Recommendations for Design Parameters for Central Composite Designs with Restricted Randomization

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ABSTRACT

In response surface methodology, the central composite design is the most popular choice for fitting a second order model. The choice of the distance for the axial runs, α, in a central composite design is very crucial to the performance of the design. In the literature, there are plenty of discussions and recommendations for the choice of α, among which a rotatable α and an orthogonal blocking α receive the greatest attention. Box and Hunter (1957) discuss and calculate the values for α that achieve rotatability, which is a way to stabilize prediction variance of the design. They also give the values for α that make the design orthogonally blocked, where the estimates of the model coefficients remain the same even when the block effects are added to the model. In the last ten years, people have begun to realize the importance of a split-plot structure in industrial experiments. Constructing response surface designs with a split-plot structure is a hot research area now. In this dissertation, Box and Hunters' choice of α for rotatablity and orthogonal blocking is extended to central composite designs with a split-plot structure. By assigning different values to the axial run distances of the whole plot factors and the subplot factors, we propose two-strata rotatable split-plot central composite designs and orthogonally blocked split-plot central composite designs. Since the construction of the two-strata rotatable split-plot central composite design involves an unknown variance components ratio d, we further study the robustness of the two-strata rotatability on d through simulation. Our goal is to provide practical recommendations for the value of the design parameter α based on the philosophy of traditional response surface methodology.

Dedication

To my beloved parents Yunguang Wang and Junli Chen.

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Chapter 1

Introduction

Box and Wilson (1951) lay the basic foundations for response surface methodology (RSM), which is an integration of experimental design, regression, and optimization theory. RSM is widely used to explore and to optimize response surfaces in industrial experiments. For many industrial experiments, the response can be obtained immediately. The results from small exploratory experiments can then be used as a guide to more complicated or larger follow-up experiments. In RSM, it is common to begin with a screening experiment to identify important factors or variables. Follow-up experiments seek to improve the performance of the response. Therefore, knowledge of the whole experimental system increases. It is a dynamic, continuous learning process instead of a one-shot static strategy, hence, the "sequential" nature of RSM. For more details on RSM, see Myers and Montgomery (2002) and Khuri and Cornell (1996).

The goal of RSM is to find a parametric model for response prediction over the given experimental region. RSM uses first and second order Taylor series approximations and regression techniques to describe the relationship between the response of interest and the quantitative factors. The different orders of models lead to different response surface designs with different properties. Among first order designs, full factorial and fractional factorial designs are used extensively in preliminary experiments to identify potentially important factors. For the second order case, the class of central composite designs (CCD) is the most popular. Box and Wilson (1951) defined the CCD as a set of two-level factorial or Resolution V fractional factorial points together with another set of $2k$ axial points and n_c center runs. The distance of the axial runs from the center is defined as α. The choice of α is crucial to the performance of the design. Box and Hunter (1957) discuss the choice of α extensively for the CCD when the runs are completely randomized. They derive the conditions required to make a design "rotatable". A rotatable design ensures that the quality of the prediction is a function of the distance, ρ, from the design center. Therefore, since the location for prediction within the design space is unknown, equally good predicted values will be obtained for points that are the same distance from the design center in any direction.

When all experimental runs can not be performed under homogeneous conditions, blocks are often constructed to increase the power for testing the treatment effects. However, the estimation of the polynomial effects are often influenced by the block effect. Orthogonal blocking provides the same estimator of the polynomial effects as the one that would be obtained by ignoring the blocks. Box and Hunter (1957) discuss the orthogonal blocking strategy for second order rotatable designs. They provide a catalog of orthogonally blocked CCDs based on their condition, which depends on the choice of the α and the number of center runs within each block. Khuri (1992) provides the matrix notation for the orthogonal blocking condition of a completely randomized design. Currently, most software packages and many practitioners still use rotatability and orthogonal blocking as guidelines for the choice of α.

Often times industrial experiments involve factors that separate into two classes: hard-to-change (HTC) and easy-to-change (ETC) factors. HTC factors are those factors that are difficult, time consuming, and costly to manipulate. ETC factors are relatively easy to manipulate. To minimize cost, practitioners fix the levels of the HTC factors and then run partial or complete combinations of the ETC factors levels, which leads to a split-plot experiment. In this split-plot experiment, each experimental unit (EU) for the HTC factors is divided into the experiment units for the ETC factors. The experiment unit for the hard-to-change factors is called the whole plot (WP), and the experiment unit for the easy-to-change factors is called the subplot (SP). The hard-to-change factors are also referred as WP factors and the easy-to-change factors are referred as SP factors. The split-plot experiment leads to two randomization procedures and two random error terms. First, the hard-to-change factors are randomly assigned to the whole plots, leading to the whole plot error term, σ_δ^2. Secondly within each whole plot, the easy-to-change factors are randomly assigned to subplots, leading to the subplot error term, σ^2.

Only recently have researchers begun to consider the impacts of split-plot structure on response surface designs. Most of the recent work has been done for first-order split-plot designs. More work is needed to extend split-plot analysis techniques to second-order industrial experiments (Myers *et al*, 2004). Box and Hunter (1957) discussed the rotatable design, the choice of α, and the orthogonal blocking strategy for the completely randomized second-order design case. We extend their results to split-plot second-order designs, especially the CCD. We intend to explore more fully the impact of a split-plot structure on traditional central composite designs and to make concrete and practical recommendations on the choice of α for both WP factors and SP factors.

The rest of the dissertation is organized as follows. In Chapter 2, we will review the work currently done in response surface designs, especially the research done by Box and Hunter (1957), and the research done in split-plot response surface designs, especially the work done by Vining, Kowalski and Montgomery (2005). In Chapter 3, we will study the impact of different variance components on the prediction variance for split-plot central composite designs. Since the rotatability condition can not be achieved in these designs, we propose two-strata rotatable split-plot central composite designs, where the prediction variance is a function of the whole plot distance and the subplot distance separately. The construction of the two-strata rotatable split-plot central composite design depends on an unknown variance components ratio d. In Chapter 4, we will study the robustness of proposed two-strata rotatable split-plot central composite design to d. We provide two methods to evaluate the robustness. One is a R^2 like measure to quantify the two-strata rotatability. The other method is graphical using contour plots in both the whole plot space and the subplot space. Simulation results are shown. In Chapter 5, we derive the conditions to achieve orthogonal blocking in split-plot central composite designs. First-order and second-order orthogonally blocked split-plot central composite designs are discussed. Catalogs of α and β for orthogonally blocked split-plot central composite designs are given. In Chapter 6, we will summarize our research on recommending the axial run distances α and β for a split-plot central composite design and close dissertation with a proposal for future research.

Chapter 2

Literature Review

2.1 Response Surface Methodology

Box and Wilson (1951) describe the sequential nature of RSM, which allows us to find the conditions for the "optimum" (better) response step by step. For a k-factor experiment, when the experimental error is small, the experimenter may explore a small sub-region of the whole experimental region adequately with only a few experiments. Based on the results of these experiments, more experiments can be conducted in another sub-region where the response is better. Thus, a "path" can be found from one sub-region to another until it reaches the neighborhood of the optimum. This idea naturally leads to the method of steepest ascent. The method of steepest ascent requires fitting a first order model based on the initial experiment. Let $\hat{y}$ be the predicted value for the response, and let x_i represent the independent factors. The fitted first order response surface model can be written as

$$\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 x_1 + \hat{\beta}_2 x_2 + \cdots + \hat{\beta}_k x_k$$

where $\hat{\beta}_0$ is the intercept estimate and $\hat{\beta}_j$ is the estimate of the unknown coefficient for the j^{th} factor. We seek the points $x_1, x_2, ..., x_k$ for which our response is optimized over all the points that are a fixed distance r from the center. Therefore, we optimize the response through the use of one Lagrange multiplier subject to the constraint $\sum_{j=1}^{k} x_j^2 = r^2$. Let λ be the appropriate Lagrange multiplier, and define the objective function, L, by

$$L(x_1, x_2, \cdots, x_k) = \hat{\beta}_0 + \sum_{j=1}^{k} \hat{\beta}_j x_j + \lambda \left(\sum_{j=1}^{k} x_j^2 - r^2 \right).$$

Setting the partial derivative of L with respect to x_j to 0, the coordinates of x_j along the steepest ascent are given as $x_j = \frac{\hat{\beta}_j}{2\lambda}$. The movement in factor x_j along the path of steepest ascent is proportional to the magnitude of the regression coefficient $\hat{\beta}_j$ with the direction based on the sign of the coefficient. Define a key factor, x_{j^*}. With a one unit increase in the key factor, the change of the other variables is $x_j = \frac{\hat{\beta}_j}{\hat{\beta}_{j^*}} x_{j^*}$. Increasing the key factor unit by unit produces a “path” through the region of interest. When the response ceases to improve, the process is stopped. One disadvantage of this method is that it must assume a strict first order model. When curvature or lack of fit is significant, one might expect little or no success with steepest ascent.

Typically for steepest ascent, practitioners use full factorial and fractional factorial designs in the design phase. These first-order designs have the property of orthogonality. Under appropriate and easily obtained conditions, these designs are the variance optimal designs, which means that they give the smallest variance of the effect estimates. It is readily shown that they are both D-optimal and G-optimal with respect to the alphabetic optimality criteria introduced by Kiefer (1959)

For the second-order case, several other important designs have been proposed. The CCD is the most popular response surface design currently used in industrial experiments.

The CCD is constructed by two sets of points plus n_c center runs. One set is a 2^k or a 2^{k-p} Resolution V fractional factorial design for all factors. The other set is the $2k$ axial runs for each factor with a distance of α from the center. The two axial runs for each x_j are of the form: $(0, 0, \cdots, 0, \alpha, 0, \cdots, 0)$ and $(0, 0, \cdots, 0, -\alpha, 0, \cdots, 0)$, where the j^{th} place is not 0. The CCD can be constructed sequentially with the second set of runs if the analysis of the data from the first set indicates the presence of significant curvature. The CCD was proposed as a more economical alternative to a 3^k design. Each factor has either three or five levels, and α can be adjusted to fit either a cuboidal or a spherical design region. The choice of α is discussed in the literature in great detail.

Myers and Montgomery (2002) discuss three basic choices for α: spherical, face-centered cube, and rotatable. The spherical choice for α is $\sqrt{k}$, which places all of the runs, other than the center runs, on the surface of the sphere defined by the factorial points. When the experimental region is spherical, the spherical choice of α makes the CCD the most D-efficient. The face-centered cube (FCC), $\alpha = 1$, places all of the runs, other than the center runs, on the surface of the cube defined by the factorial runs. This choice of α is typically the most D-efficient one for cuboidal regions. The rotatable choice of α is $\sqrt[4]{F}$, where F is the number of factorial runs in CCD. Box and Hunter (1957) derive the general condition to achieve rotatability. When this α is chosen, all the points at the same radial distance from the center have the same magnitude of prediction variance.

Box and Hunter (1957) use the properties of derived power and product vectors and *Schläflian* matrices to ensure all the points on a hyper-sphere have the same prediction variance. They establish that the first-order rotatable design has the moment matrix $N^{-1}\boldsymbol{X}'\boldsymbol{X} = \boldsymbol{I}_{k+1}$, which is the exactly the same moment matrix of the design that minimizes the variance of coefficients β_is. Therefore a first-order rotatable design is also a "best" design in the sense of estimation. Rotatable designs include such popular designs as fractional factorial, full factorial, etc.

Let the design matrix, $\boldsymbol{D}$, be defined by

$$\boldsymbol{D} = \begin{bmatrix} x_{11} & x_{12} & \cdots & x_{1k} \\ x_{21} & x_{22} & \cdots & x_{2k} \\ \vdots & \vdots & \vdots & \vdots \\ x_{N1} & x_{N2} & \cdots & x_{Nk} \end{bmatrix}.$$

Define the design moments as

$$\begin{aligned} [i] &= N^{-1} \sum_{u=1}^{N} x_{ui} \\ [ii] &= N^{-1} \sum_{u=1}^{N} x_{ui}^2 \\ [ij] &= N^{-1} \sum_{u=1}^{N} x_{ui} x_{uj} \\ [iii] &= N^{-1} \sum_{u=1}^{N} x_{ui}^3 \\ [iiii] &= N^{-1} \sum_{u=1}^{N} x_{ui}^4 \\ [iijj] &= N^{-1} \sum_{u=1}^{N} x_{ui}^2 x_{uj}^2 \\ & etc. \end{aligned}$$

A second order design is rotatable if

$$
\begin{aligned}
[ii] =& \lambda_2 \\
[iiii] =& 3[iijj] = 3\lambda_4 \\
[i] = [ij] = [iij] = [iii] = [ijj] =& [ijk] = [ijjj] = [iijk] = [ijkl] = 0,
\end{aligned} \tag{2.1}
$$

which means that all odd moments up to order four are zero, all pure second order moments are the same, and $[iiii] = 3[iijj]$.

Box and Hunter (1957) find that no single equiradial set of points can provide a rotatable design of order greater than 1, because the resulting moment matrix will be singular and the quadratic coefficients and the intercept term can not be estimated separately. By considering different sets of points with different radii from the center, they construct classes of two-dimensional second order designs. Hexagonal designs with center points, pentagonal designs with center points, and designs with two rings of points are the most well-known designs from this class. It is easy to find the conditions for a rotatable CCD based on Equation 2.1. For any factor x_i in a central composite design, the moment $[ii] = F + 2\alpha^2$, $[iiii] = F + 2\alpha^4$ and $[iijj] = F$, where F is the number of factorial runs in the design. To make a CCD rotatable, we need to have $[iiii] = 3[iijj]$, which leads to

$$
\begin{aligned}
[iiii] &= 3[iijj] \\
F + 2\alpha^4 &= 3F \\
2\alpha^4 &= 2F \\
\alpha &= \sqrt[4]{F}.
\end{aligned}
$$

When a design's moments can not conform to the rotatable conditions in Equation 2.1, the design is said to be non-rotatable. Quite often the non-rotatable design's prediction variance surface will be near spherical. In this case, the design can be called near rotatable. It can be caused when the rotatable design setting is incorrectly calculated or executed. To evaluate the rotatability of the non-rotatable design, Khuri (1988) and Draper and Pulkesheim (1990) develop different numerical measures to evaluate "how rotatable" a design is. Khuri's measure is invariant to the coding scheme and is a function of the levels of the independent variables in the design. Draper and Pulkesheim's measure is invariant to rotation.

The main idea of Khuri (1988) is to compare the standardized scale free moments of the non-rotatable design $\boldsymbol{D}$ with those of a rotatable design $\boldsymbol{R}$ of the same number of design runs, and to determine how well the moments in $\boldsymbol{D}$ can be approximated by the moments in $\boldsymbol{R}$. A measure based on the difference between the moments of these two designs is developed. An assumption in this measure is that the non-rotatable design's odd moments are zero. The difference can be written as $Q_n(D) = \|u^*(\boldsymbol{Z'Z}) - \sum_{m=2}^{d} \kappa_{2m}\omega_{2m}\|^2$, where $u^*(\boldsymbol{Z'Z})$ is the vector containing all moments except those of order 0 and 2 in the non-rotatable design and $\sum_{m=2}^{d} \kappa_{2m}\omega_{2m}$ is the vector containing all moments except those of order 0 and 2 in a rotatable design, and $\|\cdot\|$ is the Euclidean norm. The measure is defined as

$$\begin{aligned}\Phi_n(D) &= 100\left(\frac{\|u^*(\boldsymbol{Z'Z})\|^2 - min[Q_n(D)]}{\|u^*(\boldsymbol{Z'Z})\|^2}\right)\\ &= 100\left(\frac{\sum_{m=2}^{d}[u^*(\boldsymbol{Z'Z})\omega_{2m}]^2\|\omega_{2m}\|^2}{\|u^*(\boldsymbol{Z'Z})\|^2}\right).\end{aligned}$$

If a design is rotatable, $min[Q_n(D)] = 0$ and $\Phi_n(D) = 100$. A larger value for $\Phi_n(D)$ is therefore an indication that the design $\boldsymbol{D}$ is near rotatable.

Draper and Pukelsheim (1990) develop another rotatability measure Q^* using a similar idea. They mainly discuss it in the second-order case and they claim that it can be easily extended to higher order cases. They also compare the non-rotatable design's higher order even moments with a rotatable design's higher order even moments. Instead of using a vector of moments, they use the moment matrix $\boldsymbol{V}$. For a second-order rotatable design, $\boldsymbol{V} = \boldsymbol{V}_0 + \lambda_2(3k)^{1/2}\boldsymbol{V}_2 + \lambda_4(3k(k+2))^{1/2}\boldsymbol{V}_4$, where $\boldsymbol{V}_0$ is a matrix containing moments of order 0 only, $\boldsymbol{V}_2$ is a matrix containing moments of order 2 only, $\boldsymbol{V}_4$ is a matrix containing moments of order 4 only, $\lambda_2 = [ii]$, and $\lambda_4 = [iijj]$. For an arbitrary design with moment matrix $\boldsymbol{A}$, they average $\boldsymbol{A}$ over all possible rotations in the $\boldsymbol{x}$ space to get $\bar{\boldsymbol{A}} = \boldsymbol{V}_0 + tr(\boldsymbol{A}\boldsymbol{V}_2)\boldsymbol{V}_2 + tr(\boldsymbol{A}\boldsymbol{V}_4)\boldsymbol{V}_4$. Notice that the form of $\bar{\boldsymbol{A}}$ is quite similar to the $\boldsymbol{V}$ in a rotatable design. Therefore they call $\bar{\boldsymbol{A}}$ the *rotatable component* of $\boldsymbol{A}$ and define 2 measures. The first one is $Q^* = \|\bar{\boldsymbol{A}} - \boldsymbol{V}_0\|^2/\|\boldsymbol{A} - \boldsymbol{V}_0\|^2$. The idea of Q^* is similar to $\Phi(D)$ from Khuri. It measures the proportion of rotatability explained by the rotation component and when the design is rotatable, $Q^* = 1$. The second measure is the distance between $\boldsymbol{A}$ and $\bar{\boldsymbol{A}}$, $\delta = \|\boldsymbol{A} - \bar{\boldsymbol{A}}\| = [tr(\boldsymbol{A} - \bar{\boldsymbol{A}})^2]^{1/2}$.

All measures from Khuri (1988) and Draper and Pukelsheim (1990) are based on the even moments of order 2 or higher of the design and use the Euclidean norm. Khuri uses the norm for a vector and Draper uses it for a matrix. Both measures are of the form of a ratio. The numerator is the part explained by the rotatable component. The denominator is the norm of the higher order moments of the arbitrary design. The idea of both measures is similar to R^2 in regression. By "regressing" the moments in a non-rotatable design against the moments in a rotatable design, we can say the design is R^2% rotatable. Their measures are both based on a *rotatable component* from a rotatable design, whose vector and matrix form is derived from the rotatable condition given in Box and Hunter (1957), $[iiii] = 3[iijj]$.

There are times when conducting an experimental design that all of the experimental runs can not be performed under homogenous conditions. For example, the yield of a chemical process may depend on the batch of raw material used since different batches can have different impacts on the yield. To control this extraneous source of variation, the experimental runs can be arranged into blocks so that the experimental runs within each block are more homogenous. The batch is considered a block variable. However, the estimation of the experimental factor effects can be influenced by this blocking effect. A desired blocking strategy is to minimize the blocking effect on the model coefficients. In traditional response surface designs, orthogonal blocking is discussed in great detail in the literature. Orthogonal blocking allows for the same estimate of the model coefficients as the one that would have been obtained by ignoring the blocks.

