{QC}{3} + R \right) \rho_z^2 + T\rho_z^4 + U \sum_{k=1}^{S} z_k^4(\underset{\sim}{\theta}) \right] \sqrt{|W|} d\underset{\sim}{\theta}, \\
W &= \rho_z^{2(S-1)} \prod_{t=1}^{S-2} \sin^{2(S-1-t)}(\theta_t),
\end{aligned}$$

and $|W|$ is the Jacobian of the transformation. This implies

$$\sqrt{|W|} = \rho_z^{(S-1)} \prod_{t=1}^{S-2} \sin^{(S-1-t)}(\theta_t) \tag{5.5}$$

Then, by substituting (5.5) into $\mathcal{I}$, we find that the integral can be written as

$$\mathcal{I} = \int_{S^*} \left[\left(\frac{QC}{3} + R \right) \rho_z^2 + T\rho_z^4 + U \sum_{k=1}^{S} z_k^4(\underset{\sim}{\theta}) \right] \rho_z^{(S-1)} \prod_{t=1}^{S-2} \sin^{(S-1-t)}(\theta_t) d\underset{\sim}{\theta}$$

$$
\begin{aligned}
&= \int_{S^*} \left[\left(\frac{QC}{3} + R \right) \rho_z^{S+1} + T\rho_z^{S+3} + U\rho_z^{S-1} \sum_{k=1}^{S} z_k^4(\underset{\sim}{\theta}) \right] \prod_{t=1}^{S-2} \sin^{(S-1-t)}(\theta_t) d\underset{\sim}{\theta} \\
&= \left\{ \int_0^{2\pi} \int_0^{\alpha} g(\underset{\sim}{\theta}^*) \left[\left(\frac{QC}{3} + R \right) \rho_z^{S+1} + T\rho_z^{S+3} \right] d\rho_z d\theta_{S-1} \right. \\
&\qquad \left. + \int_{S^*} U\rho_z^{S-1} \sum_{k=1}^{S} z_k^4(\underset{\sim}{\theta}) \prod_{t=1}^{S-2} \sin^{(S-1-t)}(\theta_t) d\underset{\sim}{\theta} \right\} \qquad (5.6)
\end{aligned}
$$

where

$$
g(\underset{\sim}{\theta}^*) = \int_0^{\pi} \cdots \int_0^{\pi} \prod_{t=1}^{S-2} \sin^{(S-1-t)}(\theta_t) d\underset{\sim}{\theta}^* \qquad (5.7)
$$

$$
\underset{\sim}{\theta}^* = (\theta_1, \theta_2, \ldots, \theta_{S-2}) \qquad (5.8)
$$

In order to calculate $g(\underset{\sim}{\theta}^*)$, we use the following trigonometric integral identities found in Gradshteyn and Ryzhik [6]:

$$
\int_0^{\pi} \sin^{2n}(t) dt = \frac{(2n)!}{2^{2n}(n!)^2} \pi \qquad (5.9)
$$

$$
\int_0^{\pi} \sin^{2n+1}(t) dt = \frac{2^{2n+1}(n!)^2}{(2n+1)!} \qquad (5.10)
$$

By applying these identities to (5.7), we have found values of $g(\underset{\sim}{\theta}^*)$ for between 2 and 10 factors. These values are given in Table 5.1. Next, (5.6) can be simplified to

$$
\mathcal{I} = 2\pi g(\underset{\sim}{\theta}^*) \left[\left(\frac{QC}{3} + R \right) \frac{\alpha^{S+2}}{S+2} + T \frac{\alpha^{S+4}}{S+4} \right] + \int_0^{\alpha} U \cdot h^*(\rho_z) \cdot \rho_z^{S+3} d\rho_z \qquad (5.11)
$$

where

$$
h^*(\rho_z) = \frac{1}{\rho_z^{S+3}} \int_0^{\pi} \cdots \int_0^{\pi} \int_0^{2\pi} \sum_{k=1}^{S} z_k^4(\underset{\sim}{\theta}) \sqrt{|W|} d\underset{\sim}{\theta} \qquad (5.12)
$$

Borkowski [2] found values for $h^*(\rho_z)$ recursively and obtained values for between 2 and 15 design variables. Because the research for this thesis considers up to 10 factors, we give the values of $h^*(\rho_z)$ for between 2 and 10 factors in Table 5.1.

Next, by calculating the integral in (5.11), we find that $\mathcal{I}$ simplifies to

$$
\mathcal{I} = 2\pi g(\underset{\sim}{\theta}^*) \left[\left(\frac{QC}{3} + R \right) \frac{\alpha^{S+2}}{S+2} + T \frac{\alpha^{S+4}}{S+4} \right] + U \frac{\alpha^{S+4}}{S+4} h^*(\rho_z) \qquad (5.13)
$$

Table 5.1: Values of $g(\theta^*)$ and $h^*(\rho)$ for $S = 2$ to 10 factors

S	$g(\underset{\sim}{\theta}^*)$	$h^*(\rho)$	S	$g(\underset{\sim}{\theta}^*)$	$h^*(\rho)$
2	1	$\frac{3\pi}{2}$	7	$\frac{8\pi^2}{15}$	$\frac{10\pi^3}{45}$
3	2	$\frac{12\pi}{5}$	8	$\frac{\pi^3}{6}$	$\frac{\pi^4}{10}$
4	π	π^2	9	$\frac{16\pi^3}{105}$	$\frac{32\pi^4}{315}$
5	$\frac{4\pi}{3}$	$\frac{8\pi^2}{7}$	10	$\frac{\pi^4}{24}$	$\frac{\pi^5}{48}$
6	$\frac{\pi^2}{2}$	$\frac{3\pi^3}{8}$			

Finally, by substituting (5.13) into (5.4), we have the closed form for the average prediction variance which we state in Theorem 5.1.

Theorem 5.1 *For a cylindrical design with C cuboidal factors and S spherical factors, the average prediction variance (APV) is given by:*

$$\begin{aligned} APV &= K + \frac{LC}{3} + \frac{M\binom{C}{2}}{9} + \frac{PC}{3} + \frac{\Gamma\left(\frac{S}{2}+1\right)}{\alpha^S \pi^{\frac{S}{2}}} \\ &\times \left\{ 2\pi g(\underset{\sim}{\theta}^*) \left[\left(\frac{QC}{3} + R \right) \frac{\alpha^{S+2}}{S+2} + T \frac{\alpha^{S+4}}{S+4} \right] + U \frac{\alpha^{S+4}}{S+4} h^*(\rho_z) \right\} \end{aligned} \quad (5.14)$$

IV-efficiencies for Cylindrical Designs

Using the statistical software package R and applying (5.14), we have found IV-efficiencies for cylindrical designs with between 3 and 10 factors having 1 to 5 center points. These values are given in Table 5.2. Recall that IV-efficiencies are not given as percents as in the other three efficiencies. The IV-efficiencies are simply the values of the average prediction variance for each design. Thus, a design is more efficient than another design by the IV-criterion if it has a lower average prediction variance value. IV-efficiencies for cylindrical designs with 1 and 5 center points are displayed in Figure 5.1. We again use the notation CCD(c) and CCD(s) to define central composite designs with cuboidal and spherical regions, respectively. For cylindrical designs with 3 to 5 factors, there is an increasing trend in the average prediction variance as the number of spherical factors increases. Thus, by the IV-criterion, it is more efficient to use a CCD(c) instead of a cylindrical design if there are strict ranges on any of the factors. For 6 factors, the CCD(s) has the highest average prediction variance while the various cylindrical designs and the CCD(c) have very similar values (see Table 5.2 for actual values). For 7 to 10 factors, the average prediction variance is generally highest in the CCD(c), except for the case of 8 factors and 1 center point using the fractional factorial design in which case the CCD(s) has a slightly larger average prediction variance. As the number of spherical factors increases, the average prediction variance drops until almost all factors are spherical. What is important to note is that in each of these situations, the average prediction variance is lower in cylindrical designs than the CCD(c). Therefore, if an experiment is being conducted in 7 or more factors, it is advantageous to use a cylindrical design with the appropriate number of cuboidal factors instead of the CCD(c).

We realize that in response surface studies which utilize the second-order model, experiments in 7 or more factors are rare which means that in most cases, it would be best for the experimenter to use the CCD(c), according to the IV-criterion. However, we also realize that the IV-criterion is just one piece of information that aids in selecting a good design. One should also consider the other efficiencies studied in previous chapters as well as graphical techniques that allow a more in-depth look at design performance throughout the design space. We discuss other graphical techniques for design performance evaluation in the final chapter.

Table 5.2: IV-efficiencies for between 3 and 10 factors with between 1 and 5 center points

$N_0 = 1$						
Factors	C	S	APV (Full)	APV (Frac)	N (Full)	N (Frac)
3	0	3	8.12		15	
	1	2	6.30			
	3	0	5.51			
4	0	4	12.15		25	
	1	3	9.59			
	2	2	8.84			
	4	0	8.44			
5	0	5	17.75	16.13	43	27
	1	4	14.42	13.03		
	2	3	13.87	11.94		
	3	2	14.00	11.43		
	5	0	14.01	10.97		
6	0	6	25.80	22.02	77	45
	1	5	21.65	18.24		
	2	4	21.88	17.35		
	3	3	23.15	17.25		
	4	2	24.56	17.37		
	6	0	25.32	17.30		
7	0	7	34.45	29.42	143	79
	1	6	32.93	25.70		
	2	5	35.12	25.62		
	3	4	38.92	26.61		
	4	3	43.13	28.01		
	5	2	46.97	29.36		
	7	0	49.18	30.03		
8	0	8	57.14	36.18	273	81
	1	7	42.40	30.48		
	2	6	57.85	30.67		
	3	5	66.99	31.18		
	4	4	76.94	32.22		
	5	3	86.84	33.53		
	6	2	95.46	34.75		
	8	0	100.54	35.29		
9	0	9	98.01	49.11	531	147
	1	8	81.80	42.50		
	2	7	78.95	40.48		
	3	6	118.29	47.12		
	4	5	139.92	50.84		
	5	4	161.90	54.95		
	6	3	183.07	59.11		
	7	2	201.21	62.74		
	9	0	211.98	64.73		
10	0	10	142.14	55.37	1045	149
	1	9	155.01	50.59		
	2	8	171.03	50.55		
	3	7	174.34	49.36		
	4	6	259.17	56.20		
	5	5	305.38	59.89		
	6	4	351.32	63.90		
	7	3	394.98	67.93		
	8	2	432.05	71.40		
	10	0	454.12	73.26		

Table 5.2 Continued

$N_0 = 2$						
Factors	C	S	APV (Full)	APV (Frac)	N (Full)	N (Frac)
3	0	3	6.83		16	
	1	2	5.98			
	3	0	5.45			
4	0	4	10.47		26	
	1	3	9.21			
	2	2	8.78			
	4	0	8.45			
5	0	5	15.37	14.94	44	28
	1	4	13.83	12.93		
	2	3	13.72	12.09		
	3	2	13.98	11.63		
	5	0	14.02	11.17		
6	0	6	22.24	20.21	78	46
	1	5	20.70	17.93		
	2	4	21.55	17.38		
	3	3	23.02	17.38		
	4	2	24.50	17.54		
	6	0	25.28	17.47		
7	0	7	28.87	26.56	144	80
	1	6	31.38	25.05		
	2	5	34.51	25.47		
	3	4	38.60	26.62		
	4	3	42.95	28.10		
	5	2	46.84	29.48		
	7	0	49.05	30.15		
8	0	8	48.22	33.89	274	82
	1	7	39.84	30.05		
	2	6	56.77	30.67		
	3	5	66.38	31.31		
	4	4	76.54	32.42		
	5	3	86.54	33.76		
	6	2	95.19	34.99		
	8	0	100.25	35.53		
9	0	9	83.31	45.30	532	148
	1	8	77.63	41.60		
	2	7	77.07	40.20		
	3	6	117.20	47.08		
	4	5	139.17	50.90		
	5	4	161.31	55.07		
	6	3	182.56	59.28		
	7	2	200.68	62.92		
	9	0	211.40	64.90		
10	0	10	117.37	52.17	1046	150
	1	9	148.05	49.92		
	2	8	167.92	50.42		
	3	7	174.42	49.39		
	4	6	257.84	56.35		
	5	5	304.33	60.10		
	6	4	350.40	64.15		
	7	3	394.09	68.21		
	8	2	431.09	71.68		
	10	0	453.04	73.54		