Box and Hunter (1957) algebraically develop the condition for orthogonal blocking. Khuri (1992) uses matrix notation to derive the same conditions for a general block design. Consider the model

$$y = \mu \mathbf{1}_n + \bar{\boldsymbol{Z}}\gamma + \tilde{\boldsymbol{X}}\tilde{\boldsymbol{\beta}}$$

where $\bar{\boldsymbol{Z}} = (\boldsymbol{I}_n - n^{-1}\mathbf{1}_n\mathbf{1}_n')\boldsymbol{Z}$, $\boldsymbol{Z}$ is the block effect matrix, and $\tilde{\boldsymbol{X}}$ is the model matrix without block effects and intercept terms. If the design is orthogonal, then $\bar{\boldsymbol{Z}}'\tilde{\boldsymbol{X}} = \mathbf{0}$. This leads to

$$\begin{aligned}
\bar{\boldsymbol{Z}}'\tilde{\boldsymbol{X}} &= \boldsymbol{Z}'(\boldsymbol{I}_n - n^{-1}\mathbf{1}_n\mathbf{1}_n')'\tilde{\boldsymbol{X}} \\
&= \boldsymbol{Z}'(\tilde{\boldsymbol{X}} - n^{-1}\mathbf{1}_n\mathbf{1}_n'\tilde{\boldsymbol{X}}) \\
&= \boldsymbol{Z}'\tilde{\boldsymbol{X}} - n^{-1}\boldsymbol{Z}'\mathbf{1}_n\mathbf{1}_n'\tilde{\boldsymbol{X}} \\
&= \begin{pmatrix} \mathbf{1}_{k_1}'\tilde{\boldsymbol{X}}_1 \\ \mathbf{1}_{k_2}'\tilde{\boldsymbol{X}}_2 \\ \vdots \\ \mathbf{1}_{k_b}'\tilde{\boldsymbol{X}}_b \end{pmatrix} - \frac{1}{n}\begin{pmatrix} k_1 \\ k_2 \\ \vdots \\ k_b \end{pmatrix}\mathbf{1}_n'\tilde{\boldsymbol{X}}
\end{aligned} \tag{2.2}$$

and the condition for orthogonal blocking becomes

$$\frac{1}{k_i}\tilde{\boldsymbol{X}}_i'\mathbf{1}_{k_i} = \frac{1}{n}\tilde{\boldsymbol{X}}'\mathbf{1}_n.$$

In other words, for any given factor effect, in the model matrix, its average value is the same within each block, and equal to its overall average.

The average of the interaction effects in $\tilde{\boldsymbol{X}}$ is $\sum_{u=1}^{N} x_{ui}x_{uj}/N = [ij]$ and the average of the quadratic effects in $\tilde{\boldsymbol{X}}$ is $\sum_{u=1}^{N} x_{ui}^2/N$. Since a second-order rotatable design has $[ij] = 0$, then the conditions for an orthogonal blocked second-order rotatable design becomes

1. the sum of products of $x_1, x_2, \ldots, x_k$ are zero within each block

2. $\sum_{u=1}^{k_i} x_{ui}^2/k_i = \sum_{u=1}^{N} x_{ui}^2/N$

which are the conditions derived from Box and Hunter (1957). For most experiments, exact rotatability and orthogonal blocking can not be satisfied simultaneously. We can consider the construction of orthogonal blocked designs that are either rotatable or "near rotatable".

Box and Hunter (1957) also provide one strategy to achieve orthogonal blocking in a CCD. They treat a CCD as having two main blocks: one block of factorial runs and one with the axial runs. Based on the above theorem and conditions, an orthogonally blocked CCD can be constructed by adding center runs into the blocks of factorial runs and axial runs. Let n_{c0} be the number of center runs in the blocks of factorial runs, n_a be the number of axial runs in the blocks of axial runs and n_{a0} be the number of center runs in the blocks of axial runs. To achieve both rotatability and orthogonal blocking, we need

$$\frac{F^{1/2}}{2} = \frac{F + n_{c0}}{n_a + n_{a0}}.$$

For example, when we have 4 factors, the above condition becomes

$$2 = \frac{16 + n_{c0}}{8 + n_{a0}}$$

and choosing n_{c0}=4 and $n_{a0} = 2$ satisfies the condition.

Box and Draper (1975) discuss 14 criteria of the "goodness of a response surface design":

1. Ensure the difference between predicted response and the observed response is as small as possible.

2. Have ability to test lack of fit.

3. Allow experiments to be performed in blocks.

4. Allow design to be built up sequentially.

5. Provide for "pure error" estimation.

6. Be sensitive to outliers.

7. Require a minimum number of design points.
8. Provide a check on the homogeneous variance assumption.
9. Be robust to errors in the control of design levels.
10. Provide a good distribution of $Var(\hat{y}(x))/\sigma^2$.
11. Give a satisfactory distribution of information throughout the region of interest.
12. Allow transformations to be estimated.
13. Provide simple data patterns that allow ready visual appreciation.
14. Ensure simplicity of calculation.

As one can readily see, not all of the 14 points can be satisfied simultaneously, and users need the ability to choose a design with enough good properties to satisfy the special needs of the situation. They point out that a statistician must have the ability to make "sensible subjective compromises" between the competing criteria in the design construction process. Among these criteria, Numbers 2, 5, 6 and 10 are very important. Box and Draper discuss Number 6, the criteria of robustness, in great detail. To find a design that is robust to the outliers in the data, they try to minimize the measure of the discrepancy

$$V = c^4(r - p^2/n)/n$$

where c is added to the u^{th} response to make it an outlier, p is the number of parameters in the model, n is the the size of the design and r is the sum of the square of the diagonal elements in $\boldsymbol{X}(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{X}'$. For CCDs, the number of center runs and the value of α to minimize V are tabulated. From their table, for k=2, 4, and 8, the "best" number of center runs is 2, and the corresponding α is equal to the rotatable α. In other cases, the robust α is not equal to the rotatable α. Also, in terms of robustness the recommendation for center runs is either one or two.

Many other researchers have studied and recommended values for α by constructing and comparing designs using the determinant of $\boldsymbol{X}'\boldsymbol{X}$. Under the $|\boldsymbol{X}'\boldsymbol{X}|$ criterion, the resulting design tends to favor the points on the boundary. Box and Draper (1971) show that for a CCD with all explanatory variables held within $[-1, 1]$, the design that maximize $|\boldsymbol{X}'\boldsymbol{X}|$ is the one with $\alpha = 1$, a FCC. Lucas (1974) further compares different CCDs using the $|\boldsymbol{X}'\boldsymbol{X}|$ criterion. For a CCD design using a 2^{k-p} Resolution V fractional factorial design and n_c center runs, the determinant can be written as

$$|\boldsymbol{X}'\boldsymbol{X}| = (2^{k-p} + 2\alpha^2)^k (2\alpha^4)^{k-1} (2^{k-p})^{\binom{k}{2}} \cdot [2^{k-p+1}(\alpha^2 - k)^2 + 2n_c\alpha^4 + kn_c 2^{k-p}]$$

which is obtained by reducing the $\boldsymbol{X}'\boldsymbol{X}$ matrix using the identity

$$\begin{vmatrix} \boldsymbol{A}_{11} & \boldsymbol{A}_{12} \\ \boldsymbol{A}_{21} & \boldsymbol{A}_{22} \end{vmatrix} = |\boldsymbol{A}_{11}| \cdot |\boldsymbol{A}_{22} - \boldsymbol{A}_{21}\boldsymbol{A}_{11}^{-1}\boldsymbol{A}_{12}|.$$

In a traditional CCD, $\boldsymbol{A}_{11}$ is of the form

$$\begin{pmatrix} A & B\mathbf{1}' \\ B\mathbf{1} & (G - D)\boldsymbol{I} + D\boldsymbol{J} \end{pmatrix}$$

where $A = N = 2^{k-p} + 2k + n_c$, $B = 2^{k-p} + 2\alpha^2$, $G = 2^{k-p}$ and $D = 2^{k-p} + 2\alpha^4$.

When $n_c \geq 1$, the determinant is an increasing function of α. Lucas (1974) and Box and Draper (1971) show that it is better to increase the space contained in the experimental region rather than to increase α. This is because the magnitude gained in $|\boldsymbol{X}'\boldsymbol{X}|$ is always larger due to a proportion π increase in the size of the space contained in the experimental region rather than a proportion increase in the size of α. Consequently, for an optimum CCD, the fractional factorial part should be on the largest hypercube that will fit inside the experimental region. When the CCD is restricted to a hypercube, the optimum axial run distance is $\alpha = 1$. When the CCD is on a spherical region with radius $\sqrt{k}$, the optimum axial run distance is $\alpha = \sqrt{k}$. It can be shown that when $k \leq 5$, the D-efficiency of the optimal CCD is at least 0.9 and when k becomes larger than 11, the D-efficiency decreases to 0.83. Therefore, the optimum CCD is very comparable to D-optimum designs. In addition, the optimum CCD has lots of the other advantages mentioned in Box and Draper (1975) over the D-optimum design.

As an alternative to the CCD, Box and Behnken (1960) introduced a three-level design called the Box-Behnken Design (BBD). The design is constructed by combining a balanced incomplete block design (BIBD) and a two-level factorial design. All the points except center runs are at a distance of either $\sqrt{2}$ or $\sqrt{3}$ from the center. Consequently, BBD works better in a spherical design region than in a cuboidal design region. When $k = 4$ and $k = 7$, the BBD is exactly rotatable based on Box and Hunter (1957)'s condition.

2.2 Split-Plot Response Surface Designs

In a split-plot industrial experiment, we have hard-to-change factors and easy-to-change factors. As an example, Kowalski, Borror and Montgomery (2005) describe a five factor experiment that examines the image quality of a printing process. The factors are blanket type, paper type, cylinder gap, ink flow and press speed. Since changing the cylinder gap, ink flow and press speed only requires a modification on the control panel without stopping the machine, they are ETC/SP factors. On the other hand, changing the blanket type and/or paper type requires stopping the machine and then manually changing the types of blanket and/or paper. Thus, these two factors are HTC/WP factors. To save money, a split-plot design is used instead of a completely randomized design.

Consider a split plot design with m whole plots each with n_i subplots. Thus we have $N = \sum_{i=1}^{m} n_i$ observations. The general model form is:

$$\boldsymbol{y} = \boldsymbol{X\beta} + \boldsymbol{M\gamma} + \boldsymbol{\epsilon}$$

where $\boldsymbol{y}$ is the $N \times 1$ vector of responses, $\boldsymbol{X}$ is the $N \times p$ design matrix, $\boldsymbol{\beta}$ is the $p \times 1$ parameter vector associated with the p effects in the design, $\boldsymbol{M}$ is the $N \times m$ index matrix consisting of zeros and ones assigning the individual observations to the whole plots, $\boldsymbol{\gamma}$ is the $m \times 1$ vector of whole plot errors, and $\boldsymbol{\epsilon}$ is the $N \times 1$ vector of subplot errors. If we group the observations by different whole plots, then $\boldsymbol{M} = Diag(\boldsymbol{1}_{n_1}, \boldsymbol{1}_{n_2}, ..., \boldsymbol{1}_{n_m})$, where $\boldsymbol{1}_{n_i}$ is a $n_i \times 1$ vector of 1's. Assume that

$$E(\boldsymbol{\gamma}) = \boldsymbol{0}_m, \qquad Cov(\boldsymbol{\gamma}) = \sigma_\delta^2 \boldsymbol{I}_m$$

$$E(\boldsymbol{\epsilon}) = \boldsymbol{0}_N, \qquad Cov(\boldsymbol{\epsilon}) = \sigma^2 \boldsymbol{I}_N$$

$$Cov(\boldsymbol{\gamma}, \boldsymbol{\epsilon}) = \boldsymbol{0}_{m \times N},$$

then the resulting variance-covariance matrix for the observation vector $\boldsymbol{y}$ is:

$$Var(\boldsymbol{y}) = \boldsymbol{\Sigma} = \sigma^2 \boldsymbol{I} + \sigma_\delta^2 \boldsymbol{MM}'$$

where $\boldsymbol{MM}'$ is a block diagonal matrix with diagonal matrices of $\boldsymbol{J}_{n_1}, \boldsymbol{J}_{n_2}, ..., \boldsymbol{J}_{n_m}$ and $\boldsymbol{J}_{n_i}$ is a $n_i \times n_i$ matrix of 1's. The ordinary least square (OLS) estimator of $\boldsymbol{\beta}$ is defined as $(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{X}'\boldsymbol{y}$ and the generalized least square (GLS) estimator of $\boldsymbol{\beta}$ is defined as $(\boldsymbol{X}'\boldsymbol{\Sigma}^{-1}\boldsymbol{X})^{-1}\boldsymbol{X}'\boldsymbol{\Sigma}^{-1}\boldsymbol{y}$. For later use, we can define the unknown variance component ratio as,

$$d = \frac{\sigma_\delta^2}{\sigma^2}.$$

Two popular choices of split-plot designs are the two-level minimum aberration fractional factorial split plot designs (MAFFSPD) and D-optimal split-plot designs. MAFFSPD is constructed by minimizing the word length pattern in the defining contrast. Since the effects in the defining contrast involve both WP factors and SP factors, the alias structure is more complicated than the completely randomized case. Huang, Chen and Voelkel (1998) propose two methods of constructing MAFFSPD. The first one constructs a FFSP based on the known table of MA FF designs by Franklin (1984) or by a computer generated MA FF designs. The first method can be hand calculated, but it may not contain all possible MA FFSP designs for a fixed number of whole plot factors and subplot factors. The other method uses a linear integer programming to search over all minimum aberration designs with no priority of MA or near MA in the whole plot designs. Their paper gives a catalog of designs. Another construction approach is done by Bingham and Sitter (1999a) with the theoretical background found in Bingham and Sitter (1999b). They propose three different methods to construct a MA FFSP: a search table approach (Franklin and Bailey 1975); a sequential approach suggested by Chen et al. (1993); and a new method-combined approach, which takes advantage of the two previous approaches. They focus on the non-isomorphic FFSPs, and their catalog is more complete than Huang, Chen and Voelkel's (1998). Bingham and Sitter (2001) discuss the criteria to be considered when choosing a "best" MAFFSPD. Bisgaard (2000) discussed the partial alias structure in a fractional factorial split-plot design. He gave the rules for the partial alias structure for WP factors and SP factors. Theoretically the combination of minimum aberration fractional factorial designs and a split-plot structure seems reasonable. However, the application of the MAFFSPD is not always satisfactory. Some criticisms are that the MA criterion is based on the smallest word of the overall defining contrast group and is an overall resolution criterion instead of a partial criterion. The designs generated tend to have a large number of whole plots with a small number of subplots, which conflicts with the idea of having HTC factors and tends to be too costly.

D-optimal split-plot designs are constructed based on an optimality criterion introduced by Kiefer (1975). The D-optimal split-plot design maximizes the determinant of the information matrix $\boldsymbol{X}'\boldsymbol{\Sigma}^{-1}\boldsymbol{X}$. Under the normality assumption, the D-optimal design minimizes the volume of the confidence ellipsoid of the estimated coefficient vector. Goos and Vandebroek (2001) propose an exchange algorithm for constructing a D-optimal split-plot design without constraints on the number of whole plots or the whole plot size. Goos and Vandebroek (2002) have shown that for a given set of whole plot and subplot treatments, the D-optimal split-plot design can be constructed by crossing a design in the subplot factors with another design in the whole plots, which means that the whole plot size is the same for each whole plot, and the levels of subplot factors are the same within each whole plot unit. Goos and Vandebroek (2003) improve the exchange algorithm to accommodate the restriction of the whole plot size, the number of whole plots, and the total number of observations. One main result is that for any D-optimal design in the completely randomized case where the runs can be rearranged into m whole plots of size n such that the sum of the design settings for the subplot factors is 0 within each whole plot, then the resulting split-plot design is a D-optimal split-plot design. As a result, 2^m, 2^{m-p}, and Plackett-Burman Designs are D-optimal among all feasible split-plot designs with m whole plots of size n, when the allocation of points satisfies the sum of each subplot factor in design matrix is 0 within each whole plot. Practically, this result works better for a first-order model but not for second order models since the D-optimal design for the second-order model can not always be found. Therefore, they use a computer algorithm to construct a "D-optimal split-plot" design for the second-order case when the allocation of points is not possible. Goos and Vandebroek (2004) discussed the advantages of increasing the number of whole plots. Increasing the number of whole plots ensures that the resulting split-plot design has a higher D-efficiency and more degrees of freedom for the whole plot error, comparing to the design with less whole plots. However, when practitioners have no idea of the number of runs to use, or the number of whole plots to use, their procedure tends to produce designs that increase the number of whole plots to achieve the high D-criteria value and smaller variance estimate, which is not always acceptable if the whole plots are expensive. The other criticism is that for different values of d and a fixed total number of observations, the resulting D-optimal split-plot designs can be quite different in terms of number of whole plots, m, the reallocation of the design points, and even the design points. Goos and Vandebroek (2004) never justify how to choose the best D-optimal split-plot design among the different D-optimal designs. How to choose a "good" split-plot design is still an open issue.

2.3 Split-Plot Second Order Response Surface Designs

Cornell (1988) discusses a mixture design run as a split-plot with the process variables as the whole plot factors. Kowalski, Cornell and Vining (2002) also study the impact of a split-plot structure on mixture designs with process variables. They construct a design by combining a CCD in the process variables with a fractionated simplex-centroid mixture design, which is used to fit a second order model. They use three estimation methods to estimate the variance components: OLS, restricted maximum likelihood (REML) and pure-error. They find that when three or more replicates of the center of the design in the process variables are performed, REML and pure-error methods are quite comparable. Therefore, when practitioners can afford at least three WP center runs, they suggest using pure-error methods since it does not require specifying the model.

Letsinger, Myers and Lentner (1996) (LML) propose "bi-randomization designs" (BRD) and studied various methods for estimating variance components. They assume in the second-order non-crossed BRD case that designs that maintain the equivalence between OLS estimates of the parameters and GLS estimates of the parameters do not exist. As a result, they use an asymptotic estimation method which depends on the specified model to estimate variance components and to construct formal tests. Vining, Kowalski and Montgomery (VKM) (2005) find the conditions for the existence of second-order split-plot designs where the OLS estimates of the coefficients is equivalent to the GLS estimates, which will be referred to as OLS-GLS equivalent designs. VKM will be discussed in more detail later in this section. Vining and Kowalski (VK) (2006) further find that exact tests for all the model parameters can be constructed when all sub-plot effects are completely orthogonal to the whole plot terms and it does not depend on the model assumption. If all sub-plot effects are not completely orthogonal to all the whole plot terms, VK outline a Satterthwaite's procedure to adjust the degrees of freedoms. Trinca and Gilmour (2001) propose "multistratum" designs where the split-plot design is a special case. They develop a computer algorithm to construct designs stratum by stratum. In each stratum, they try to arrange the experimental runs as orthogonal to the higher stratum as possible. Compared with Letsinger, Myers and Lentner (1996), their designs have smaller variances for parameter estimation. Draper and John (1998) study the impact of split-plot structure on BBD type designs, star designs and cube designs. They found that rotatability is not achievable in these types of designs. Therefore, they utilize the measure Q introduced by Draper and Pukelsheim (1990) to measure "how rotatable" the design is. They use REML to estimate unknown variance components first. By discussing different scenarios with different variance component ratios and the numbers of factors, they find the best value in the design to maximize the measure Q.