Table 5.2 Continued

$N_0 = 3$						
Factors	C	S	APV (Full)	APV (Frac)	N (Full)	N (Frac)
3	0	3	6.61		17	
	1	2	5.95			
	3	0	5.50			
4	0	4	10.13		27	
	1	3	9.13			
	2	2	8.83			
	4	0	8.53			
5	0	5	14.76	14.86	45	29
	1	4	13.62	13.06		
	2	3	13.70	12.31		
	3	2	14.02	11.88		
	5	0	14.08	11.41		
6	0	6	21.20	19.87	79	47
	1	5	20.26	17.90		
	2	4	21.40	17.51		
	3	3	22.99	17.57		
	4	2	24.52	17.75		
	6	0	25.30	17.67		
7	0	7	27.12	25.81	145	81
	1	6	30.58	24.79		
	2	5	34.14	25.45		
	3	4	38.42	26.71		
	4	3	42.85	28.23		
	5	2	46.78	29.63		
	7	0	48.99	30.30		
8	0	8	45.34	33.38	275	83
	1	7	38.42	29.95		
	2	6	56.07	30.78		
	3	5	65.97	31.50		
	4	4	76.27	32.65		
	5	3	86.33	34.02		
	6	2	95.00	35.26		
	8	0	100.04	35.79		
9	0	9	78.50	44.22	533	149
	1	8	75.26	41.18		
	2	7	75.79	40.08		
	3	6	116.41	47.12		
	4	5	138.60	51.02		
	5	4	160.87	55.24		
	6	3	182.16	59.47		
	7	2	200.27	63.12		
	9	0	210.93	65.10		
10	0	10	109.17	51.32	1047	151
	1	9	144.04	49.66		
	2	8	165.77	50.43		
	3	7	170.97	49.49		
	4	6	256.80	56.55		
	5	5	303.48	60.34		
	6	4	349.65	64.42		
	7	3	393.35	68.50		
	8	2	430.27	71.99		
	10	0	452.12	73.83		

Table 5.2 Continued

$N_0 = 4$						
Factors	C	S	APV (Full)	APV (Frac)	N (Full)	N (Frac)
3	0	3	6.66		18	
	1	2	6.04			
	3	0	5.61			
4	0	4	10.11		28	
	1	3	9.19			
	2	2	8.94			
	4	0	8.64			
5	0	5	14.61	15.06	46	30
	1	4	13.57	13.29		
	2	3	13.76	12.58		
	3	2	14.12	12.15		
	5	0	14.18	11.67		
6	0	6	20.81	19.89	80	48
	1	5	20.06	18.01		
	2	4	21.35	17.69		
	3	3	23.01	17.79		
	4	2	24.57	17.98		
	6	0	25.36	17.89		
7	0	7	26.32	25.57	146	82
	1	6	30.12	24.73		
	2	5	33.93	25.52		
	3	4	38.33	26.84		
	4	3	42.82	28.40		
	5	2	46.77	29.82		
	7	0	48.98	30.48		
8	0	8	43.97	33.32	276	84
	1	7	37.53	30.01		
	2	6	55.60	30.95		
	3	5	65.68	31.72		
	4	4	76.08	32.91		
	5	3	86.20	34.30		
	6	2	94.88	35.55		
	8	0	99.90	36.07		
9	0	9	76.16	43.82	534	150
	1	8	73.75	41.00		
	2	7	74.88	40.06		
	3	6	115.82	47.21		
	4	5	138.18	51.17		
	5	4	160.53	55.43		
	6	3	181.85	59.69		
	7	2	199.95	63.35		
	9	0	210.56	65.32		
10	0	10	105.11	51.05	1048	153
	1	9	141.45	49.60		
	2	8	164.21	50.52		
	3	7	169.85	49.64		
	4	6	255.98	56.77		
	5	5	302.80	60.60		
	6	4	349.04	64.71		
	7	3	392.74	68.81		
	8	2	429.59	72.31		
	10	0	451.33	74.15		

Table 5.2 Continued

$N_0 = 5$						
Factors	C	S	APV (Full)	APV (Frac)	N (Full)	N (Frac)
3	0	3	6.81		19	
	1	2	6.19			
	3	0	5.75			
4	0	4	10.23		29	
	1	3	9.31			
	2	2	9.09			
	4	0	8.79			
5	0	5	14.62	15.36	47	31
	1	4	13.63	13.58		
	2	3	13.87	12.88		
	3	2	14.25	12.45		
	5	0	14.31	11.95		
6	0	6	20.66	20.06	81	49
	1	5	19.98	18.20		
	2	4	21.37	17.92		
	3	3	23.08	18.03		
	4	2	24.67	18.23		
	6	0	25.46	18.14		
7	0	7	25.91	25.55	147	83
	1	6	29.85	24.77		
	2	5	33.82	25.64		
	3	4	38.30	27.00		
	4	3	42.84	28.59		
	5	2	46.81	30.02		
	7	0	49.01	30.68		
8	0	8	43.21	33.43	277	85
	1	7	36.94	30.15		
	2	6	55.28	31.16		
	3	5	65.50	31.97		
	4	4	75.97	33.19		
	5	3	86.13	34.59		
	6	2	94.81	35.85		
	8	0	99.81	36.37		
9	0	9	74.80	43.69	535	151
	1	8	72.72	40.95		
	2	7	74.20	40.10		
	3	6	115.39	47.35		
	4	5	137.86	51.35		
	5	4	160.28	55.65		
	6	3	181.63	59.93		
	7	2	199.70	63.60		
	9	0	210.26	65.56		
10	0	10	102.72	51.02	1049	154
	1	9	139.67	49.65		
	2	8	163.03	50.66		
	3	7	168.97	49.82		
	4	6	255.32	57.01		
	5	5	302.26	60.88		
	6	4	348.54	65.02		
	7	3	392.23	69.14		
	8	2	429.01	72.64		
	10	0	450.65	74.48		

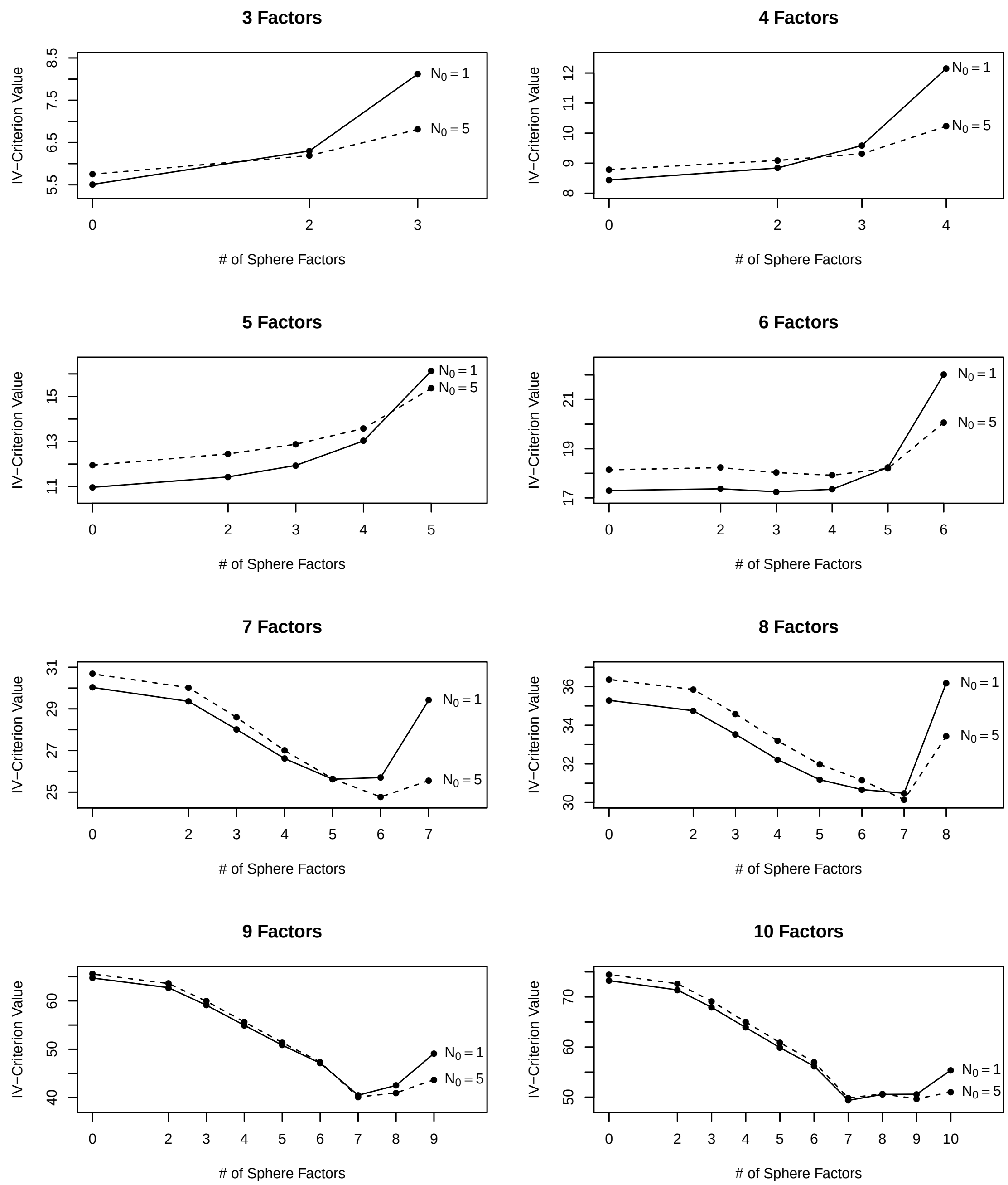

Figure 5.1: IV-efficiencies (Average Prediction Variance (APV) values for between 3 and 10 factors comparing use of 1 and 5 center points. For 5 or more factors, it is assumed that the appropriate fractional factorial design is used.

CONCLUSIONS

Summary of Results

We developed a new class of designs for response surface studies where quadratic regression modeling is desired and some but not all of the factors under consideration have strict ranges on their levels. We derived closed forms for the determinant and inverse of the $\mathbf{X}'\mathbf{X}$ matrix of a cylindrical design. In addition, we found the trace of the $(\mathbf{X}'\mathbf{X})^{-1}$ matrix and found closed forms for the maximum spherical prediction variance and average prediction variance. All of these derivations allowed us to study four of the alphabetic design optimality criteria for cylindrical designs. Design efficiencies were calculated and we compared performance of cylindrical designs to central composite designs.

According to both the D-criterion and the A-criterion, the cylindrical design outperformed the CCD with a cuboidal region, regardless of the number of factors or the number of center points used. For cylindrical designs, both D- and A-efficiency increased as the number of spherical factors increased. Therefore, if some but not all factors have strict bounds, then the most efficient design to use according to these two criteria is the cylindrical design where the factors that have bounded levels are the cuboidal factors and the unbounded factors are the spherical factors.

For experiments in 3 or 4 factors, the CCD with a cuboidal region was more efficient than the cylindrical design by the G-criterion, regardless of the number of center points used. However, for experiments with 5 or more factors, cylindrical designs with relatively few cuboidal factors outperformed the CCD with a cuboidal region. In general, the larger the number of total factors in an experiment, the more cuboidal factors a cylindrical design could have and still outperform the CCD with a cuboidal region, according to the G-criteiron. To see exactly when the cylindrical design was better than the CCD with a cuboidal region, refer to the G-efficiencies in Table 4.1 on page 59.

In addition to studying the maximum prediction variance which finds the absolute largest prediction variance in the entire design space, we studied the maximum spherical prediction variance. Specifically, we looked at variance dispersion graphs for central composite designs and created contour plots of maximum spherical prediction variance for cylindrical designs. We gave one example of an experiment done in 5 factors with 3 center points. The maximum spherical prediction variance was lower in greater portions of the design space for cylindrical designs with more spherical factors.

The results from studying the IV-criterion indicated that for 3 to 5 factors, the CCD with a cuboidal region would be a better choice than a cylindrical design. For 6-factor experiments, the CCD with a cuboidal region was nearly equivalent to each of the 6-factor cylindrical designs, according to the IV-criterion. However, for 7 or more factors, each of the cylindrical designs was better than the CCD with a cuboidal region.