LML's contribution is that they were the first to study the split-plot structure for second-order response surface designs and propose a way to estimate the variance components. However, their designs have some unattractive properties. For example, there are several whole plots with only one subplot run. VKM point out that in split-plot designs where the whole plot factors are really hard to change and the whole plot runs are more expensive than the sub-plot runs, it is a waste of resources to run only one observation in a whole plot. In addition, the LML design has no replication of whole plots to gain pure-error estimates of whole plot variance. The asymptotic methods used to estimate the variance components are model dependent. Also, geometrically it is not balanced. Finally, second-order OLS-GLS equivalent designs actually exist.

VKM construct the equivalent designs based on Graybill (1976) (Theorem 6.8.1). In VKM designs, replicates of the overall center runs can be added to the design without violating the equivalence between OLS and GLS. There is no constraint on the number of center runs in the design. The resulting design fills the blank in Letsinger, Myers and Lentner's work and makes the derivation of design properties a much more tractable mathematical problem. In addition, they also propose a pure-error approach, which is model-independent, to estimate the unknown variance components. OLS-GLS equivalence is an attractive property since REML is an asymptotic and iterative estimation method that always depends on the specified model. VKM also point out that the cost is very essential in the construction of the design.

Parker (2005) expands VKM's design to the unbalanced (unequal whole plot size) case. He finds that the whole plot size of the overall center runs does not need to be equal to other whole plots size. Therefore, the number of subplot runs at the whole plot center can be reduced. He also proposes minimum whole plot (MWP) OLS-GLS equivalent designs where the number of whole plots is the minimum number possible. For a 2^k CCD, the number of whole plots is $2^k + 2k$. In MWP designs, subplot center runs can be added into the whole plots with WP factor factorial runs. This technique reduces the overall size of the design while keeping the equivalence between the OLS and GLS estimates.

The VKM derivation will serve as the foundation of the current research so it is worthwhile to review here. The assumptions are that the model contains an intercept term and that the design is balanced. Parker (2005) relaxes the requirement of balance. Graybill (1976) show that the OLS and GLS estimates are equivalent if and only if there exists a nonsingular matrix $\boldsymbol{F}$ such that

$$\boldsymbol{\Sigma X} = \boldsymbol{XF}.$$

Since $\boldsymbol{\Sigma} = \sigma^2\boldsymbol{I} + \sigma_\delta^2\boldsymbol{MM}'$, we have

$$\boldsymbol{\Sigma X} = [\sigma^2\boldsymbol{I} + \sigma_\delta^2\boldsymbol{MM}']\boldsymbol{X}.$$

The goal is to find an $\boldsymbol{F}$ to satisfy the theorem. VKM partitioned the model matrix $\boldsymbol{X}$ as

$$\boldsymbol{X} = \begin{bmatrix} \mathbf{1}_1 & \boldsymbol{W}_1 & \boldsymbol{S}_{D_1} & \boldsymbol{S}_{O_1} \\ \mathbf{1}_2 & \boldsymbol{W}_2 & \boldsymbol{S}_{D_2} & \boldsymbol{S}_{O_2} \\ \vdots & \vdots & \vdots & \vdots \\ \mathbf{1}_m & \boldsymbol{W}_m & \boldsymbol{S}_{D_m} & \boldsymbol{S}_{O_m} \end{bmatrix}$$

where $\boldsymbol{W}_i$ is the whole plot model matrix including the WP first order terms, the WP $\times$ WP interactions and the WP second order terms, $\boldsymbol{S}_{D_i}$ is the subplot model matrix including the SP first order terms, the SP $\times$ SP interactions and the SP $\times$ WP interactions, $\boldsymbol{S}_{O_i}$ is the subplot model matrix including the SP quadratic terms. The first condition of the equivalent design is $\boldsymbol{S}'_{D_i}\mathbf{1} = \boldsymbol{q}$, $i = 1, \ldots, m$, where $\boldsymbol{q}$ is a vector of constants. Note that although $\boldsymbol{S}'_{D_i}$ may not be exactly the same for each whole plot, the sum of the columns of $\boldsymbol{S}'_{D_i}$ needs to be the same for all the whole plots. So even if $\boldsymbol{S}'_{D_i} \neq \boldsymbol{S}'_{D_i^*}$, we have

$$\boldsymbol{S}'_{D_i}\mathbf{1} = \boldsymbol{S}'_{D_i^*}\mathbf{1} = \boldsymbol{q}, \quad i = 1, \ldots, m.$$

Now the left side in the theorem becomes

$$\begin{aligned}
\boldsymbol{\Sigma X} &= [\sigma^2 \boldsymbol{I} + \sigma_\delta^2 \boldsymbol{M M'}]\boldsymbol{X} \\
&= \sigma^2 \boldsymbol{X} + \sigma_\delta^2 \begin{bmatrix} \mathbf{1}_{n_1}\mathbf{1}'_{n_1}\mathbf{1}_{n_1} & \mathbf{1}_{n_1}\mathbf{1}'_{n_1}\boldsymbol{W}_1 & \mathbf{1}_{n_1}\mathbf{1}'_{n_1}\boldsymbol{S}_{D_1} & \mathbf{1}_{n_1}\mathbf{1}'_{n_1}\boldsymbol{S}_{O_1} \\ \mathbf{1}_{n_2}\mathbf{1}'_{n_2}\mathbf{1}_{n_2} & \mathbf{1}_{n_2}\mathbf{1}'_{n_2}\boldsymbol{W}_2 & \mathbf{1}_{n_2}\mathbf{1}'_{n_2}\boldsymbol{S}_{D_2} & \mathbf{1}_{n_2}\mathbf{1}'_{n_2}\boldsymbol{S}_{O_2} \\ \vdots & \vdots & \vdots & \vdots \\ \mathbf{1}_{n_m}\mathbf{1}'_{n_m}\mathbf{1}_{n_m} & \mathbf{1}_{n_m}\mathbf{1}'_{n_m}\boldsymbol{W}_m & \mathbf{1}_{n_m}\mathbf{1}'_{n_m}\boldsymbol{S}_{D_m} & \mathbf{1}_{n_m}\mathbf{1}'_{n_m}\boldsymbol{S}_{O_m} \end{bmatrix} \\
&= \sigma^2 \boldsymbol{X} + \sigma_\delta^2 \begin{bmatrix} \mathbf{1}_{n_1}\mathbf{1}'_{n_1}\mathbf{1}_{n_1} & \mathbf{1}_{n_1}\mathbf{1}'_{n_1}\boldsymbol{W}_1 & \mathbf{1}_{n_1}\boldsymbol{q}' & \mathbf{1}_{n_1}\mathbf{1}'_{n_1}\boldsymbol{S}_{O_1} \\ \mathbf{1}_{n_2}\mathbf{1}'_{n_2}\mathbf{1}_{n_2} & \mathbf{1}_{n_2}\mathbf{1}'_{n_2}\boldsymbol{W}_2 & \mathbf{1}_{n_2}\boldsymbol{q}' & \mathbf{1}_{n_2}\mathbf{1}'_{n_2}\boldsymbol{S}_{O_2} \\ \vdots & \vdots & \vdots & \vdots \\ \mathbf{1}_{n_m}\mathbf{1}'_{n_m}\mathbf{1}_{n_m} & \mathbf{1}_{n_m}\mathbf{1}'_{n_m}\boldsymbol{W}_m & \mathbf{1}_{n_m}\boldsymbol{q}' & \mathbf{1}_{n_m}\mathbf{1}'_{n_m}\boldsymbol{S}_{O_m} \end{bmatrix}. \qquad (2.3)
\end{aligned}$$

When the design is balanced with whole plot size n, we have $\mathbf{1}_{n_i} = \mathbf{1}$. Also, since the rows within a whole plot are the same, we have $\boldsymbol{W}_i = \mathbf{1}\boldsymbol{w}'_i$, where $\boldsymbol{w}'_i$ is the row vector in the i^{th} whole plot. This leads to

$$\mathbf{1}\mathbf{1}'\boldsymbol{W}_i = \mathbf{1}\mathbf{1}'\mathbf{1}\boldsymbol{w}'_i = n\mathbf{1}\boldsymbol{w}'_i = n\boldsymbol{W}_i.$$

Now we have

$$\boldsymbol{\Sigma X} = \sigma^2 \boldsymbol{X} + \sigma_\delta^2 \begin{bmatrix} n\mathbf{1} & n\boldsymbol{W}_1 & \mathbf{1}\boldsymbol{q} & \mathbf{1}\mathbf{1}'\boldsymbol{S}_{O_1} \\ n\mathbf{1} & n\boldsymbol{W}_2 & \mathbf{1}\boldsymbol{q} & \mathbf{1}\mathbf{1}'\boldsymbol{S}_{O_2} \\ \vdots & \vdots & \vdots & \vdots \\ n\mathbf{1} & n\boldsymbol{W}_m & \mathbf{1}\boldsymbol{q} & \mathbf{1}\mathbf{1}'\boldsymbol{S}_{O_m} \end{bmatrix}. \qquad (2.4)$$

Let $\boldsymbol{F}$ be given by

$$\boldsymbol{F} = \sigma^2 \boldsymbol{I} + \sigma_\delta^2 \begin{bmatrix} n & \boldsymbol{0}' & \boldsymbol{q}' & \boldsymbol{0}' \\ \boldsymbol{0} & n\boldsymbol{I} & \boldsymbol{0} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{0} & \boldsymbol{0} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{0} & \boldsymbol{0} & \boldsymbol{G} \end{bmatrix}.$$

Then

$$\begin{aligned} \boldsymbol{XF} &= \sigma^2 \boldsymbol{X} + \sigma_\delta^2 \begin{bmatrix} \boldsymbol{1} & \boldsymbol{W}_1 & \boldsymbol{S}_{D_1} & \boldsymbol{S}_{O_1} \\ \boldsymbol{1} & \boldsymbol{W}_2 & \boldsymbol{S}_{D_2} & \boldsymbol{S}_{O_2} \\ \vdots & \vdots & \vdots & \vdots \\ \boldsymbol{1} & \boldsymbol{W}_m & \boldsymbol{S}_{D_m} & \boldsymbol{S}_{O_m} \end{bmatrix} \begin{bmatrix} n & \boldsymbol{0}' & \boldsymbol{q}' & \boldsymbol{0}' \\ \boldsymbol{0} & n\boldsymbol{I} & \boldsymbol{0} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{0} & \boldsymbol{0} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{0} & \boldsymbol{0} & \boldsymbol{G} \end{bmatrix} \\ &= \sigma^2 \boldsymbol{X} + \sigma_\delta^2 \begin{bmatrix} n\boldsymbol{1} & n\boldsymbol{W}_1 & \boldsymbol{1}\boldsymbol{q}' & \boldsymbol{S}_{O_1}\boldsymbol{G} \\ n\boldsymbol{1} & n\boldsymbol{W}_2 & \boldsymbol{1}\boldsymbol{q}' & \boldsymbol{S}_{O_2}\boldsymbol{G} \\ \vdots & \vdots & \vdots & \vdots \\ n\boldsymbol{1} & n\boldsymbol{W}_m & \boldsymbol{1}\boldsymbol{q}' & \boldsymbol{S}_{O_m}\boldsymbol{G} \end{bmatrix}. \end{aligned}$$

Thus $\boldsymbol{\Sigma X} = \boldsymbol{XF}$ if for some $\boldsymbol{G}$

$$\boldsymbol{1}\boldsymbol{1}'\boldsymbol{S}_{O_i} = \boldsymbol{S}_{O_i}\boldsymbol{G}, \quad i = 1, \ldots, m.$$

So as long as the design satisfies

1. the design is balanced
2. the sum of columns in each $\boldsymbol{S}_{D_i}$ is a constant vector $\boldsymbol{q}$
3. $\boldsymbol{1}\boldsymbol{1}'\boldsymbol{S}_{O_i} = \boldsymbol{S}_{O_i}\boldsymbol{G}$

then the design is an OLS-GLS equivalent design.

Chapter 3

Two-Strata Rotatability in Split-Plot Central Composite Designs

3.1 Rotatability in Central Composite Designs with a Split-Plot Structure

3.1.1 Split-Plot Central Composite Designs

Letsinger, Myers and Lentner (1996) (LML) propose "bi-randomization designs". Vining, Kowalski, Montgomery (2005) propose second order OLS-GLS equivalent split-plot response surface designs and Vining and Kowalski (VK) (2006) further find second order split-plot response surface designs that yield exact tests for the model parameters. Parker (2005) proposes second order minimum whole plot (MWP) OLS-GLS equivalent designs where the number of whole plots is the minimum number possible.

As an example, for two whole plot factors and two subplot factors, the VKM equivalent design is shown in Table 3.1 and MWP equivalent design is shown in Table 3.2. Both designs are balanced (the same number of subplots in each whole plot) and the sum of the columns in each $\boldsymbol{S}_{D_i}$ is zero in every whole plot, even though the split-plot designs within each whole plot are not the same. The MWP design has subplot center runs within each whole plot and it has 9 whole plots rather than 12 whole plots in VKM. However, the VKM design has the additional ability to estimate model independent pure error at the whole plot level while MWP design doesn't. A VK (2006) CCD is shown in Table 3.3. Comparing Table 3.3 to Table 3.1 shows that the subplot design for the subplot axial runs are different. The advantage of the VK (2006) design is that it provides an exact test on the subplot quadratic effects. The LML type CCD is shown in Table 3.5. Another possible unbalanced split-plot CCD is shown in Table 3.4.

Comparing the 5 designs shows that Tables 3.1, 3.2 and 3.3 are balanced while Tables 3.4 and 3.5 are unbalanced. Another important design structure will be whether or not $\boldsymbol{S}_O$ is a subset of the whole plot effects.

We define this important design structure as:

If in a split-plot design, the pure quadratic terms for any subplot factor are not constant within each whole plot, then $\boldsymbol{S}_O$ of this design is not a subset of the whole plot effects. If in a split-plot design, the pure quadratic terms for all subplot factors are constant within each whole plot, then $\boldsymbol{S}_O$ of this design is a subset of the whole plot effects.

In Tables 3.1, 3.2 and 3.5, $\boldsymbol{S}_O$ is not a subset of the whole plot effects and in Tables 3.3 and 3.4, $\boldsymbol{S}_O$ is a subset of the whole plot effects. The factorial runs are all full factorial runs.

We will restrict our work in balanced and unbalanced split-plot CCDs to those with full factorial runs or Resolution V fractional factorial runs with respect to all factors. We will also examine MWP split-plot designs, which is a small deviation from split-plot CCD and OLS-GLS equivalent. We will separately examine the two cases that can occur for the axial runs, that is, $\boldsymbol{S}_O$ is either a subset of the whole plot effects or not a subset of the whole plot effects. Since the rotatability criterion is based on the sum of the columns in design matrix $\boldsymbol{X}$, including overall center runs will not affect the sum. In the following discussion, we won't discuss adding center runs to the designs.

As a summary of the examples, Tables 3.1 and 3.2 are balanced and $\boldsymbol{S}_O$ is not a subset of the WP effects; Table 3.3 is balanced and $\boldsymbol{S}_O$ is a subset of the WP effects; Table 3.4 is unbalanced and $\boldsymbol{S}_O$ is a subset of the WP effects; Table 3.5 is unbalanced and $\boldsymbol{S}_O$ is not a subset of the WP effects.

Table 3.1: The VKM CCD for Two Whole Plot and Two Subplot Factors

WP	z_1	z_2	x_1	x_2	WP	z_1	z_2	x_1	x_2
	-1	-1	-1	-1		0	$-\alpha$	0	0
1	-1	-1	-1	1	7	0	$-\alpha$	0	0
	-1	-1	1	-1		0	$-\alpha$	0	0
	-1	-1	1	1		0	$-\alpha$	0	0
	-1	1	-1	-1		0	α	0	0
2	-1	1	-1	1	8	0	α	0	0
	-1	1	1	-1		0	α	0	0
	-1	1	1	1		0	α	0	0
	1	-1	-1	-1	9	0	0	$-\beta$	0
3	1	-1	-1	1		0	0	β	0
	1	-1	1	-1		0	0	0	$-\beta$
	1	-1	1	1		0	0	0	β
	1	1	-1	-1	10	0	0	0	0
4	1	1	-1	1		0	0	0	0
	1	1	1	-1		0	0	0	0
	1	1	1	1		0	0	0	0
	$-\alpha$	0	0	0	11	0	0	0	0
5	$-\alpha$	0	0	0		0	0	0	0
	$-\alpha$	0	0	0		0	0	0	0
	$-\alpha$	0	0	0		0	0	0	0
	α	0	0	0	12	0	0	0	0
6	α	0	0	0		0	0	0	0
	α	0	0	0		0	0	0	0
	α	0	0	0		0	0	0	0

Table 3.2: The MWP Design for Two Whole Plot and Two Subplot Factors

WP	z_1	z_2	x_1	x_2	WP	z_1	z_2	x_1	x_2
1	-1	-1	-1	-1	6	α	0	0	0
	-1	-1	-1	1		α	0	0	0
	-1	-1	1	-1		α	0	0	0
	-1	-1	1	1		α	0	0	0
	-1	-1	0	0		α	0	0	0
2	-1	1	-1	-1	7	0	$-\alpha$	0	0
	-1	1	-1	1		0	$-\alpha$	0	0
	-1	1	1	-1		0	$-\alpha$	0	0
	-1	1	1	1		0	$-\alpha$	0	0
	-1	1	0	0		0	$-\alpha$	0	0
3	1	-1	-1	-1	8	0	α	0	0
	1	-1	-1	1		0	α	0	0
	1	-1	1	-1		0	α	0	0
	1	-1	1	1		0	α	0	0
	1	-1	0	0		0	α	0	0
4	1	1	-1	-1	9	0	0	$-\beta$	0
	1	1	-1	1		0	0	β	0
	1	1	1	-1		0	0	0	$-\beta$
	1	1	1	1		0	0	0	β
	1	1	0	0		0	0	0	0
5	$-\alpha$	0	0	0					
	$-\alpha$	0	0	0					
	$-\alpha$	0	0	0					
	$-\alpha$	0	0	0					
	$-\alpha$	0	0	0					

Table 3.3: VK(2006) CCD for Two Whole Plot and Two Subplot Factors

WP	z_1	z_2	x_1	x_2	WP	z_1	z_2	x_1	x_2
	-1	-1	-1	-1		0	$-\alpha$	0	0
1	-1	-1	-1	1	7	0	$-\alpha$	0	0
	-1	-1	1	-1		0	$-\alpha$	0	0
	-1	-1	1	1		0	$-\alpha$	0	0
	-1	1	-1	-1		0	α	0	0
2	-1	1	-1	1	8	0	α	0	0
	-1	1	1	-1		0	α	0	0
	-1	1	1	1		0	α	0	0
	1	-1	-1	-1		0	0	$-\beta$	0
3	1	-1	-1	1	9	0	0	β	0
	1	-1	1	-1		0	0	$-\beta$	0
	1	-1	1	1		0	0	β	0
	1	1	-1	-1		0	0	0	$-\beta$
4	1	1	-1	1	10	0	0	0	β
	1	1	1	-1		0	0	0	$-\beta$
	1	1	1	1		0	0	0	β
	$-\alpha$	0	0	0	11	0	0	0	0
5	$-\alpha$	0	0	0		0	0	0	0
	$-\alpha$	0	0	0		0	0	0	0
	$-\alpha$	0	0	0		0	0	0	0
	α	0	0	0	12	0	0	0	0
6	α	0	0	0		0	0	0	0
	α	0	0	0		0	0	0	0
	α	0	0	0		0	0	0	0