Overall, the results of this research indicate that when some but not all factors are bounded, a cylindrical design can be more efficient than the cuboidal CCD in certain situations, according to the various design optimality criteria. In some cases, the cylindrical design will have better estimation of the model parameters and have better prediction capabilities than the CCD with a cuboidal region. Because we have provided design efficiencies for 4 of the design optimality criteria, practitioners encountering experiments where a cylindrical design could prove useful can choose a design based on some or all of the criteria we have discussed.

Future Research

We discussed the use of graphical techniques to assess design performance. While we were able to study maximum prediction variance over a cylindrical design's entire space, we did not examine minimum spherical prediction variance or average spherical prediction variance. Recall that variance dispersion graphs utilize the maximum, minimum, and average spherical prediction variance. Further work that could be done would be to find closed forms for the minimum and average spherical prediction variance in order to further assess the behavior of the prediction variance throughout a cylindrical design's space. In addition to these graphical techniques, fraction of design space (FDS) plots would be useful in assessing design performance. Zahran et al. (2003) developed these graphs which plot the scaled prediction variance against the fraction of the design space. Myers et al. (2009) summarize the construction and implementation of the FDS plot well in terms of the scaled prediction variance $v(\mathbf{x})$:

> "The curve of an FDS plot matches the value of $v(\mathbf{x})$ against the fraction of the design space that has prediction variance less than or equal to the given value. A graph of the cumulative fraction provides the user with a sketch of the prediction variance throughout the appropriate design region. The plot can be constructed by taking a random sample of design locations throughout the design space, and calculating $v(\mathbf{x})$ at these locations. These values are then sorted and plotted against the quantiles from 0 to 1, in a manner similar to a cumulative distribution function for a statistical distribution."

The benefit of using an FDS plot in comparing CCDs to cylindrical designs would be that the graphs would be created similarly. Comparing the variance dispersion graphs to the contour plots that we made in chapter 4 was difficult. For a given number of factors, one FDS plot could be made which compared the cuboidal and spherical CCDs to the various cylindrical designs for easy comparison.

In addition to studying performance by use of plots, other future research could include examining how results change when replication of design points other than center points is allowed. For example, how would the design efficiencies change if factorial points or axial points were replicated? How would graphical assessment change? Another interesting question is how should one form blocks for a cylindrical design and still retain important properties such as orthogonality. Finally, in our research of the D-criterion, we considered all N of the design points to be equally weighted. Recall that there are 4 types of points in a cylindrical design: factorial points, cuboidal axial points, spherical axial points, and center points. Thus, another topic of future research could be based on the following question. What are the optimal weights for these points to produce the optimal design by the D-criterion?

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APPENDICES

APPENDIX A

R CODE FOR GENERATING DESIGN EFFICIENCIES

D-efficiencies

The R code shown below generates D-efficiencies in a 10 by 10 matrix of values. The output is shown below the code. The row labels (0-10) represent the values for C, the number of cuboidal factors, while the column labels (also 1-10) represent the value for S, the number of spherical factors. Thus, the D-efficiency for a cylindrical design with 3 cuboidal factors and 4 spherical factors is found by looking at the intersection of row 3 with column 4, and the value given in the output is 58.41.

To obtain D-efficiencies for designs with numbers of center points other than 1, change the value of `N.0` in the R code. For designs which utilize fractional factorials, subtract the appropriate number in the exponent of the `F[i,j]` matrix. For example, for a design with 8 factors, the appropriate fractional factorial is a 2_V^{8-2} design. Therefore, to obtain D-efficiencies for cylindrical designs with 8 factors which use this fractional factorial, subtract 2 from `C[i]+S[j]` in the line of code for `F[i,j]`. To study the D-efficiency of designs where either C or S is greater than 10, increase the number of rows or columns in each of the matrices defined in the R code.

```
N.0=1
F=matrix(0,ncol=11,nrow=11)
N=matrix(0,ncol=11,nrow=11)
alpha=matrix(0,ncol=11,nrow=11)
p=matrix(0,ncol=11,nrow=11)
d.eff=matrix(0,ncol=11,nrow=11)
C=0:10
S=0:10
for(i in 1:11){
```

```
for(j in 1:11){
F[i,j]=2^(C[i]+S[j])
N[i,j]=F[i,j]+2*(C[i]+S[j])+N.0
alpha[i,j]=max(sqrt(S[j]),1)
p[i,j]=1+2*(C[i]+S[j])+choose(C[i],2)+choose(S[j],2)+C[i]*S[j]
d.eff[i,j]=(2^(C[i]+S[j]-1)*alpha[i,j]^(4*S[j]-4)*(F[i,j]+2)^C[i]*
            (F[i,j]+2*alpha[i,j]^2)^S[j]*
            F[i,j]^(choose(C[i],2)+choose(S[j],2)+C[i]*S[j])*
            (2*N[i,j]*alpha[i,j]^4+C[i]*alpha[i,j]^4*(N[i,j]*F[i,j]-
            (F[i,j]+2)^2)+S[j]*(N[i,j]*F[i,j]-(F[i,j]+
            2*alpha[i,j]^2)^2)-2*C[i]*S[j]*F[i,j]*
            (1-alpha[i,j]^2)^2))^(1/p[i,j])/N[i,j]
}
}
rownames(d.eff)=0:10
colnames(d.eff)=0:10
round(100*d.eff,2)
```

	0	1	2	3	4	5	6	7	8	9	10
0	100.00	50.40	62.85	71.13	76.73	80.16	81.43	80.82	78.90	76.26	73.35
1	50.40	46.22	54.83	63.55	69.90	73.45	74.53	73.87	72.16	69.97	67.61
2	46.22	44.72	51.73	58.69	63.51	65.98	66.60	66.01	64.73	63.14	Inf
3	44.72	44.52	50.13	55.17	58.41	59.93	60.21	59.72	58.80	57.66	Inf
4	44.52	44.84	48.87	52.19	54.19	55.07	55.17	54.79	54.13	Inf	Inf
5	44.84	44.84	47.41	49.45	50.64	51.15	51.17	50.89	Inf	Inf	Inf
6	44.84	44.29	45.75	46.94	47.65	47.95	47.96	Inf	Inf	Inf	Inf
7	44.29	43.29	44.02	44.70	45.14	45.34	Inf	Inf	Inf	Inf	Inf
8	43.29	42.05	42.35	42.75	43.04	Inf	Inf	Inf	Inf	Inf	Inf
9	42.05	40.75	40.82	41.06	Inf	Inf	Inf	Inf	Inf	Inf	Inf
10	40.75	39.50	39.46	Inf	Inf	Inf	Inf	Inf	Inf	Inf	Inf