Table 3.4: An Unbalanced CCD in a Split-Plot Structure for Two Whole Plot Factors and Two Subplot Factors

WP	z_1	z_2	x_1	x_2
	-1	-1	-1	-1
1	-1	-1	-1	1
	-1	-1	1	-1
	-1	-1	1	1
	-1	1	-1	-1
2	-1	1	-1	1
	-1	1	1	-1
	-1	1	1	1
	1	-1	-1	-1
3	1	-1	-1	1
	1	-1	1	-1
	1	-1	1	1
	1	1	-1	-1
4	1	1	-1	1
	1	1	1	-1
	1	1	1	1
5	$-\alpha$	0	0	0
	$-\alpha$	0	0	0
	$-\alpha$	0	0	0
6	α	0	0	0
	α	0	0	0
	α	0	0	0
7	0	$-\alpha$	0	0
	0	$-\alpha$	0	0
	0	$-\alpha$	0	0
8	0	α	0	0
	0	α	0	0
	0	α	0	0
9	0	0	$-\beta$	0
	0	0	β	0
10	0	0	0	$-\beta$
	0	0	0	β

Table 3.5: The LML Type CCD in a Split-Plot Structure for Two Whole Plot Factors and Two Subplot Factors

WP	z_1	z_2	x_1	x_2
	-1	-1	-1	-1
1	-1	-1	-1	1
	-1	-1	1	-1
	-1	-1	1	1
	-1	1	-1	-1
2	-1	1	-1	1
	-1	1	1	-1
	-1	1	1	1
	1	-1	-1	-1
3	1	-1	-1	1
	1	-1	1	-1
	1	-1	1	1
	1	1	-1	-1
4	1	1	-1	1
	1	1	1	-1
	1	1	1	1
5	$-\alpha$	0	0	0
	$-\alpha$	0	0	0
6	α	0	0	0
	α	0	0	0
7	0	$-\alpha$	0	0
	0	$-\alpha$	0	0
8	0	α	0	0
	0	α	0	0
9	0	0	$-\beta$	0
	0	0	β	0
	0	0	0	$-\beta$
	0	0	0	β

3.1.2 Rotatable Conditions in Split-Plot Central Composite Designs

Suppose we have k factors and k_1 of them are whole plot factors and k_2 of them are subplot factors. Following the idea in VKM, we can partition the design matrix for a second order design with a split-plot structure as

$$\boldsymbol{X} = \begin{bmatrix} \mathbf{1}_1 & \boldsymbol{W}_{Q_1} & \boldsymbol{S}_{O_1} & \boldsymbol{W}_{F_1} & \boldsymbol{S}_{D_1} \\ \mathbf{1}_2 & \boldsymbol{W}_{Q_2} & \boldsymbol{S}_{O_2} & \boldsymbol{W}_{F_2} & \boldsymbol{S}_{D_2} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \mathbf{1}_m & \boldsymbol{W}_{Q_m} & \boldsymbol{S}_{O_m} & \boldsymbol{W}_{F_m} & \boldsymbol{S}_{D_m} \end{bmatrix} = [[\boldsymbol{T}, \boldsymbol{W}_F], \boldsymbol{S}_D] = [\boldsymbol{W}^*, \boldsymbol{S}_D]$$

where $\boldsymbol{W}_Q$ is the $N \times k_1$ model matrix containing the WP factor quadratic effects, $\boldsymbol{W}_F$ is the $N \times (k_1 + \binom{k_1}{2})$ model matrix containing the WP factor first order effects and the WP×WP interaction effects, $\boldsymbol{S}_D$ is the $N \times (k_2 + \binom{k_2}{2} + k_1 k_2)$ model matrix containing the SP factor first order, SP×SP two-way interaction and SP×WP two-way interaction effects, and $\boldsymbol{S}_O$ is the $N \times k_2$ model matrix containing the SP factor quadratic effects, $\boldsymbol{T} = [\mathbf{1}, \boldsymbol{W}_Q, \boldsymbol{S}_O]$ and $\boldsymbol{W}^* = [\boldsymbol{T}, \boldsymbol{W}_F]$. The matrix with subscript i is the corresponding model matrix in the i^{th} whole plot. Suppose each subplot sub-design within each whole plot is orthogonal to the mean, then we have $\mathbf{1}'\boldsymbol{S}_{D_i} = \mathbf{0}'$, which implies that $\boldsymbol{M}'\boldsymbol{S}_D = \boldsymbol{S}_D'\boldsymbol{M} = \mathbf{0}$.

Since the prediction variance $Var(\hat{y}(\boldsymbol{x}_0))$ is now calculated as $\boldsymbol{x}_0'(\boldsymbol{X}'\boldsymbol{\Sigma}^{-1}\boldsymbol{X})^{-1}\boldsymbol{x}_0$, we need to study the moment matrix $\boldsymbol{X}'\boldsymbol{\Sigma}^{-1}\boldsymbol{X}$ instead of $\boldsymbol{X}'\boldsymbol{X}$. We do this for four different, general scenarios.

Balanced Split-Plot CCD Where $\boldsymbol{S}_O$ Is a Subset of the Whole Plot Effects

Table 3.3 is one example of this design. Since the whole plots are equal-sized,

$$\boldsymbol{\Sigma}^{-1} = \frac{1}{\sigma^2}\boldsymbol{I}_N - \frac{\sigma_\delta^2}{\sigma^2(\sigma^2 + n\sigma_\delta^2)}\boldsymbol{M}\boldsymbol{M}'.$$

In this case, since $\boldsymbol{S}_O$ is effectively a subset of the WP effects, then $\boldsymbol{W}_i^* = \boldsymbol{1}_n \boldsymbol{w}_i^{*'}$ and $\boldsymbol{X} = [\boldsymbol{W}^*, \boldsymbol{S}_D]$. Therefore $\boldsymbol{M}\boldsymbol{M}'\boldsymbol{X} = [\boldsymbol{M}\boldsymbol{M}'\boldsymbol{W}^*, \boldsymbol{M}\boldsymbol{M}'\boldsymbol{S}_D] = [n\boldsymbol{W}^*, \boldsymbol{0}]$. Hence,

$$\begin{aligned}\boldsymbol{X}'\boldsymbol{\Sigma}^{-1}\boldsymbol{X} &= \frac{1}{\sigma^2}\begin{bmatrix} \boldsymbol{W}^{*'}\boldsymbol{W}^* & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{S}_D'\boldsymbol{S}_D \end{bmatrix} - \frac{\sigma_\delta^2}{\sigma^2(\sigma^2 + n\sigma_\delta^2)}\begin{bmatrix} n\boldsymbol{W}^{*'}\boldsymbol{W}^* & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{0} \end{bmatrix} \\ &= \begin{bmatrix} \frac{1}{\sigma^2 + n\sigma_\delta^2}\boldsymbol{W}^{*'}\boldsymbol{W}^* & \boldsymbol{0} \\ \boldsymbol{0} & \frac{1}{\sigma^2}\boldsymbol{S}_D'\boldsymbol{S}_D \end{bmatrix}. \end{aligned} \tag{3.1}$$

Furthermore,

$$\begin{aligned}\boldsymbol{W}^{*'}\boldsymbol{W}^* &= [\boldsymbol{T}, \boldsymbol{W}_F]'[\boldsymbol{T}, \boldsymbol{W}_F] \\ &= \begin{bmatrix} \boldsymbol{T}'\boldsymbol{T} & \boldsymbol{T}'\boldsymbol{W}_F \\ \boldsymbol{W}_F'\boldsymbol{T} & \boldsymbol{W}_F'\boldsymbol{W}_F \end{bmatrix}. \end{aligned} \tag{3.2}$$

For a CCD, the first-order effect is always orthogonal to all other terms, thus, $\boldsymbol{T}'\boldsymbol{W}_F = \boldsymbol{W}_F'\boldsymbol{T} = \boldsymbol{0}$, and Equation (3.1) becomes

$$\boldsymbol{X}'\boldsymbol{\Sigma}^{-1}\boldsymbol{X} = \begin{bmatrix} \frac{1}{\sigma^2 + n\sigma_\delta^2}\begin{bmatrix} \boldsymbol{T}'\boldsymbol{T} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{W}_F'\boldsymbol{W}_F \end{bmatrix} & \boldsymbol{0} \\ \boldsymbol{0} & \frac{1}{\sigma^2}\boldsymbol{S}_D'\boldsymbol{S}_D \end{bmatrix}.$$

Using the example design in Table 3.3, we have

$$\boldsymbol{T}'\boldsymbol{T} = \begin{pmatrix} N & F+8\alpha^2 & F+8\alpha^2 & F+4\beta^2 & F+4\beta^2 \\ F+8\alpha^2 & F+8\alpha^4 & F & F & F \\ F+8\alpha^2 & F & F+8\alpha^4 & F & F \\ F+4\beta^2 & F & F & F+4\beta^4 & F \\ F+4\beta^2 & F & F & F & F+4\beta^4 \end{pmatrix} \tag{3.3}$$

$$\boldsymbol{W}'_F\boldsymbol{W}_F = \begin{pmatrix} F+8\alpha^2 & 0 & 0 \\ 0 & F+8\alpha^2 & 0 \\ 0 & 0 & F \end{pmatrix} \tag{3.4}$$

$$\boldsymbol{S}'_D\boldsymbol{S}_D = \begin{pmatrix} F+4\beta^2 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & F+4\beta^2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & F & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & F & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & F & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & F & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & F \end{pmatrix} \tag{3.5}$$

where F is the number of factorial points in the design, which is $2^4 = 16$.

For the other three scenarios, the moment matrix is of a similar format. Detailed derivations are provided in the Appendix. A summary of the results is given here.

Balanced Split-Plot CCD Where S_O Is Not a Subset of the Whole Plot Effects

The moment matrix is

$$\frac{1}{\sigma^2}\begin{bmatrix} \boldsymbol{T}'\boldsymbol{T} - \frac{d}{1+nd}\boldsymbol{T}'\boldsymbol{M}\boldsymbol{M}'\boldsymbol{T} & \boldsymbol{0} & \boldsymbol{0} \\ \boldsymbol{0} & \frac{1}{1+nd}\boldsymbol{W}'_F\boldsymbol{W}_F & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{0} & \boldsymbol{S}'_D\boldsymbol{S}_D \end{bmatrix}.$$

Unbalanced Split-Plot CCD Where S_O Is a Subset of the Whole Plot Effects

The moment matrix is

$$\boldsymbol{X}'\boldsymbol{\Sigma}^{-1}\boldsymbol{X} = \begin{pmatrix} \boldsymbol{W}'Diag(\frac{1}{\sigma^2+n_i\sigma_\delta^2}\boldsymbol{I}_{n_i})\boldsymbol{W} & \boldsymbol{0} \\ \boldsymbol{0} & \frac{1}{\sigma^2}\boldsymbol{S}'_D\boldsymbol{S}_D \end{pmatrix}.$$

where $\boldsymbol{W}'Diag(\frac{1}{\sigma^2+n_i\sigma_\delta^2}\boldsymbol{I}_{n_i})\boldsymbol{W}$ is

$$\begin{pmatrix} \boldsymbol{T}'Diag(\frac{1}{\sigma^2+n_i\sigma_\delta^2}\boldsymbol{I}_{n_i})\boldsymbol{T} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{W}'_F Diag(\frac{1}{\sigma^2+n_i\sigma_\delta^2}\boldsymbol{I}_{n_i})\boldsymbol{W}_F \end{pmatrix}.$$

Unbalanced Split-Plot CCD Where S_O Is Not a Subset of the Whole Plot Effects

The moment matrix is

$$\boldsymbol{X}'\boldsymbol{\Sigma}^{-1}\boldsymbol{X} = \begin{pmatrix} \frac{1}{\sigma^2}\boldsymbol{T}'\boldsymbol{T} - \boldsymbol{T}'Diag(\frac{\sigma_\delta^2}{\sigma^2(\sigma^2+n_i\sigma_\delta^2)}\boldsymbol{I}_{n_i})\boldsymbol{M}\boldsymbol{M}'\boldsymbol{T} & \boldsymbol{0} & \boldsymbol{0} \\ \boldsymbol{0} & \sum_{i=1}^{m}\frac{1}{\sigma^2+n_i\sigma_\delta^2}\boldsymbol{W}'_{F_i}\boldsymbol{W}_{F_i} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{0} & \frac{1}{\sigma^2}\boldsymbol{S}'_D\boldsymbol{S}_D \end{pmatrix}.$$

As a summary, if we denote the diagonal submatrix involving $\boldsymbol{T}$ in the moment matrix as $\boldsymbol{Q}$, and the submatrix involving $\boldsymbol{W}_F$ as $\boldsymbol{W}_F^*$, the moment matrices in these four scenarios can be expressed as

$$\boldsymbol{X}'\boldsymbol{\Sigma}^{-1}\boldsymbol{X} = \begin{bmatrix} \begin{matrix} \boldsymbol{Q} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{W}_F^* \end{matrix} & \boldsymbol{0} \\ \boldsymbol{0} & \frac{1}{\sigma^2}\boldsymbol{S}'_D\boldsymbol{S}_D \end{bmatrix}.$$

We can see from the Appendix that the $\boldsymbol{Q}$s in all scenarios are of the same format

$$\begin{pmatrix} A & B\boldsymbol{1}' & C\boldsymbol{1}' \\ B\boldsymbol{1} & (P-G)\boldsymbol{I} + G\boldsymbol{J}_{k_1} & G\boldsymbol{J}_{k_1\times k_2} \\ C\boldsymbol{1} & G\boldsymbol{J}_{k_2\times k_1} & (E-H)\boldsymbol{I} + H\boldsymbol{J}_{k_2} \end{pmatrix}$$

where A,B,...,H are scalars, and all $\boldsymbol{W}_F^*$ and $\boldsymbol{S}'_D\boldsymbol{S}_D$ are diagonal matrices. From Equation 3.1 and Equation 3.3, we can see that the different variance components have different impacts on the WP factors and the SP factors. The factors are not treated equally as in the completely randomized case because of the split-plot structure. Moreover, the overall rotatability condition can not be achieved in this kind of design because the moments of the original design matrix are divided into two parts with two different multipliers. For example, the pure second-order moment for the i^{th} SP factor that resides in $\boldsymbol{S}'_D\boldsymbol{S}_D$, $[ii]^S_{sp}$, is obtained by multiplying the original $[ii]_{sp}$ by $\frac{1}{\sigma^2}$. However, $[ii]^W_{sp}$, the pure second-order moment for the i^{th} SP factor that resides in $\boldsymbol{W}'\boldsymbol{W}$ is obtained by multiplying the original $[ii]_{sp}$ by $\frac{1}{\sigma^2+n\sigma^2_\delta}$. A rotatable design requires that $[ii]^S_{sp} = [ii]^W_{sp}$ and $[ii] = [jj], i \neq j$. Here $[ii]^S_{sp} = [ii]^W_{sp}$ only when $\sigma^2_\delta = 0$ which is the completely randomized case. When σ^2_δ is not zero, it is impossible to achieve the conditions in Box and Hunter (1957) for a split-plot design. Although it is hard to see directly from the latter three scenarios, we can safely draw the same conclusion of rotatability based on the result in the Appendix. Therefore, the idea of considering rotatability as one combined measure for both whole plot and subplot factors is not appropriate.

3.2 Two-Strata Rotatability in Response Surface Designs with a Split-Plot Structure

3.2.1 Two-Strata Rotatability conditions in Split-Plot Central Composite Designs

Since rotatability is not achievable, we propose a concept of two-strata rotatability. It has similar properties, and it is more logical in the split-plot case. In a two-strata rotatable design, there are two axial distances instead of one. First is the whole plot axial distance, ρ^2_w and the second is the subplot axial distance, ρ^2_s. A two-strata rotatable design will allow all the points with same ρ^2_w and ρ^2_s to have same prediction variance, which means the prediction variance is a function of ρ^2_w and ρ^2_s. The design space is divided into the WP space and the SP space. The design is rotatable separately in whole plot space and in subplot space. The idea of separating the space is consistent with split-plot designs in the literature. Liang and

Anderson-Cook (2004) use separate distance measures in the WP space and the SP space to construct a 3D variance dispersion graph (VDG) to evaluate split-plot designs. Kowalski, Borror and Montgomery (2005) modify the path of the steepest ascent method by using separate distance measures in the WP space and the SP space.

We define the two-strata rotatable designs as:

In a k-factor split-plot design with k_1 WP factors and k_2 SP factors, let z_i be the i^{th} WP factor and x_i be the i^{th} SP factor. If for any two design runs t_0=$(z_{10}, z_{20}, ..., z_{k_{1,0}}, x_{10}, ..., x_{k_{2,0}})$ and t_1=$(z_{11}, z_{21}, ..., z_{k_{1,1}}, x_{11}, ..., x_{k_{2,1}})$ satisfying $\sum_{i=1}^{i=k1} z_{i0}^2 = \sum_{i=1}^{i=k1} z_{i1}^2 = \rho_w^2$ and $\sum_{j=1}^{j=k2} x_{j0}^2 = \sum_{j=1}^{j=k2} x_{j1}^2 = \rho_s^2$, the corresponding prediction variances $Var(\hat{y}(t_0))$ and $Var(\hat{y}(t_1))$ are equal, the design is called a two-strata rotatable split-plot design.

Consider $\boldsymbol{x}_0$ as the entire vector of factor settings (both whole plot and subplot). In a rotatable design, $Var(\hat{y}(\boldsymbol{x}_0)) = f(\rho_w^2 + \rho_s^2)$, which is a function of the overall distance. In a two-strata rotatable design, $Var(\hat{y}(\boldsymbol{x}_0)) = f^*(\rho_w^2, \rho_s^2)$, a function of two separate distances. Therefore, the stronger assumption in the rotatable designs is being relaxed to accommodate the split-plot structure.