A-efficiencies

The R code and output for A-efficiencies is similar the code for D-efficiencies. Thus, we only give the code and no output. To study A-efficiencies beyond what is shown in the code, follow the same guidelines provided in the above section on D-efficiencies.

```
N.0=1
F=matrix(0,ncol=12,nrow=12)
N=matrix(0,ncol=12,nrow=12)
alpha=matrix(0,ncol=12,nrow=12)
gamma.1=matrix(0,ncol=12,nrow=12)
gamma.1.new=matrix(0,ncol=12,nrow=12)
gamma.2=matrix(0,ncol=12,nrow=12)
```

```
gamma.3=matrix(0,ncol=12,nrow=12)
p=matrix(0,ncol=12,nrow=12)
a.eff=matrix(0,ncol=12,nrow=12)
C=0:11
S=0:11
for(i in 0:11){
for(j in 0:11){
F[i,j]=2^(C[i]+S[j])
N[i,j]=F[i,j]+2*(C[i]+S[j])+N.0
alpha[i,j]=max(sqrt(S[j]),1)
gamma.1[i,j]=(2*alpha[i,j]^4+S[j]*F[i,j]+C[i]*F[i,j]*alpha[i,j]^4)/
             (2*N[i,j]*alpha[i,j]^4+N[i,j]*F[i,j]*S[j]+
             C[i]*N[i,j]*F[i,j]*alpha[i,j]^4-C[i]*alpha[i,j]^4*
             (F[i,j]+2)^2-S[j]*(F[i,j]+2*alpha[i,j]^2)^2-
             2*C[i]*S[j]*F[i,j]*(alpha[i,j]^2-1)^2)
gamma.2[i,j]=(2*alpha[i,j]^4*(N[i,j]*F[i,j]-(F[i,j]+2)^2)-
             4*S[j]*F[i,j]*(alpha[i,j]^2-1)^2)/(2*N[i,j]*alpha[i,j]^4+
             S[j]*N[i,j]*F[i,j]-S[j]*(F[i,j]+2*alpha[i,j]^2)^2)
gamma.3[i,j]=(2*(N[i,j]*F[i,j]-(F[i,j]+2*alpha[i,j]^2)^2)-4*C[i]*
             F[i,j]*(alpha[i,j]^2-1)^2)/(2*N[i,j]+C[i]*N[i,j]*
             F[i,j]-C[i]*(F[i,j]+2)^2)
p[i,j]=1+2*(C[i]+S[j])+choose(C[i],2)+choose(S[j],2)+C[i]*S[j]
a.eff[i,j]=p[i,j]/(N[i,j]*(gamma.1[i,j]+C[i]/(F[i,j]+2)+S[j]/(F[i,j]+
             2*alpha[i,j]^2)+(choose(C[i],2)+choose(S[j],2)+
             C[i]*S[j])/F[i,j]+(C[i]/2)*((2+(C[i]-1)*gamma.2[i,j])/
             (2+C[i]*gamma.2[i,j]))+(S[j]/(2*alpha[i,j]^4))*
```

```
            ((2*alpha[i,j]^4+(S[j]-1)*gamma.3[i,j])/
            (2*alpha[i,j]^4+S[j]*gamma.3[i,j]))))
}
}
a.eff=a.eff[-12,]
a.eff=a.eff[,-12]
colnames(a.eff)=0:10
rownames(a.eff)=0:10
round(100*a.eff,2)
```

G-efficiencies

Because a closed form for the G-efficiency for cylindrical designs was not found, the method of generating G-efficiencies using R was different than the other design efficiencies. The R code and output shown below were used to find the G-efficiency for a cylindrical design with 2 cuboidal factors and 2 spherical factors with 1 center point. We created two sequences of values, each of length 1000, for the two radii and made all possible combinations of values for those two radii. Then, using R, we calculated the maximum spherical prediction variance for each set of radii and searched for the overall maximum prediction variance within that set of radii. The results are below.

```
> N.0=1
> C=2
> S=2
> F=2^(C+S)
> N=F+2*(C+S)+N.0
```

```
> alpha=max(1,sqrt(S))
> p=1+2*(C+S)+choose(C,2)+choose(S,2)+C*S
> gamma.1=(2*alpha^4+S*F+C*F*alpha^4)/(2*N*alpha^4+N*F*S+
+          C*N*F*alpha^4-C*alpha^4*(F+2)^2-S*(F+2*alpha^2)^2-
+          2*C*S*F*(alpha^2-1)^2)
> gamma.2=(2*alpha^4*(N*F-(F+2)^2)-4*S*F*(alpha^2-1)^2)/
+         (2*N*alpha^4+S*N*F-S*(F+2*alpha^2)^2)
> gamma.3=(2*(N*F-(F+2*alpha^2)^2)-4*C*F*(alpha^2-1)^2)/
+         (2*N+C*N*F-C*(F+2)^2)
> gamma.4=-(N*F-(F+2)*(F+2*alpha^2))/
+         (S*(N*F-(F+2*alpha^2)^2)+C*alpha^4*(N*F-(F+2)^2)+
+          2*(N*alpha^4-C*S*F*(alpha^2-1)^2))
> gamma.5=-(2*(F+2)+S*gamma.4*(F+2*alpha^2)*(2+C*gamma.2))/
+          (2*N*(2+C*gamma.2))
> gamma.6=-(2*(F+2*alpha^2)+C*gamma.4*(F+2)*(2*alpha^4+S*gamma.3))/
+         (2*N*(2*alpha^4+S*gamma.3))
> A=gamma.1
> B=2*gamma.5+1/(F+2)
> D=2*gamma.6+1/(F+2*alpha^2)
> E=(1/2)*(1/F-gamma.2/(2+C*gamma.2))
> G=(1/2)*(1/F-gamma.3/(alpha^4*(2*alpha^4+S*gamma.3)))
> H=1/F+gamma.4
> I=(1/2)*(1-1/F)
> J=(1/2)*(1/alpha^4-1/F)
> rho.1.seq=seq(0,sqrt(C),length.out=1000)
> rho.2.seq=seq(0,sqrt(S),length.out=1000)
```

```
> rho.1=rep(rho.1.seq,length(rho.2.seq))
> rho.2=rep(rho.2.seq,each=length(rho.1.seq))
> V.rho=N*(A+B*rho.1^2+D*rho.2^2+E*rho.1^4+G*rho.2^4++H*rho.1^2*rho.2^2+
+          I*(floor(rho.1^2)+(rho.1^2-floor(rho.1^2))^2)+J*rho.2^4)
> cbind(rho.1[which(V.rho==max(V.rho))],rho.2[which(V.rho==max(V.rho))])
         [,1]     [,2]
[1,] 1.000850 1.414214
```