We can write any design run $\boldsymbol{x}$ as $\boldsymbol{x}' = (\boldsymbol{x}'_Q, \boldsymbol{x}'_{W_F}, \boldsymbol{x}'_{S_D})$ where

$$\begin{aligned}
\boldsymbol{x}'_Q &= (1, z_1^2, ..., z_{k_1}^2, x_1^2, ..., x_{k_2}^2)' = (1, \boldsymbol{q}'_w, \boldsymbol{q}'_s), \\
\boldsymbol{x}'_{W_F^*} &= (z_1, ..., z_{k_1}, z_1 z_2, ..., z_{k_1-1} z_{k_1})' = (\boldsymbol{f}'_w, \boldsymbol{f}'_{ww}), \\
\boldsymbol{x}'_{S_D} &= (x_1, ..., x_{k_2}, x_1 x_2, ..., x_{k_2-1} x_{k_2}, x_1 z_1, ..., x_1 z_{k_1}, ..., x_{k_2} z_1, ..., x_{k_2} z_{k_1})' = (\boldsymbol{f}'_s, \boldsymbol{f}'_{ss}, \boldsymbol{f}'_{ws}).
\end{aligned}$$

In our scenarios, the prediction variance is

$$\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{\Sigma}^{-1}\boldsymbol{X})^{-1}\boldsymbol{x} = (\boldsymbol{x}'_Q, \boldsymbol{x}'_{W_F^*}, \boldsymbol{x}'_{S_D}) \begin{bmatrix} \boldsymbol{Q} & \boldsymbol{0} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{W}_F^* & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{0} & \frac{1}{\sigma^2}\boldsymbol{S}'_D\boldsymbol{S}_D \end{bmatrix}^{-1} (\boldsymbol{x}'_Q, \boldsymbol{x}'_{W_F^*}, \boldsymbol{x}'_{S_D})'$$

$$= \boldsymbol{x}'_Q\boldsymbol{Q}^{-1}\boldsymbol{x}_Q + \boldsymbol{x}'_{W_F^*}(\boldsymbol{W}_F^*)^{-1}\boldsymbol{x}_{W_F^*} + \sigma^2(\boldsymbol{x}'_{S_D}(\boldsymbol{S}'_D\boldsymbol{S}_D)^{-1}\boldsymbol{x}_{S_D}) \tag{3.6}$$

Both $(\boldsymbol{S}'_D\boldsymbol{S}_D)^{-1}$ and $(\boldsymbol{W}_F^*)^{-1}$ are diagonal matrices (since Resolution V or better is assumed), therefore the inverses can be easily calculated. However, $\boldsymbol{Q}$ is not diagonal and it is shown in the Appendix that

$$\boldsymbol{Q}^{-1} = \begin{pmatrix} a & b\boldsymbol{1}' & c\boldsymbol{1}' \\ b\boldsymbol{1} & (p-e)\boldsymbol{I} + e\boldsymbol{J}_{k_1} & g\boldsymbol{J}_{k_1 \times k_2} \\ c\boldsymbol{1} & g\boldsymbol{J}_{k_2 \times k_1} & (f-h)\boldsymbol{I} + h\boldsymbol{J}_{k_2} \end{pmatrix}.$$

The magnitude of the scalars in the inverse matrix are quite complicated. However, we can see that $p - e = \frac{1}{P-G}$ and $f - h = \frac{1}{E-H}$. Fortunately, in the derivation of two-strata rotatability below, only the relationship between these scalars is used, which simplifies the problem.

For general notation, we denote the sum of WP interactions in one column as F_w^* and the sum of WP×SP interaction in one column as F_s. Also we denote the diagonal elements other than F_w^* in $\boldsymbol{W}_F^*$ as w and the ones in $\boldsymbol{S}'_D\boldsymbol{S}_D$ denoted as s. The inverse of $\boldsymbol{W}_F^*$ can be written as:

$$\begin{pmatrix} \frac{1}{w} & \cdots & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & \cdots & \frac{1}{w} & 0 & \cdots & 0 \\ 0 & \cdots & 0 & \frac{1}{F_w^*} & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & \cdots & 0 & 0 & \cdots & \frac{1}{F_w^*} \end{pmatrix}$$

and the inverse of $\boldsymbol{S}'_D \boldsymbol{S}_D$ is:

$$\begin{pmatrix} \frac{1}{s} & \cdots & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & \cdots & \frac{1}{s} & 0 & \cdots & 0 \\ 0 & \cdots & 0 & \frac{1}{F_s} & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & \cdots & 0 & 0 & \cdots & \frac{1}{F_s} \end{pmatrix}.$$

Now for any vector $\boldsymbol{x}'$, we have

$$\boldsymbol{x}_Q'\boldsymbol{Q}^{-1}\boldsymbol{x}_Q = \begin{pmatrix} 1 & \boldsymbol{q}_w' & \boldsymbol{q}_s' \end{pmatrix} \begin{pmatrix} a & b\boldsymbol{1}' & c\boldsymbol{1}' \\ b\boldsymbol{1} & (p-e)\boldsymbol{I} + e\boldsymbol{J}_{k_1} & g\boldsymbol{J}_{k_1\times k_2} \\ c\boldsymbol{1} & g\boldsymbol{J}_{k_2\times k_1} & (f-h)\boldsymbol{I} + h\boldsymbol{J}_{k_2} \end{pmatrix} \begin{pmatrix} 1 \\ \boldsymbol{q}_w \\ \boldsymbol{q}_s \end{pmatrix}$$

$$\begin{aligned}
&= a + 2b\boldsymbol{q}_w'\boldsymbol{1} + 2c\boldsymbol{q}_s'\boldsymbol{1} + 2g\boldsymbol{q}_s'\boldsymbol{J}\boldsymbol{q}_w + (p-e)\boldsymbol{q}_w'\boldsymbol{q}_w + e\boldsymbol{q}_w'\boldsymbol{J}\boldsymbol{q}_w + (f-h)\boldsymbol{q}_s'\boldsymbol{q}_s + h\boldsymbol{q}_s'\boldsymbol{J}\boldsymbol{q}_s \\
&= a + 2b\rho_w^2 + 2c\rho_s^2 + 2g(\rho_w^2\rho_s^2) + (p-e)\left(\rho_w^4 - 2\sum_{i<j} z_i^2 z_j^2\right) \\
&\quad + e(\rho_w^4) + (f-h)\left(\rho_s^4 - 2\sum_{i<j} x_i^2 x_j^2\right) + h(\rho_s^4) \\
&= a + 2b\rho_w^2 + 2c\rho_s^2 + 2g(\rho_w^2\rho_s^2) + p(\rho_w^4) + f(\rho_s^4) \\
&\quad + (2e-2p)\sum_{i<j} z_i^2 z_j^2 + (2h-2f)\sum_{i<j} x_i^2 x_j^2, \qquad (3.7)
\end{aligned}$$

$$\begin{aligned}
\boldsymbol{x}_{W_F^*}'(\boldsymbol{W}_F^*)^{-1}\boldsymbol{x}_{W_F^*} &= \frac{1}{w}\boldsymbol{f}_w'\boldsymbol{f}_w + \frac{1}{F_w^*}(\boldsymbol{f}_{ww}'\boldsymbol{f}_{ww}) \\
&= \frac{1}{w}\rho_w^2 + \frac{1}{F_w^*}\left(\sum_{i<j} z_i^2 z_j^2\right), \qquad (3.8)
\end{aligned}$$

$$\begin{aligned}
\boldsymbol{x}_{S_D}'(\boldsymbol{S}_D'\boldsymbol{S}_D)^{-1}\boldsymbol{x}_{S_D} =& \frac{1}{s}(\boldsymbol{f}_s'\boldsymbol{f}_s) + \frac{1}{F_s}(\boldsymbol{f}_{ws}')(\boldsymbol{f}_{ws}) + \frac{1}{F_s}(\boldsymbol{f}_{ss}'\boldsymbol{f}_{ss}) \\
=& \frac{1}{s}\rho_s^2 + \frac{1}{F_s}(\rho_s^2\rho_w^2) + \frac{1}{F_s}\left(\sum_{i<j} x_i^2 x_j^2\right) \qquad (3.9)
\end{aligned}$$

Using Equations (3.6) with Equations (3.7), (3.8) and (3.9), gives an expression which is a function of ρ_w^2, ρ_s^2, $\sum_{i<j} x_i^2 x_j^2$ and $\sum_{i<j} z_i^2 z_j^2$. In order to achieve two-strata rotatability, the

prediction variance should be a function of ρ_w^2 and ρ_s^2 only. Therefore, we need to cancel the interaction terms with $\sum_{i<j} x_i^2 x_j^2$ and $\sum_{i<j} z_i^2 z_j^2$, which by Equations 3.7-3.9 gives

$$interaction = 0 \Longleftrightarrow \begin{cases} 2e - 2p + \frac{1}{F_w^*} = 0, \\ 2h - 2f + (\sigma^2)\frac{1}{F_s} = 0. \end{cases}$$

Using the relationships in the Appendix gives the main result to achieve two-strata rotatability as

$$\begin{cases} \frac{2}{G-P} + \frac{1}{F_w^*} = 0, \\ \frac{2}{G-E} + (\sigma^2)\frac{1}{F_s} = 0, \end{cases} \tag{3.10}$$

In each of our four scenarios, the magnitude and the expression of G, E, P, F_w^* and F_s are different. We derive these values in the Appendix and the results are summarized in Table 3.6.

Table 3.6: The Summary of the Main Result to Achieve Two-Strata Rotatability In Split-Plot CCDs

	Balanced	Unbalanced
S_O is a subset of WP effects	Table 3.3 $\begin{cases} \alpha = \sqrt[4]{\frac{F_w}{n}}, \\ \beta = \sqrt[4]{\frac{2(1+nd)F_s}{n}} \end{cases}$	Table 3.4 $\begin{cases} \alpha = \sqrt[4]{\frac{2C_1F_w}{rC_2}} = \sqrt[4]{\frac{2F_w(1+n_{WA}d)}{r(1+n_{WF}d)}} \\ \beta = \sqrt[4]{\frac{2F_s}{a\sigma^2 C_3}} = \sqrt[4]{\frac{2F_s(1+n_{SA}d)}{a}} \end{cases}$
S_O is not a subset of WP effects	Table 3.1,3.2 $\begin{cases} \alpha = \sqrt[4]{\frac{F_w}{n}} \\ \beta = \sqrt[4]{\frac{4F_s}{n}} \end{cases}$	Table 3.5 $\begin{cases} \alpha = \sqrt[4]{\frac{2C_1F_w}{rC_2}} = \sqrt[4]{\frac{2F_w(1+n_{WA}d)}{r(1+n_{WF}d)}} \\ \beta = \sqrt[4]{\frac{2F_s}{a}} \end{cases}$

This result gives us several interesting findings. First notice that the format of the given

α and β are quite similar to Box and Hunter (1957)'s rotatable value. This is not surprising since our two-strata rotatable design inherits most of the properties in Box and Hunter (1957). Second, the balanced scenarios are special cases of the unbalanced scenarios. The derived balanced condition is exactly the same as the one from the unbalanced condition, when the parameters in the balanced design are correctly rewritten as the parameters in the unbalanced design. For example, for the balanced design in Table 3.3, using the notation and the result from the unbalanced scenarios, which is $C_1 = C_2 = C_3$, $r = 2n$, $a = n$, the reduced condition is the same as the one listed in Table 3.6. For the design in Table 3.1, similarly, the balanced condition can also be derived by using $C_1 = C_2$, $r = 2n$ and $a = \frac{n}{2}$. Third, it should be noted that the conditions for α and β in the balanced designs in Table 3.6 are derived without whole plot replication for the whole plots containing axial runs. If the whole plots containing axial runs are replicated, then G and H in moment matrix will not be the same function of n as derived in the Appendix. Instead, they will be the same function of r and a in the conditions for the unbalanced designs. Therefore we can safely use the unbalanced condition as a general condition for both balanced and unbalanced designs, see Table 3.7. Finally, for most of the scenarios, the condition depends on unknown variance component ratio d. When the design is balanced and $\boldsymbol{S}_O$ is not whole plot effects, the condition does not depend on d, which is a desirable property. However, it loses the ability to do exact test for pure subplot quadratic effects.

Table 3.7: The General Condition to Achieve Two-Strata Rotatability In Balanced and Unbalanced Split-Plot CCDs

S_O is a subset of WP effects	$\begin{cases} \alpha = \sqrt[4]{\frac{2C_1F_w}{rC_2}} = \sqrt[4]{\frac{2F_w(1+n_{WA}d)}{r(1+n_{WF}d)}} \\ \beta = \sqrt[4]{\frac{2F_s}{a\sigma^2C_3}} = \sqrt[4]{\frac{2F_s(1+n_{SA}d)}{a}} \end{cases}$
S_O is not a subset of WP effects	$\begin{cases} \alpha = \sqrt[4]{\frac{2C_1F_w}{rC_2}} = \sqrt[4]{\frac{2F_w(1+n_{WA}d)}{r(1+n_{WF}d)}} \\ \beta = \sqrt[4]{\frac{2F_s}{a}} \end{cases}$

3.2.2 Results and Discussions

Rotatable CCD and Two-Strata Rotatable Split-Plot CCD

Effectively, a completely randomized CCD can be treated as a balanced split-plot CCD with $d = 0$. So the design can be thought of as having every design point allocated into whole plots of size one with $N = F + 2k + n_c$ whole plots. Now $n_i = 1$, $r = 2$, $a = 2$ and $\boldsymbol{S}_O$ is part of the whole plot effects. Box and Hunter (1957) give the exact condition to make such CCD rotatable as $\alpha = \beta = \sqrt[4]{F}$. Based on our general condition in Table 3.7, now we have $C_1 = C_2 = C_3 = 1$, then our $\alpha = \sqrt[4]{\frac{2F_w}{r}} = \sqrt[4]{F}$ and $\beta = \sqrt[4]{\frac{2F_s(1+nd)}{a}} = \sqrt[4]{F}$, which is exactly the same as the Box and Hunter (1957) condition. Therefore, when d is equal to zero and thus the subplot quadratic effects are effectively the whole plot effects, the rotatable CCD is the same design given by two-strata rotatable split-plot CCD. Actually it can be seen from the definition too. Rotatable designs require that the prediction variance be a function of $\rho_w^2 + \rho_s^2$ and the two-strata rotatable design requires that the prediction variance is a function of ρ_w^2 and ρ_s^2. Any function of $\rho_w^2 + \rho_s^2$ must be a function of ρ_w^2 and ρ_s^2. However, any function of ρ_w^2 and ρ_s^2 is not necessarily a function of $\rho_w^2 + \rho_s^2$. Thus two-strata rotatable designs are a more general class of designs. It is a natural extension of the traditional rotatable design to the second-order split-plot case.

Alias Structure in Two-Strata Rotatable split-plot CCD

Since the idea of two-strata rotatable split-plot CCD is similar to a rotatable CCD, these two class of designs share similar properties and limitations. In a second-order rotatable CCD, the factorial part has to be a full factorial or a Resolution V fractional factorial design. The reason for this is to ensure that all the odd moments are zero. For example, suppose the resolution in a five-factor rotatable CCD is less than V. Consider a Resolution III design with a design generator of $I = ABC$. Therefore, the main effect A is aliased with two-way interaction BC. Thus, in moment matrix $\boldsymbol{X'X}$, the moment between A and BC, [123], can be easily derived as F instead of 0. Similarly, in a Resolution IV CCD with a design generator of $I = ABCD$, the moment [1234] is F instead of 0. Hence the third condition in Equation 2.1 for achieving Box and Hunter (1957)'s rotatability is not satisfied. Therefore, when the factorial part of the CCD is not at least resolution V, even when $\alpha = \sqrt[4]{F}$ is chosen, the design is not rotatable.

The same result is true for two-strata rotatable split-plot CCDs. To achieve two-strata rotatability, the odd moments up to order of four must be zero. Therefore, if the resolution in fractional factorial part is not at least V, some corresponding odd moments will not be zero and thus two-strata rotatability can not be achieved.

Model Dependence

Rotatable designs require the model to be a full k^{th} order model, which means it contains main effects, all the interactions and pure k^{th} order effects. For example, from Box and Hunter's condition, we know that a 2-factor factorial design is a first-order rotatable design. However, if the model contains first-order interaction effects in addition to first-order main effects, this factorial design is not rotatable since the prediction variance will involve interaction effects which can not be canceled. Specifically, $Var(\hat{y}(x)) = \frac{\sigma^2}{4}(1 + x_1^2 + x_2^2 + x_1^2 * x_2^2) \neq f(x_1^2 + x_2^2)$.

Two-strata rotatable split-plot designs require similar but more relaxed model assumptions. In the same example above, the 2-factor factorial design is not rotatable but it is two-strata rotatable since $Var(\hat{y}(x)) = \frac{\sigma^2}{4}(1 + z_1^2 + x_1^2 + z_1^2 * x_1^2) = f(z_1^2, x_1^2)$. For a second-order model with no whole plot and subplot interaction effects, the proposed CCDs can still be two-strata rotatable using the same conditions previously derived.

Center Runs

In both rotatable designs and two-strata rotatable split-plot designs, the condition depends on moments, which are the sum of the columns in design matrix. No matter how many center runs are added to the design, the sum of the columns will remain the same. Thus, the condition for rotatability and two-strata rotatability will not change. For this reason, we do not discuss the addition of center runs to the design.

3.2.3 Summary

Since rotatability is not achievable in split-plot central composite designs, we have proposed two-strata rotatable split-plot central composite designs. In our proposed designs, the prediction variance is a function of the whole plot distance and the subplot distance separately. We have discussd several scenarios and derived the conditions for axial distances α and β that achieve two-strata rotatability in split-plot central composite designs. The unbalanced condition has the balanced condition as a special case. Based on the definition, two-strata rotatable split-plot designs are a natural extension of the rotatable designs in split-plot case. A completely randomized CCD can be effectively treated as a split-plot CCD with $d = 0$ and our conditions reduce to the same result as the one by Box and Hunter (1957). Two-strata rotatable designs require less restriction on model. Finally, the number of center runs will not affect two-strata rotatability.

Chapter 4

Robustness of Two-Strata Rotatability in Split-Plot Central Composite Designs

4.1 Introduction

In practice, it is often impossible to set the factors at the required α-level for rotatability. Thus, the resulting design is not rotatable. In the completely randomized case, Khuri (1988) and Draper and Pulkesheim (1990) propose different measures to quantify "how rotatable" a non-rotatable design is. They compare the moments of a non-rotatable design to the corresponding moments of the rotatable design and propose a R^2 like measure. The non-rotatable design is more rotatable when the measure is closer to 100%.

In some two-strata rotatable split-plot central composite designs, the design setting depends on the unknown variance components ratio, $d = \frac{\sigma_\delta^2}{\sigma^2}$. When d is correctly specified, the design is exactly two-strata rotatable. However, in reality, d is often unknown before the set up of the design. Therefore, there is a great possibility for a practitioner to misspecify d. If a misspecified d is used instead of the true variance components ratio d_0 to construct two-strata rotatable split-plot central composite design, then the resulting α and β will deviate from the true two-strata rotatable level. Hence, the prediction variance will not be a function of whole plot distance and subplot distance alone. The resulting design is not two-strata rotatable. To deal with this natural problem, there are several possible approaches. One approach to correct misspecification of d is to use historical data and estimate historical d using statistical software. It is the most natural and the easiest way to obtain a reasonable estimate of d. However, it has several disadvantages. First, the historical data may not reflect the most current experimental situation. Thus, the historical d may not be accurate for the current situation. Second, in most industrial situations, historical data is not readily available. For example, an exploratory experiment in the pharmaceutical industry is often new. In these situations, the historical approach will not work. Another approach is a sequential approach, which is based on the "sequential" nature of the response surface methodology. In the completely randomized case, the central composite design is a popular choice for fitting a second-order model. The practitioners can run a full factorial or Resolution V factorial design with center runs first. Then a test for curvature can be conducted. If the sum of the squares for curvature is significant, then a first-order design may not be a good approximation of the true response surface. Axial runs can then be added to estimate the second order effect. We can employ the same sequential idea in the two-strata rotatable split-plot design case. The practitioners can run a full factorial or Resolution V fractional factorial split-plot design with center runs first and calculate the sum of squares for curvature. If the curvature effect is significant, then the whole plots of axial runs can be augmented to the initial design. A sequential estimate of d can be calculated in the first step and the values of whole plot axial runs and subplot axial runs can be calculated based on the sequential estimate of d. These two approaches are the solutions from the view of experimental process. Another approach from a design point of view is to study the robustness of the two-strata rotatable split-plot design. If the performance of the two-strata rotatable design, which is in terms of prediction variance, is roughly the same across a wide range of d, then the design is robust to the misspecification of d.