The values in the output (`1.000850` and `1.414214`) give the location of the maximum prediction variance among the radii given in the sequences. Note that the cuboidal factors' radius (`rho.1`) is near 1 and the spherical factors' radius (`rho.2`) is at $\sqrt{2} = \alpha$. We then set `rho.1` to be 1 and `rho.2` to be $\sqrt{2}$ and calculated the maximum spherical prediction variance using these values and compared that to the maximum spherical prediction variance found with the above values. The R code and output are below.

```
> rho.1=1
> rho.2=sqrt(S)
> V.rho.new=N*(A+B*rho.1^2+D*rho.2^2+E*rho.1^4+G*rho.2^4++H*rho.1^2*rho.2^2+
+          I*(floor(rho.1^2)+(rho.1^2-floor(rho.1^2))^2)+J*rho.2^4)
> cbind(max(V.rho),V.rho.new)
              V.rho.new
[1,] 21.41100  21.42565
> 100*p/V.rho.new
[1] 70.00953
```

Notice how the maximum spherical prediction variance is larger with the new values of 1 and $\sqrt{2}$. A radius of 1 for the cuboidal factors and $\sqrt{2}$ for the spherical factors indicates that the maximum prediction variance occurs at $(x_1, x_2|z_1, z_2) = (\pm 1, 0| \pm \sqrt{2}, 0)$ or at points determined by permuting the x or z coordinates. This maximum prediction variance location and those found for other cylindrical designs are similar to what is seen in CCDs with cuboidal and spherical regions. Thus, we believe the G-efficiencies given in this research are, in fact, exact.

The last value in the output is the G-efficiency for this particular design. To study G-efficiencies of other designs, change the values of `N.0`, `C`, or `S` in the code and adjust the second set of code to reflect the location of the maximum for the particular design under consideration.

IV-efficiencies

The IV-efficiencies were found in a manner similar to the D- and A-efficiencies. Recall from Equation 5.14 that the average prediction variance involves $g(\underset{\sim}{\theta}^*)$ and $h^*(\rho_z)$. The values in the vectors `h.rho` and `g.theta` in the R code come from Table 5.1. Because the output is similar to what was found for D-efficiencies, we only give the R code that generates the IV-efficiencies.

```
N.0=1
C=0:10
S=0:10
h.rho=c(0,0,3*pi/2,12*pi/5,pi^2,8*pi^2/7,3*pi^3/8,10*pi^3/45,pi^4/10,
        32*pi^4/315,pi^5/48)
g.theta=c(1,1,1,2,pi,4*pi/3,pi^2/2,8*pi^2/15,pi^3/6,16*pi^3/105,pi^4/24)
F=matrix(0,nrow=11,ncol=11)
N=matrix(0,nrow=11,ncol=11)
alpha=matrix(0,nrow=11,ncol=11)
```

```
p=matrix(0,nrow=11,ncol=11)
gamma.1.num=matrix(0,nrow=11,ncol=11)
gamma.1.denom=matrix(0,nrow=11,ncol=11)
gamma.2.num=matrix(0,nrow=11,ncol=11)
gamma.2.denom=matrix(0,nrow=11,ncol=11)
gamma.3.num=matrix(0,nrow=11,ncol=11)
gamma.3.denom=matrix(0,nrow=11,ncol=11)
gamma.4.num=matrix(0,nrow=11,ncol=11)
gamma.4.denom=matrix(0,nrow=11,ncol=11)
gamma.5=matrix(0,nrow=11,ncol=11)
gamma.6=matrix(0,nrow=11,ncol=11)
M=matrix(0,nrow=11,ncol=11)
P=matrix(0,nrow=11,ncol=11)
T=matrix(0,nrow=11,ncol=11)
iv.eff=matrix(0,nrow=11,ncol=11)
for(i in 1:11){
for(j in 1:11){
F[i,j]=2^(C[i]+S[j])
N[i,j]=F[i,j]+2*(C[i]+S[j])+N.0
alpha[i,j]=max(1,sqrt(S[j]))
p[i,j]=1+2*(C[i]+S[j])+choose(C[i],2)+choose(S[j],2)+C[i]*S[j]
gamma.1.num[i,j]=(2*alpha[i,j]^4+S[j]*F[i,j]+C[i]*F[i,j]*alpha[i,j]^4)
gamma.1.denom[i,j]=(2*N[i,j]*alpha[i,j]^4+N[i,j]*F[i,j]*S[j]+
                   C[i]*N[i,j]*F[i,j]*alpha[i,j]^4-C[i]*alpha[i,j]^4*
                   (F[i,j]+2)^2-S[j]*(F[i,j]+2*alpha[i,j]^2)^2-
                   2*C[i]*S[j]*F[i,j]*(alpha[i,j]^2-1)^2)
```

```
gamma.2.num[i,j]=(2*alpha[i,j]^4*(N[i,j]*F[i,j]-(F[i,j]+2)^2)-
                  4*S[j]*F[i,j]*(alpha[i,j]^2-1)^2)
gamma.2.denom[i,j]=(2*N[i,j]*alpha[i,j]^4+S[j]*N[i,j]*F[i,j]-S[j]*(F[i,j]+
                    2*alpha[i,j]^2)^2)
gamma.3.num[i,j]=(2*N[i,j]*(N[i,j]*F[i,j]-(F[i,j]+2*alpha[i,j]^2)^2)-
                  4*C[i]*N[i,j]*F[i,j]*(alpha[i,j]^2-1)^2)
gamma.3.denom[i,j]=(N[i,j]*(2*N[i,j]+C[i]*N[i,j]*F[i,j]-C[i]*(F[i,j]+2)^2))
gamma.4.num[i,j]=((F[i,j]+2)*(F[i,j]+2*alpha[i,j]^2)-N[i,j]*F[i,j])
gamma.4.denom[i,j]=(S[j]*(N[i,j]*F[i,j]-(F[i,j]+2*alpha[i,j]^2)^2)+
                    C[i]*alpha[i,j]^4*(N[i,j]*F[i,j]-(F[i,j]+2)^2)+
                    2*(N[i,j]*alpha[i,j]^4-
                    C[i]*S[j]*F[i,j]*(alpha[i,j]^2-1)^2))
gamma.1=gamma.1.num/gamma.1.denom
gamma.2=gamma.2.num/gamma.2.denom
gamma.3=gamma.3.num/gamma.3.denom
gamma.4=gamma.4.num/gamma.4.denom
gamma.5[i,j]=-(2*(F[i,j]+2)+S[j]*gamma.4[i,j]*(F[i,j]+
               2*alpha[i,j]^2)*(2+C[i]*gamma.2[i,j]))/
              (N[i,j]*(2+C[i]*gamma.2[i,j]))/2
gamma.6[i,j]=-(2*(F[i,j]+2*alpha[i,j]^2)+C[i]*gamma.4[i,j]*(F[i,j]+2)*
              (2*alpha[i,j]^4+S[j]*gamma.3[i,j]))/(N[i,j]*(2*alpha[i,j]^4+
               S[j]*gamma.3[i,j]))/2
K=gamma.1
L=2*gamma.5+1/(F+2)
M[i,]=1/F[i,]-gamma.2[i,]/(2+C[i]*gamma.2[i,])
P[i,]=(1/2)*(1-gamma.2[i,]/(2+C[i]*gamma.2[i,]))
```

```
Q=(1/F)+gamma.4

R=2*gamma.6+1/(F+2*alpha^2)

T[,j]=(1/2)*(1/F[,j]-gamma.3[,j]/(alpha[,j]^4*(2*alpha[,j]^4+
       S[j]*gamma.3[,j])))

U=(1/2)*(1/alpha^4-1/F)

iv.eff[i,j]=N[i,j]*(K[i,j]+L[i,j]*C[i]/3+M[i,j]*choose(C[i],2)/9+P[i,j]*
                    C[i]/5+
                    (gamma(S[j]/2+1)/(S[j]^(S[j]/2)*pi^(S[j]/2)))*
                    (2*pi*g.theta[j]*((Q[i,j]*C[i]/3+R[i,j])*
                    S[j]^((S[j]+2)/2)/(S[j]+2)+
                    T[i,j]*S[j]^((S[j]+4)/2)/(S[j]+4))+
                    U[i,j]*S[j]^((S[j]+4)/2)/(S[j]+4)*h.rho[j]))
}
}
colnames(iv.eff)=0:10
rownames(iv.eff)=0:10
round(iv.eff,2)
```