4.2 Two Methods to Measure Robustness

We propose two methods to measure "how two-strata rotatable" a split-plot central composite design is when d is misspecified. The first method is a numerical measure, which quantifies the two-strata rotatability. The second more intuitive method is to construct contour plots in both the whole plot and the subplot spaces. The shape of the contour plots is the actual reflection of the behavior of the prediction variance of the design. If the design is two-strata rotatable, the contour plots are perfect circles. The less two-strata rotatable the design is, the more the shape deviates from perfect circles. However, to judge "how different" the contour plots are from perfect circles is subjective. If there are two designs and the two-dimension contour plot from one design is like a square, say, and the shape from the other design is like a spade, it is hard to say which is more two-strata rotatable by visual inspection alone. Therefore, the best way to evaluate the two-strata rotatability for a two-strata rotatable split-plot central composite design is to use both methods together to get a better idea of the performance of the design.

4.2.1 Two-Strata Rotatability Measure

Following Khuri (1988) and Draper and Pulkesheim (1990), we propose a similar measure to evaluate the robustness in two-strata rotatable designs. Suppose we have two designs with different values of d. The design constructed with the true d, d_0, is denoted as D_0 and the design constructed with user specified d_1 is denoted as D_1. In two-strata rotatable split-plot central composite designs, different ds lead to different values for axial run distances and thus a different moment matrix, $\boldsymbol{X}'\boldsymbol{\Sigma}^{-1}\boldsymbol{X}$. From chapter 3, it is clear that the prediction variance depends on the entries in moment matrix, which involve d. When d changes, the whole moment matrix will change and thus the prediction variance changes. Therefore, the most natural way to compare these two designs is to compare their moment matrices. Following Khuri (1998) and Draper and Pulkesheim (1990), it seems natural and reasonable to use Euclidean norm to measure the difference between the two moment matrices. Let A_{d_i} be the moment matrix for given d_i in design D_i and $\|A_{d_i}\|$ be the Euclidean norm for matrix A_{d_i}, which is calculated by $[tr(A_{d_i})^2]^{1/2}$. We first define $Q^1 = \|(A_{d_0} - A_{d_1})\|^2$ as a difference measure which is similar to $Q_n(D)$ used in Khuri (1988). Khuri (1988) uses vectors and we use matrices. Q^1 takes all even order moments into consideration and measures the difference between the moment matrices A_{d_0} and A_{d_1}. When the user specified d_1 is exactly the same as d_0, $D_0 = D_1$ and the moment matrices are exactly the same. Correspondingly, $Q^1 = 0$. When the user specified d_1 is quite different from d_0, we expect the moment matrices to be quite different. Therefore, Q^1 will be large. This measure is quite useful when we have two user specified designs with d_1 and d_2 respectively. For a specific d_0, each design can be compared with D_0 and calculate corresponding Q^1. The design with a smaller Q^1, thus smaller departure from D_0, can be described as more "two-strata rotatable".

If there is only one user specified candidate design D_1, we can not get sufficient information about the performance of two-strata rotatability using Q^1 since there is no criterion, or a clear specification, for the value of Q^1 to distinguish whether the design is “close” to two-strata rotatable or “far from” two-strata rotatable. The value of Q^1 could be very large. Therefore, we propose another measure Q^0 to quantify its two-strata rotatability.

$$Q^0 = \frac{\|A_{d_1}\|^2 - \min(\|(A_{d_0} - A_{d_1})\|^2, \|A_{d_1}\|^2)}{\|A_{d_1}\|^2} = \frac{\|A_{d_1}\|^2 - \min(Q^1, \|A_{d_1}\|^2)}{\|A_{d_1}\|^2}.$$

Similar to Khuri (1988) and Draper and Pulkesheim (1990), Q^0 is a ratio. The denominator is the Euclidean norm of the moment matrix of the non two-strata rotatable design. The numerator is the norm of the part that can be explained by “two-strata rotatability”. Q^0 is between 0 to 1. When the user correctly specifies d_1, the difference measure Q^1 is zero, and thus, $Q^0 = 1$. Hence, the user specified design is 100% two-strata rotatable. When the user specifies d_1 far from d_0, the difference between A_{d_0} and A_{d_1} could be large. These designs can be called “totally wrong” designs in terms of d. The prediction variance calculated from these designs is severally distorted from perfect circles or hyper-sphere. Therefore, theses designs are far from two-strata rotatable. By using a minimum on the numerator, a design that is “totally wrong” will have $Q^0 = 0$, which means the design is 0% two-strata rotatable. It provides a boundary to distinguish ”total wrong” two-strata rotatable designs. Hence, a design with a value of Q^0 can be described as Q^0% two-strata rotatable. A design is more two-strata rotatable with larger values for Q^0.

4.2.2 Contour Plots in Whole Plot Space and Subplot Space

One intuitive way of judging the performance of two-strata rotatability is by using contour plots. If the design is exactly two-strata rotatable, the contour plots in the whole plot space and the subplot space should be perfect circles. If the design is "totally wrong", the contour plots should be far from perfect circles.

Calculation of Prediction Variance When d is MisSpecified

When d is correctly specified, the prediction variance $Var(\hat{y}(\boldsymbol{x}_0))$ is calculated by

$$\boldsymbol{x}_0{}'(\boldsymbol{X}'\boldsymbol{\Sigma}^{-1}\boldsymbol{X})^{-1}\boldsymbol{x}_0.$$

When d is not correctly specified, $Var(\hat{y}(\boldsymbol{x}_0))$ should be calculated by

$$\boldsymbol{x}_0{}'(\boldsymbol{X}'\boldsymbol{\Sigma}^{-1}\boldsymbol{X})^{-1}\boldsymbol{X}'\boldsymbol{\Sigma}^{-1}\boldsymbol{\Sigma}_0\boldsymbol{\Sigma}^{-1}\boldsymbol{X}(\boldsymbol{X}'\boldsymbol{\Sigma}^{-1}\boldsymbol{X})^{-1}\boldsymbol{x}_0,$$

where $\boldsymbol{\Sigma}_0 = \sigma^2(\boldsymbol{I} + d_0\boldsymbol{M}\boldsymbol{M}')$, and $\boldsymbol{\Sigma} = \sigma^2(\boldsymbol{I} + d_1\boldsymbol{M}\boldsymbol{M}')$. Without loss of generality, we can let $\sigma^2 = 1$. Thus, the prediction variance involves only the design structure, d_0 and d_1.

Choice of d and Simulation Details

Since d_0 is usually unknown, we use a simulation study to see the behavior of the contour plots and the prediction variance. To determine reasonable values of d_0, we looked at the literature. Letsinger et al. (1996) study a split-plot experiment with d=1.04. Bisgaard and Steinberg (1997) state that the whole plot variance is usually larger than subplot variance in prototype experiments for many applications. Webb, Lucas and Borkowski (2002) described an experiment with variance ratio 6.92 in a computer component manufacturing company. Vining, Kowalski and Montgomery (2005) estimate $d = 5.65$ using pure error method. The values of d that appear in the literature range from 1.04 to 6.92. Therefore, to be comprehensive we study the robustness of two-strata rotatability with d_0 going from 1 to 10 by increments of 0.5. For each d_0, we then compute Q^0 with d_1 in the same range as d_0.

When dimensionality increases, the contour plots will be very hard to visualize and not intuitive. We only show contour plots for two-dimensional designs here. The results should be able to extend to higher dimensional designs. For contour plots in the whole plot space, we fix the subplot distance at 1 and compute the scaled prediction variance in 10,000 grids from the unit square $[-1, 1] \times [-1, 1]$ in the whole plot space for each d_0 and d_1. For contour plots in the subplot space, we fix the whole plot distance at 1 and compute the scaled prediction variance in 10,000 grids from the unit square $[-1, 1] \times [-1, 1]$ in the subplot space for each d_0 and d_1.

Scaling Issue

In the completely randomized case, the prediction variance is $Var(\hat{\boldsymbol{y}}(\boldsymbol{x})) = \boldsymbol{x}'(\sigma^2(\boldsymbol{X}'\boldsymbol{X})^{-1})\boldsymbol{x}$. In graphical studies of the direct effect of the design structure on the prediction variance, it is common to scale the prediction variance by σ^2 so that the scaled prediction variance (SPV) only depends on design matrix $\boldsymbol{X}$. The scaled prediction variance is $\frac{Var(\hat{\boldsymbol{y}}(\boldsymbol{x}))}{\sigma^2} = \boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}$.

In the split-plot case, the prediction variance is $Var(\hat{\boldsymbol{y}}(\boldsymbol{x})) = \boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{\Sigma}^{-1}\boldsymbol{X})^{-1}\boldsymbol{x}$ and $\boldsymbol{\Sigma}^{-1}$ involves unknown variance components. It is needed to find a way to scale the prediction variance to minimize the effect of the unknown variance components.

We use the balanced split-plot single replicate factorial design with model having first-order terms and first-order whole plot and subplot interaction terms as a starting point. The reason we use these designs is that they are not only two-strata rotatable but also OLS-GLS equivalent. This makes the calculation for the prediction variance more mathematical tractable. It will shed light on the scaling issue for a second-order two-strata rotatable design.

When the design is OLS-GLS equivalent, we have $(\boldsymbol{X}'\boldsymbol{\Sigma}^{-1}\boldsymbol{X})^{-1}\boldsymbol{X}'\boldsymbol{\Sigma}^{-1}\boldsymbol{y} = (\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{X}'\boldsymbol{y}, \forall \boldsymbol{y}$. Therefore, we have $(\boldsymbol{X}'\boldsymbol{\Sigma}^{-1}\boldsymbol{X})^{-1}\boldsymbol{X}'\boldsymbol{\Sigma}^{-1} = (\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{X}'$. Hence, the prediction variance can be reduced to $\boldsymbol{x}_0{}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{X}'\boldsymbol{\Sigma}_0\boldsymbol{X}(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}_0$. If we write $\boldsymbol{X} = [\boldsymbol{W}, \boldsymbol{S}_D]$, similar to Equation 3.1, it can be shown that

$$(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{X}'\boldsymbol{\Sigma}_0\boldsymbol{X}(\boldsymbol{X}'\boldsymbol{X})^{-1} = \begin{bmatrix} (\sigma^2 + nd_0\sigma^2)(\boldsymbol{W}'\boldsymbol{W})^{-1} & \boldsymbol{0} \\ \boldsymbol{0} & \sigma^2(\boldsymbol{S}_D'\boldsymbol{S}_D)^{-1} \end{bmatrix}. \tag{4.1}$$

If we write $\boldsymbol{x}' = (\boldsymbol{x}_w', \boldsymbol{x}_{s_D}')$, the prediction variance can be written as

$$(\sigma^2 + nd_0\sigma^2)\boldsymbol{x}_w'(\boldsymbol{W}'\boldsymbol{W})^{-1}\boldsymbol{x}_w + \sigma^2\boldsymbol{x}_{S_D}'(\boldsymbol{S}_D'\boldsymbol{S}_D)^{-1}\boldsymbol{x}_{S_D}.$$

When $\sigma^2 = 1$, it can be written as

$$(1 + nd_0)\boldsymbol{x}_w'(\boldsymbol{W}'\boldsymbol{W})^{-1}\boldsymbol{x}_w + \boldsymbol{x}_{S_D}'(\boldsymbol{S}_D'\boldsymbol{S}_D)^{-1}\boldsymbol{x}_{S_D}.$$

In following discussion, we write d_0 as d. It is clear that there are two multipliers for the two parts: $1 + nd$ for the first part and 1 for the second part. The first part only involves the whole plot distance and the second part involves both the whole plot distance and the subplot distance. The prediction variance is a weighted average of the two parts. To see the structure clearer, suppose the split-plot factorial design we are using has k_1 whole plot factors and k_2 subplot factors. Further suppose there are $m = 2^{k_1}$ whole plots and the whole plot size is $n = 2^{k_2}$. We can write explicitly the expression for the prediction variance as

$$\begin{aligned} Var(\hat{\boldsymbol{y}}(\boldsymbol{x})) &= (1+nd)\boldsymbol{x}'_w(\boldsymbol{W}'\boldsymbol{W})^{-1}\boldsymbol{x}_w + \boldsymbol{x}'_{S_D}(\boldsymbol{S}'_D\boldsymbol{S}_D)^{-1}\boldsymbol{x}_{S_D} \\ &= \frac{1+nd}{mn}(1+\rho_w^2) + \frac{1}{mn}(\rho_s^2 + \rho_s^2 * \rho_w^2) \\ &= \frac{1+nd+\rho_s^2}{mn}(1+\rho_w^2) \end{aligned} \tag{4.2}$$

It is clear that $1 + nd$ and ρ_s^2 are inseparable and there is no way to scale out the effect of d completely. For the contour plots in the whole plot space, if we fix the subplot distance at 1, Equation 4.2 becomes

$$\begin{aligned} Var(\hat{y}(x)) &= (1+nd)\boldsymbol{x}'_w(\boldsymbol{W}'\boldsymbol{W})^{-1}\boldsymbol{x}_w + \boldsymbol{x}'_{S_D}(\boldsymbol{S}'_D\boldsymbol{S}_D)^{-1}\boldsymbol{x}_{S_D} \\ &= \frac{2+nd}{mn}(1+\rho_w^2). \end{aligned} \tag{4.3}$$

Thus if the prediction variance is scaled by $2 + nd$, it will not depend on d. For the contour plots in the subplot space, if we fix the whole plot distance at 1, Equation 4.2 becomes

$$\begin{aligned} Var(\hat{y}(x)) &= (1+nd)\boldsymbol{x}'_w(\boldsymbol{W}'\boldsymbol{W})^{-1}\boldsymbol{x}_w + \boldsymbol{x}'_{S_D}(\boldsymbol{S}'_D\boldsymbol{S}_D)^{-1}\boldsymbol{x}_{S_D} \\ &= \frac{2(1+nd+\rho_s^2)}{mn}. \end{aligned} \tag{4.4}$$

We have tried several common scaling methods for Equation 4.3 and Equation 4.4 in Mathematica, and the results are listed below in Figure 4.1. From Figure 4.1, we can see that when the prediction variance is scaled by $1 + d$, the prediction variance in the whole plot space is almost constant for a specific d. In the subplot space, the prediction variance is almost a first-order constant plane when d is approximately greater than 1. Changing d and fixing the whole plot distance at 1 does not seem to be an issue. Furthermore, scaling by $1 + d$ has a theoretical advantage over other possible scaling schemes. It will give us a compound symmetry correlation matrix for each whole plot as a neat function of d. When we assume $\sigma^2 = 1$, $\frac{\boldsymbol{X}'\boldsymbol{\Sigma}^{-1}\boldsymbol{X}}{1+d} = \frac{\boldsymbol{X}'\boldsymbol{\Sigma}^{-1}\boldsymbol{X}}{\sigma^2+\sigma_\delta^2}$. If we define $\boldsymbol{V} = \frac{\boldsymbol{\Sigma}}{\sigma^2+\sigma_\delta^2}$, the scaled prediction variance can be written as

$$SPV = \frac{Var(\hat{\boldsymbol{y}}(\boldsymbol{x}))}{1+d} = \frac{Var(\hat{\boldsymbol{y}}(\boldsymbol{x}))}{\sigma^2+\sigma_\delta^2} = \boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{V}^{-1}\boldsymbol{X})^{-1}\boldsymbol{x}.$$

Specifically,

$$\boldsymbol{V} = \boldsymbol{I}_m \bigotimes \boldsymbol{V}_i, \boldsymbol{V}_i = \begin{pmatrix} 1 & \frac{d}{1+d} & \cdots & \frac{d}{1+d} \\ \frac{d}{1+d} & 1 & \cdots & \frac{d}{1+d} \\ \vdots & \vdots & \vdots & \vdots \\ \frac{d}{1+d} & \frac{d}{1+d} & \cdots & 1 \end{pmatrix},$$

and $\frac{d}{1+d}$ equals the within-whole-plots correlation. When d is misspecified, the scaled prediction variance becomes

$$\boldsymbol{x}_0{}'(\boldsymbol{X}'\boldsymbol{\Sigma}^{-1}\boldsymbol{X})^{-1}\boldsymbol{X}'\boldsymbol{\Sigma}^{-1}\boldsymbol{V}_0\boldsymbol{\Sigma}^{-1}\boldsymbol{X}(\boldsymbol{X}'\boldsymbol{\Sigma}^{-1}\boldsymbol{X})^{-1}\boldsymbol{x}_0.$$

The contour plots in both the whole plot and the subplot space for the factorial split-plot design with two whole plot factors and two subplot factors are shown in Figure 4.2. As expected, they are perfect circles and the values on the subplot contour plots are very close as d increases.

Contour Plots of Second-Order Split-Plot Central Composite Designs

In second order split-plot central composite designs, when the design is balanced, OLS-GLS equivalent and $\boldsymbol{S}_O$ being WP effects, the prediction variance Equation 3.1 is of the same format as Equation 4.1. We can safely extend the scaling scheme recommended in first order split-plot designs to second order designs. The scaled contour plots for balanced and $\boldsymbol{S}_O$ being not WP effects second-order split-plot central composite designs are listed in Figure 4.3. In the contour plots, each column corresponds to a specific d_0. Each row corresponds a user specified d_1. It can be seen that the contour plots conform with Q^0 very well. Along every column, when $d_1 = d_0$, the contour plots are perfect circles and $Q^0 = 1$. When d_1 is further away from d_0, Q^0 becomes smaller and the contour plots become more distorted. For example, when $d_0 = 1$, Q^0 decreases from 100% to 69% if user misspecifies d from 1 to 10. From contour plots, it is clear that when $d_1 = d_0 = 1$, the contour plots are perfect circles and when d_1 is further away from d_0, the circles become more and more like a spade. When $d_0 = 10$ and $d_1 = 1$, $Q^0 = 0.06$ tells us that the design is only 6% two-strata rotatable. The contour plots are also far from perfect circles. When d_1 increases to $d_0 = 10$, Q^0 becomes larger and the contour plots are more like perfect circles, thus the design is more two-strata rotatable,

The scaled whole plot contour plots for an unbalanced split-plot CCD when S_O is not a whole plot effect are shown in Figure 4.4. The scaled subplot contour plots for an unbalanced split-plot CCD when S_O is WP effect are shown in Figure 4.5. The whole plot contour plots for the same design are shown in Figure 4.6. Again it is clear that Q^0 are in well compliance with the contour plots. The contour plots in both spaces are very close to perfect circles and the Q^0 is from 75% to 100%. Within each column, Q^0 becomes smaller as d_1 is further away from d_0.