APPENDIX B

R CODE FOR CONTOUR PLOTS OF MAXIMUM SPHERICAL PREDICTION VARIANCE

The R code for the contour plots of maximum spherical prediction variance is similar to the R code for G-efficiencies. However, instead of making all possible combinations of the two radii, we provide the appropriate sequence of numbers for each radius and create a matrix of average prediction variance values for each pair of radii. The R function `contour` requires the following arguments: each radius, the matrix of average prediction variance, and any desired graphical parameters. The example given is for a cylindrical design with 1 cuboidal factor, 4 spherical factors, and 3 center points, shown in Figure 4.3. To create similar contour plots for other cylindrical designs, change the values in first 4 lines of the R code below.

```
# 1 cuboidal and 4 spherical
N.0=1
C=1
S=4
F=2^(C+S-1)
N=F+2*(C+S)+N.0
alpha=max(1,sqrt(S))
p=1+2*(C+S)+choose(C,2)+choose(S,2)+C*S
gamma.1=(2*alpha^4+S*F+C*F*alpha^4)/(2*N*alpha^4+N*F*S+C*N*F*alpha^4-
        C*alpha^4*(F+2)^2-S*(F+2*alpha^2)^2-2*C*S*F*(alpha^2-1)^2)
gamma.2=(2*alpha^4*(N*F-(F+2)^2)-4*S*F*(alpha^2-1)^2)/
        (2*N*alpha^4+S*N*F-S*(F+2*alpha^2)^2)
gamma.3=(2*(N*F-(F+2*alpha^2)^2)-4*C*F*(alpha^2-1)^2)/
        (2*N+C*N*F-C*(F+2)^2)
gamma.4=-(N*F-(F+2)*(F+2*alpha^2))/
        (S*(N*F-(F+2*alpha^2)^2)+C*alpha^4*(N*F-(F+2)^2)+
```

```
         2*(N*alpha^4-C*S*F*(alpha^2-1)^2))
gamma.5=-(2*(F+2)+S*gamma.4*(F+2*alpha^2)*(2+C*gamma.2))/
         (2*N*(2+C*gamma.2))
gamma.6=-(2*(F+2*alpha^2)+C*gamma.4*(F+2)*(2*alpha^4+S*gamma.3))/
        (2*N*(2*alpha^4+S*gamma.3))
A=gamma.1
B=2*gamma.5+1/(F+2)
D=2*gamma.6+1/(F+2*alpha^2)
E=(1/2)*(1/F-gamma.2/(2+C*gamma.2))
G=(1/2)*(1/F-gamma.3/(alpha^4*(2*alpha^4+S*gamma.3)))
H=1/F+gamma.4
I=(1/2)*(1-1/F)
J=(1/2)*(1/alpha^4-1/F)
rho.1.seq=seq(0,sqrt(C),length.out=100)
rho.2.seq=seq(0,sqrt(S),length.out=100)
V.rho=matrix(0,ncol=100,nrow=100)
for(i in 1:100){
for(j in 1:100){
V.rho[i,j]=N*(A+B*rho.1.seq[i]^2+D*rho.2.seq[j]^2+E*rho.1.seq[i]^4+
              G*rho.2.seq[j]^4+H*rho.1.seq[i]^2*rho.2.seq[j]^2+
              I*(floor(rho.1.seq[i]^2)+(rho.1.seq[i]^2-
              floor(rho.1.seq[i]^2))^2)+J*rho.2.seq[j]^4)
}
}
contour(rho.1.seq,rho.2.seq,V.rho,xlab=expression(rho[x]),
        ylab=expression(rho[z]),main="1 Cuboidal, 4 Spherical")
```