From all second-order contour plots and Q^0 values for different non two-strata rotatable central composite designs, we can summarize that when Q^0 is approximately greater than 80%, the design is near two-strata rotatable. For the VKM CCD, the design is a little bit more sensitive to the misspecification of d, but it is still robust as long as d is estimated in a reasonable range. The unbalanced split-plot CCD is more robust to the misspecification of d.

4.3 Summary

When the unknown variance component ratio d is misspecified, the constructed split-plot design is no longer two-strata rotatable. Following Khuri (1988) and Draper and Pulkesheim (1990), we propose two methods for evaluating the two-strata rotatability of a non two-strata rotatable split-plot central composite design. The first one is a numerical measure, Q^0. Basically it compares the norm of the moment matrix of the non two-strata rotatable design to the norm of the two-strata rotatable design. As Q^0 increases, the design is more two-strata rotatable. The second method uses contour plots in both the whole plot space and the subplot space. It is more intuitive but subjective. In addition, contour plots are harder to implement in higher dimensions. We recommend scaling the prediction variance by $1 + d$. We have applied these two methods to various designs and find that they agree with each other quite well and recommend combining them together to evaluate a design.

Table 4.1: Q^0 for Balanced Non Two-Strata Rotatable VKM Split-Plot CCD (2,2)

$d_1 \backslash d_0$	1.00	1.50	2.00	2.50	3.00	3.50	4.00	4.50	5.00	5.50	6.00	6.50	7.00	7.50	8.00	8.50	9.00	9.50	10.00
1.00	1.00	0.98	0.95	0.91	0.87	0.82	0.77	0.72	0.67	0.61	0.56	0.50	0.44	0.38	0.31	0.25	0.19	0.12	0.06
1.50	0.99	1.00	0.99	0.97	0.95	0.92	0.88	0.85	0.81	0.76	0.72	0.67	0.63	0.58	0.53	0.47	0.42	0.37	0.31
2.00	0.96	0.99	1.00	0.99	0.98	0.96	0.94	0.92	0.89	0.85	0.82	0.79	0.75	0.71	0.67	0.63	0.58	0.54	0.50
2.50	0.93	0.98	1.00	1.00	1.00	0.99	0.97	0.96	0.93	0.91	0.89	0.86	0.83	0.80	0.77	0.73	0.70	0.66	0.63
3.00	0.91	0.96	0.99	1.00	1.00	1.00	0.99	0.98	0.96	0.95	0.93	0.91	0.89	0.86	0.84	0.81	0.78	0.75	0.72
3.50	0.89	0.94	0.97	0.99	1.00	1.00	1.00	0.99	0.98	0.97	0.96	0.94	0.92	0.90	0.88	0.86	0.84	0.81	0.79
4.00	0.86	0.92	0.96	0.98	0.99	1.00	1.00	1.00	0.99	0.99	0.98	0.96	0.95	0.94	0.92	0.90	0.88	0.86	0.84
4.50	0.84	0.91	0.94	0.97	0.98	0.99	1.00	1.00	1.00	0.99	0.99	0.98	0.97	0.96	0.95	0.93	0.92	0.90	0.88
5.00	0.83	0.89	0.93	0.96	0.97	0.99	0.99	1.00	1.00	1.00	1.00	0.99	0.98	0.97	0.96	0.95	0.94	0.93	0.91
5.50	0.81	0.87	0.91	0.94	0.96	0.98	0.99	1.00	1.00	1.00	1.00	1.00	0.99	0.99	0.98	0.97	0.96	0.95	0.94
6.00	0.79	0.86	0.90	0.93	0.95	0.97	0.98	0.99	1.00	1.00	1.00	1.00	1.00	0.99	0.99	0.98	0.97	0.96	0.95
6.50	0.78	0.84	0.89	0.92	0.94	0.96	0.97	0.98	0.99	1.00	1.00	1.00	1.00	1.00	0.99	0.99	0.98	0.98	0.97
7.00	0.76	0.83	0.87	0.91	0.93	0.95	0.97	0.98	0.99	0.99	1.00	1.00	1.00	1.00	1.00	0.99	0.99	0.98	0.98
7.50	0.75	0.82	0.86	0.89	0.92	0.94	0.96	0.97	0.98	0.99	0.99	1.00	1.00	1.00	1.00	1.00	0.99	0.99	0.99
8.00	0.74	0.80	0.85	0.88	0.91	0.93	0.95	0.96	0.97	0.98	0.99	0.99	1.00	1.00	1.00	1.00	1.00	1.00	0.99
8.50	0.73	0.79	0.84	0.87	0.90	0.92	0.94	0.95	0.97	0.98	0.98	0.99	0.99	1.00	1.00	1.00	1.00	1.00	1.00
9.00	0.71	0.78	0.83	0.86	0.89	0.91	0.93	0.95	0.96	0.97	0.98	0.99	0.99	1.00	1.00	1.00	1.00	1.00	1.00
9.50	0.70	0.77	0.82	0.85	0.88	0.90	0.92	0.94	0.95	0.96	0.97	0.98	0.99	0.99	1.00	1.00	1.00	1.00	1.00
10.00	0.69	0.76	0.81	0.84	0.87	0.89	0.91	0.93	0.95	0.96	0.97	0.98	0.98	0.99	0.99	1.00	1.00	1.00	1.00

Table 4.2: Q^0 for Unbalanced Non Two-Strata Rotatable Split-Plot CCD (2,2) When $\boldsymbol{S}_O$ is not WP Effect

$d_1 \backslash d_0$	1.00	1.50	2.00	2.50	3.00	3.50	4.00	4.50	5.00	5.50	6.00	6.50	7.00	7.50	8.00	8.50	9.00	9.50	10.00
1.00	1.000	0.984	0.960	0.937	0.919	0.904	0.891	0.881	0.872	0.864	0.858	0.852	0.847	0.843	0.839	0.836	0.832	0.830	0.827
1.50	0.986	1.000	0.995	0.985	0.976	0.968	0.961	0.954	0.949	0.944	0.940	0.937	0.933	0.931	0.928	0.926	0.923	0.922	0.920
2.00	0.965	0.995	1.000	0.998	0.994	0.989	0.985	0.981	0.977	0.974	0.971	0.969	0.966	0.964	0.962	0.961	0.959	0.958	0.957
2.50	0.946	0.986	0.998	1.000	0.999	0.997	0.994	0.992	0.989	0.987	0.985	0.983	0.982	0.980	0.979	0.978	0.976	0.975	0.974
3.00	0.932	0.978	0.994	0.999	1.000	0.999	0.998	0.997	0.995	0.994	0.992	0.991	0.990	0.988	0.987	0.986	0.985	0.985	0.984
3.50	0.919	0.971	0.989	0.997	0.999	1.000	1.000	0.999	0.998	0.997	0.996	0.995	0.994	0.993	0.992	0.992	0.991	0.990	0.990
4.00	0.909	0.964	0.985	0.994	0.998	1.000	1.000	1.000	0.999	0.999	0.998	0.997	0.997	0.996	0.995	0.995	0.994	0.994	0.993
4.50	0.901	0.959	0.982	0.992	0.997	0.999	1.000	1.000	1.000	1.000	0.999	0.999	0.998	0.998	0.997	0.997	0.996	0.996	0.995
5.00	0.894	0.954	0.978	0.990	0.995	0.998	0.999	1.000	1.000	1.000	1.000	0.999	0.999	0.999	0.998	0.998	0.998	0.997	0.997
5.50	0.888	0.950	0.975	0.988	0.994	0.997	0.999	1.000	1.000	1.000	1.000	1.000	1.000	0.999	0.999	0.999	0.998	0.998	0.998
6.00	0.883	0.946	0.973	0.986	0.992	0.996	0.998	0.999	1.000	1.000	1.000	1.000	1.000	1.000	0.999	0.999	0.999	0.999	0.999
6.50	0.879	0.943	0.970	0.984	0.991	0.995	0.997	0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000	0.999	0.999	0.999
7.00	0.875	0.940	0.968	0.982	0.990	0.994	0.997	0.998	0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	0.999
7.50	0.871	0.938	0.967	0.981	0.989	0.993	0.996	0.998	0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
8.00	0.868	0.935	0.965	0.980	0.988	0.992	0.995	0.997	0.998	0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
8.50	0.865	0.933	0.963	0.979	0.987	0.992	0.995	0.997	0.998	0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
9.00	0.863	0.931	0.962	0.977	0.986	0.991	0.994	0.996	0.998	0.998	0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000
9.50	0.861	0.930	0.961	0.976	0.985	0.990	0.994	0.996	0.997	0.998	0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000
10.00	0.858	0.928	0.959	0.976	0.984	0.990	0.993	0.995	0.997	0.998	0.999	0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000

Table 4.3: Q^0 for Unbalanced Non Two-Strata Rotatable Split-Plot CCD (2,2) When $\boldsymbol{S}_O$ is WP Effect

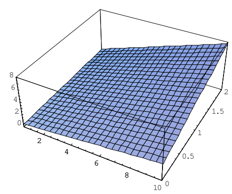
$d_1 \backslash d_0$	1.00	1.50	2.00	2.50	3.00	3.50	4.00	4.50	5.00	5.50	6.00	6.50	7.00	7.50	8.00	8.50	9.00	9.50	10.00
1.00	1.00	0.99	0.97	0.96	0.94	0.93	0.92	0.91	0.90	0.89	0.88	0.87	0.86	0.85	0.85	0.84	0.83	0.83	0.82
1.50	0.99	1.00	1.00	0.99	0.98	0.97	0.96	0.95	0.94	0.94	0.93	0.92	0.91	0.91	0.90	0.89	0.89	0.88	0.87
2.00	0.97	1.00	1.00	1.00	0.99	0.99	0.98	0.97	0.97	0.96	0.95	0.95	0.94	0.94	0.93	0.92	0.92	0.91	0.90
2.50	0.96	0.99	1.00	1.00	1.00	1.00	0.99	0.99	0.98	0.98	0.97	0.96	0.96	0.95	0.95	0.94	0.94	0.93	0.92
3.00	0.94	0.98	0.99	1.00	1.00	1.00	1.00	0.99	0.99	0.99	0.98	0.98	0.97	0.97	0.96	0.96	0.95	0.94	0.94
3.50	0.93	0.97	0.99	1.00	1.00	1.00	1.00	1.00	0.99	0.99	0.99	0.98	0.98	0.98	0.97	0.97	0.96	0.96	0.95
4.00	0.91	0.96	0.98	0.99	1.00	1.00	1.00	1.00	1.00	1.00	0.99	0.99	0.99	0.98	0.98	0.97	0.97	0.97	0.96
4.50	0.90	0.95	0.97	0.99	0.99	1.00	1.00	1.00	1.00	1.00	1.00	0.99	0.99	0.99	0.98	0.98	0.98	0.97	0.97
5.00	0.88	0.94	0.96	0.98	0.99	0.99	1.00	1.00	1.00	1.00	1.00	1.00	0.99	0.99	0.99	0.99	0.98	0.98	0.98
5.50	0.87	0.92	0.95	0.97	0.98	0.99	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	0.99	0.99	0.99	0.98	0.98
6.00	0.86	0.91	0.94	0.96	0.98	0.99	0.99	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	0.99	0.99	0.99	0.99
6.50	0.84	0.90	0.94	0.96	0.97	0.98	0.99	0.99	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	0.99	0.99	0.99
7.00	0.83	0.89	0.93	0.95	0.96	0.98	0.98	0.99	0.99	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	0.99	0.99
7.50	0.82	0.88	0.92	0.94	0.96	0.97	0.98	0.99	0.99	0.99	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	0.99
8.00	0.80	0.87	0.90	0.93	0.95	0.96	0.97	0.98	0.99	0.99	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00
8.50	0.79	0.85	0.89	0.92	0.94	0.96	0.97	0.98	0.98	0.99	0.99	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00
9.00	0.77	0.84	0.88	0.91	0.93	0.95	0.96	0.97	0.98	0.99	0.99	0.99	1.00	1.00	1.00	1.00	1.00	1.00	1.00
9.50	0.76	0.83	0.87	0.90	0.92	0.94	0.96	0.97	0.97	0.98	0.99	0.99	0.99	1.00	1.00	1.00	1.00	1.00	1.00
10.00	0.75	0.82	0.86	0.89	0.92	0.93	0.95	0.96	0.97	0.98	0.98	0.99	0.99	0.99	1.00	1.00	1.00	1.00	1.00

Figure 4.1: Scaled Prediction Variance in the Whole Plot Space and the Subplot Space as a Function of d and distance

In Whole Plot Space:

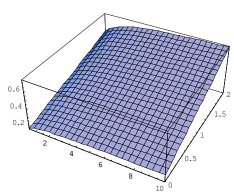
Unscaled PV:

Plot3D[((2+4x)/16)*(1+y),{x,0.5,10},{y,0,2}]



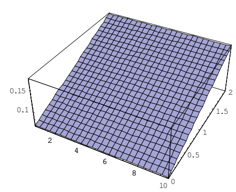
Scaled by 1+d:

Plot3D[((2+4x)/16)*(1+y)/(1+x),{x,0.5,10},{y,0,2}]



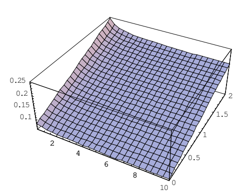
Scaled by 2+nd:

Plot3D[((2+4x)/16)*(1+y)/(2+4x),{x,0.5,10},{y,0,2}]



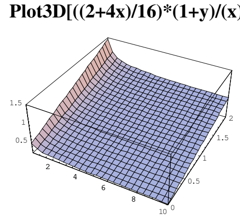
Scaled by 1+nd:

Plot3D[((2+4x)/16)*(1+y)/(1+4x),{x,0.5,10},{y,0,2}]



Scaled by d:

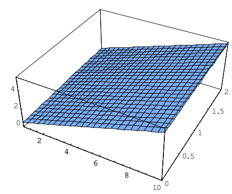
Plot3D[((2+4x)/16)*(1+y)/(x),{x,0.5,10},{y,0,2}]



In Subplot Space:

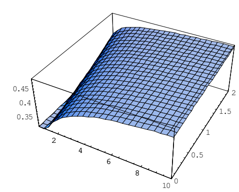
Unscaled PV:

Plot3D[((1+4x+y)/8),{x,0.5,10},{y,0,2}]



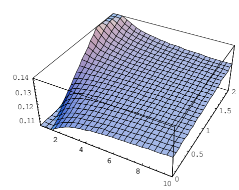
Scaled by 1+d:

Plot3D[((1+4x+y)/(8(1+x))),{x,0.5,10},{y,0,2}]



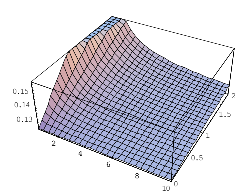
Scaled by 2+nd:

Plot3D[((1+4x+y)/(8(2+4x))),{x,0.5,10},{y,0,2}]



Scaled by 1+nd:

Plot3D[((1+4x+y)/(8(1+4x))),{x,0.5,10},{y,0,2}]



Scaled by d:

Plot3D[((1+4x+y)/(8x)),{x,0.5,10},{y,0,2}]

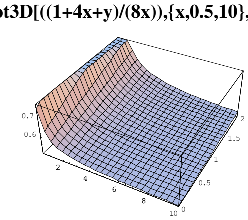
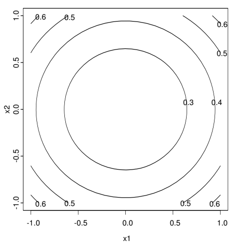


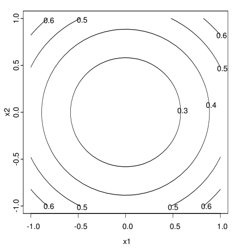
Figure 4.2: Contour Plots in the Whole Plot Space and the Subplot Space For Factorial Design (2,2) Scaled by $1 + d$

Whole Plot Contour Plots:

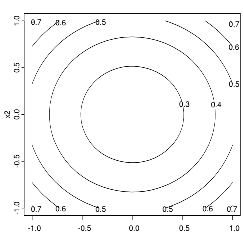
d=1



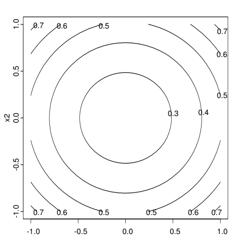
d=2



d=5

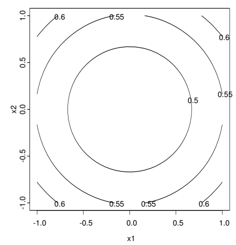


d=10

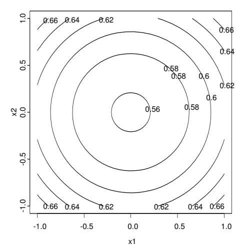


Subplot Contour Plots:

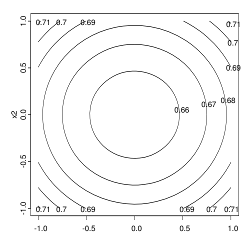
d=1



d=2



d=5



d=10

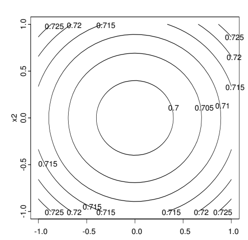


Figure 4.3: Subplot Contour Plots For the Balanced VKM CCD (2,2) Scaled by $1 + d$

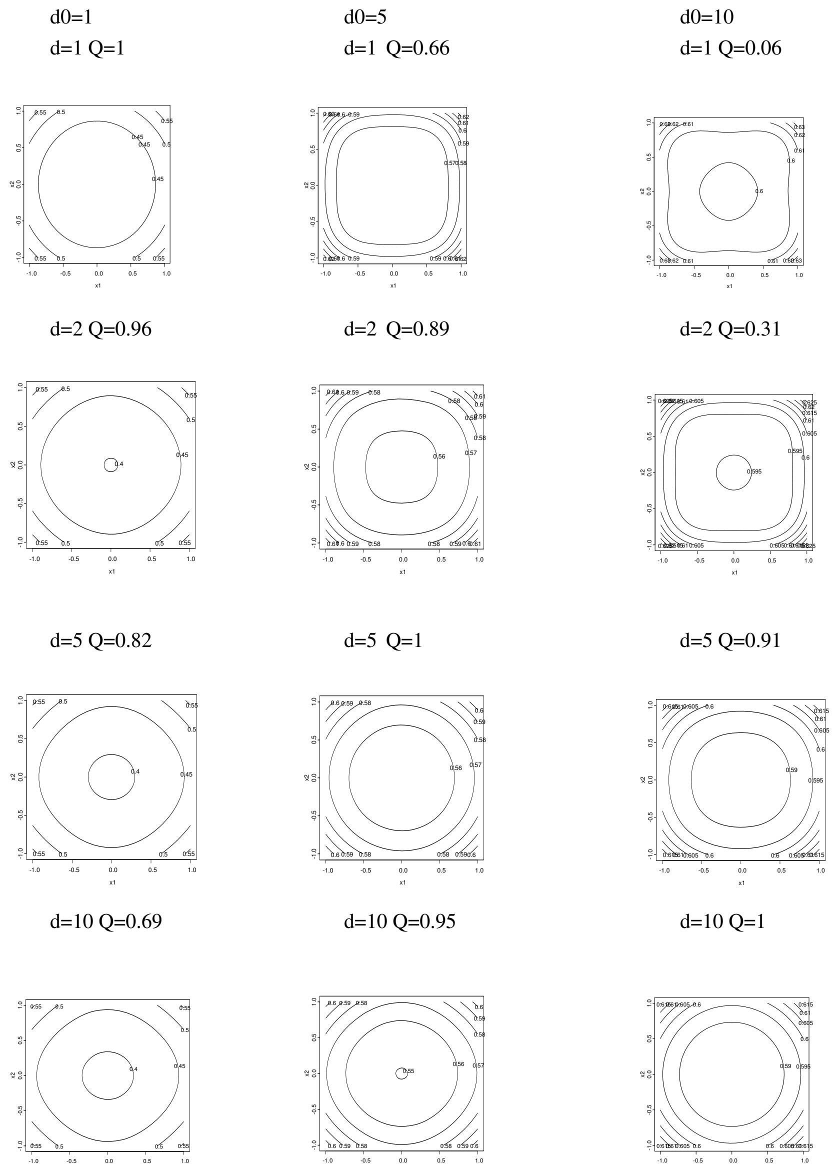


Figure 4.4: Whole Plot Contour Plots For the Unbalanced Split-Plot CCD (2,2) when S_O is not a WP Effect Scaled by $1 + d$

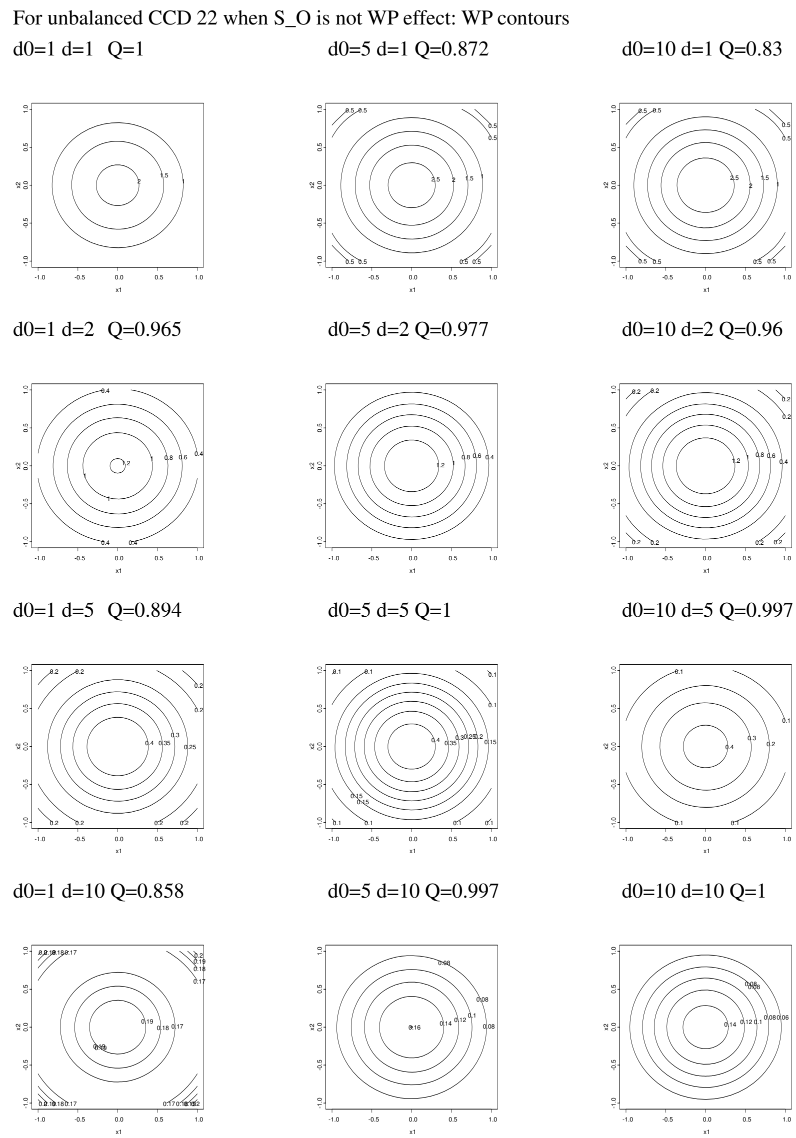


Figure 4.5: Subplot Contour Plots For the Unbalanced Split-Plot CCD (2,2) when S_O is WP Effect Scaled by $1 + d$

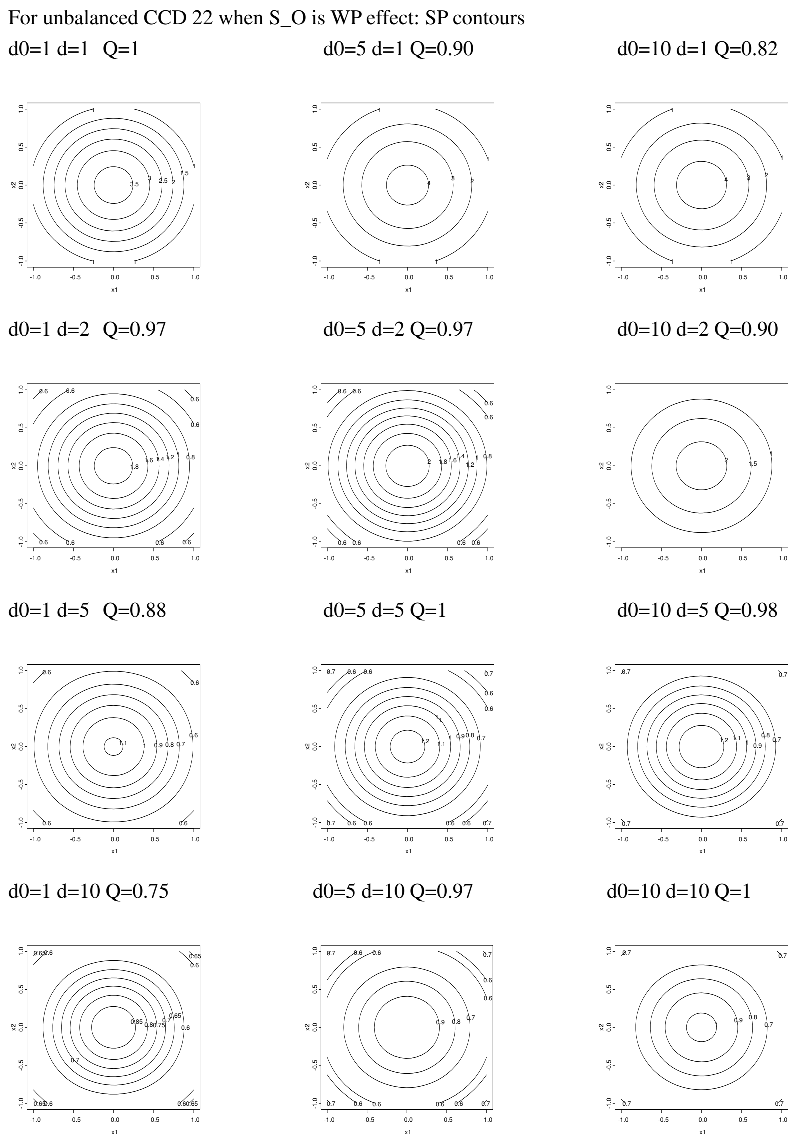
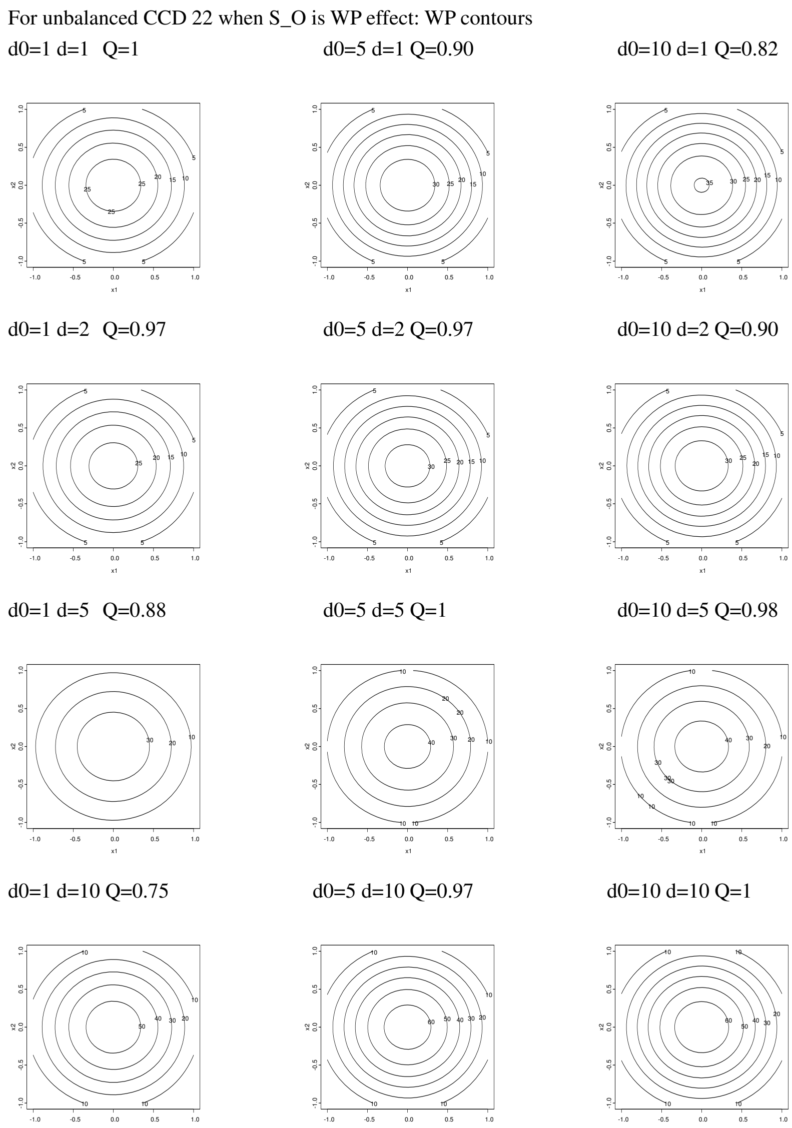


Figure 4.6: Whole Plot Contour Plots For the Unbalanced Split-Plot CCD (2,2) when S_O is WP Effect Scaled by $1 + d$



Chapter 5

Orthogonal Blocking in Split-Plot Central Composite Designs

5.1 Introduction

5.1.1 Relationships Between Orthogonal Blocking and OLS-GLS Equivalency in Split-Plot Designs

In a split-plot design, when all whole plots can not be performed under homogeneous conditions, blocks can be employed to increase the power to test treatment effects. In a blocked split-plot design, blocks are partitions of the whole plots instead of individual runs. Consider a split plot design with m whole plots each with n_i subplots. Thus we have $N = \sum_{i=1}^{m} n_i$ observations. The general model form is:

$$y = \boldsymbol{X}\boldsymbol{\beta} + \boldsymbol{M}\boldsymbol{\gamma} + \boldsymbol{\epsilon} \tag{5.1}$$

where $\boldsymbol{y}$ is the $N \times 1$ vector of responses, $\boldsymbol{X}$ is the $N \times p$ design matrix, $\boldsymbol{\beta}$ is the $p \times 1$ parameter vector associated with the p effects in the design, $\boldsymbol{M}$ is the $N \times m$ index matrix consisting of zeros and ones assigning the individual observations to the whole plots, $\boldsymbol{\gamma}$ is the $m \times 1$ vector of whole plot errors, and $\boldsymbol{\epsilon}$ is the $N \times 1$ vector of subplot errors. If we group the observations by different whole plots, then $\boldsymbol{M} = Diag(\mathbf{1}_{n_1}, \mathbf{1}_{n_2}, ..., \mathbf{1}_{n_m})$, where $\mathbf{1}_{n_i}$ is a $n_i \times 1$ vector of 1's. Assume that

$$E(\boldsymbol{\gamma}) = \mathbf{0}_m, \qquad Cov(\boldsymbol{\gamma}) = \sigma_\delta^2 \boldsymbol{I}_m$$

$$E(\boldsymbol{\epsilon}) = \mathbf{0}_N, \qquad Cov(\boldsymbol{\epsilon}) = \sigma^2 \boldsymbol{I}_N$$

$$Cov(\boldsymbol{\gamma}, \boldsymbol{\epsilon}) = \mathbf{0}_{m \times N},$$

then the resulting variance-covariance matrix for the observation vector $\boldsymbol{y}$ is:

$$Var(\boldsymbol{y}) = \boldsymbol{\Sigma} = \sigma^2 \boldsymbol{I} + \sigma_\delta^2 \boldsymbol{M}\boldsymbol{M}'$$

where $\boldsymbol{M}\boldsymbol{M}'$ is a block diagonal matrix with diagonal matrices of $\boldsymbol{J}_{n_1}, \boldsymbol{J}_{n_2}, ..., \boldsymbol{J}_{n_m}$ and $\boldsymbol{J}_{n_i}$ is a $n_i \times n_i$ matrix of 1's. The Best Linear Unbiased Estimator (BLUE) of $\boldsymbol{\beta}$ is the Generalized Least Square (GLS) estimator, $(\boldsymbol{X}'\boldsymbol{\Sigma}^{-1}\boldsymbol{X})^{-1}\boldsymbol{X}'\boldsymbol{\Sigma}^{-1}\boldsymbol{y}$. Now with fixed block effects, the model becomes

$$\begin{aligned} \boldsymbol{y} &= \bar{\boldsymbol{Z}}\boldsymbol{\xi} + \boldsymbol{X}\boldsymbol{\beta} + \boldsymbol{M}\boldsymbol{\gamma} + \boldsymbol{\epsilon} \\ &= \boldsymbol{U}\boldsymbol{\theta} + \boldsymbol{M}\boldsymbol{\gamma} + \boldsymbol{\epsilon} \end{aligned}$$

where $\boldsymbol{U} = (\bar{\boldsymbol{Z}}, \boldsymbol{X})$, $\boldsymbol{\theta} = (\boldsymbol{\xi}, \boldsymbol{\beta})$ and $\bar{\boldsymbol{Z}} = (\boldsymbol{I}_N - N^{-1}\mathbf{1}_N\mathbf{1}_N')\boldsymbol{Z}$ for block effect matrix $\boldsymbol{Z}$.

The GLS estimator of $\boldsymbol{\theta}$ becomes

$$\hat{\boldsymbol{\theta}} = \begin{pmatrix} \hat{\boldsymbol{\xi}} \\ \hat{\boldsymbol{\beta}} \end{pmatrix} = (\boldsymbol{U}'\boldsymbol{\Sigma}^{-1}\boldsymbol{U})^{-1}\boldsymbol{U}'\boldsymbol{\Sigma}^{-1}\boldsymbol{y} = \begin{pmatrix} \bar{\boldsymbol{Z}}'\boldsymbol{\Sigma}^{-1}\bar{\boldsymbol{Z}} & \bar{\boldsymbol{Z}}'\boldsymbol{\Sigma}^{-1}\bar{\boldsymbol{X}} \\ \bar{\boldsymbol{X}}'\boldsymbol{\Sigma}^{-1}\bar{\boldsymbol{Z}} & \bar{\boldsymbol{X}}'\boldsymbol{\Sigma}^{-1}\bar{\boldsymbol{X}} \end{pmatrix}^{-1} \begin{pmatrix} \bar{\boldsymbol{Z}}'\boldsymbol{\Sigma}^{-1}\boldsymbol{y} \\ \bar{\boldsymbol{X}}'\boldsymbol{\Sigma}^{-1}\boldsymbol{y} \end{pmatrix}.$$

One way to achieve orthogonal blocking is to examine the condition $\bar{\boldsymbol{X}}'\boldsymbol{\Sigma}^{-1}\bar{\boldsymbol{Z}} = 0$. However, this condition clearly depends on unknown variance components, which are needed to be estimated by REML or other techniques before constructing the design. It is often undesirable in practice.

To avoid calculating and estimating unknown variance components, we can construct OLS-GLS equivalent blocked split-plot designs to achieve orthogonal blocking. Once the blocked design is OLS-GLS equivalent, we have

$$\begin{aligned} \hat{\boldsymbol{\theta}} = \begin{pmatrix} \hat{\boldsymbol{\xi}} \\ \hat{\boldsymbol{\beta}} \end{pmatrix} &= (\boldsymbol{U}'\boldsymbol{\Sigma}^{-1}\boldsymbol{U})^{-1}\boldsymbol{U}'\boldsymbol{\Sigma}^{-1}\boldsymbol{y} = \begin{pmatrix} \bar{\boldsymbol{Z}}'\boldsymbol{\Sigma}^{-1}\bar{\boldsymbol{Z}} & \bar{\boldsymbol{Z}}'\boldsymbol{\Sigma}^{-1}\bar{\boldsymbol{X}} \\ \bar{\boldsymbol{X}}'\boldsymbol{\Sigma}^{-1}\bar{\boldsymbol{Z}} & \bar{\boldsymbol{X}}'\boldsymbol{\Sigma}^{-1}\bar{\boldsymbol{X}} \end{pmatrix}^{-1} \begin{pmatrix} \bar{\boldsymbol{Z}}'\boldsymbol{\Sigma}^{-1}\boldsymbol{y} \\ \bar{\boldsymbol{X}}'\boldsymbol{\Sigma}^{-1}\boldsymbol{y} \end{pmatrix} \\ &= (\boldsymbol{U}'\boldsymbol{U})^{-1}\boldsymbol{U}'\boldsymbol{y} = \begin{pmatrix} \bar{\boldsymbol{Z}}'\bar{\boldsymbol{Z}} & \bar{\boldsymbol{Z}}'\bar{\boldsymbol{X}} \\ \bar{\boldsymbol{X}}'\bar{\boldsymbol{Z}} & \bar{\boldsymbol{X}}'\bar{\boldsymbol{X}} \end{pmatrix}^{-1} \begin{pmatrix} \bar{\boldsymbol{Z}}'\boldsymbol{y} \\ \bar{\boldsymbol{X}}'\boldsymbol{y} \end{pmatrix}. \end{aligned}$$

It is clear that the estimates for non-block parameters are unchanged by presence of block effects if the orthogonal blocking condition $\bar{\boldsymbol{X}}'\bar{\boldsymbol{Z}} = 0$ is satisfied. Again, $\bar{\boldsymbol{X}}'\bar{\boldsymbol{Z}} = 0$ means that for any given factor effect, in the model matrix, its average value is the same within each block, and equal to its overall average.

To construct an OLS-GLS equivalent blocked split-plot design, we show below that for any partition of whole plots into blocks, as long as the original split-plot design is OLS-GLS equivalent and the whole plot sizes are the same for each whole plot, the blocked design is

OLS-GLS equivalent.

Using the model in Equation 5.1 and Theorem 6.8.1 from Graybill (1976), the OLS and GLS estimates are equivalent if and only if there exists a non-singular $\boldsymbol{F}$ such that

$$\boldsymbol{\Sigma X} = \boldsymbol{XF}.$$

Now for the model with blocks, the OLS-GLS estimates are equivalent if and only if there exists a non-singular $\boldsymbol{F}^*$ such that

$$\boldsymbol{\Sigma U} = \boldsymbol{UF}^*. \tag{5.2}$$

The left side of Equation 5.2 becomes

$$\boldsymbol{\Sigma U} = \Sigma(\bar{\boldsymbol{Z}}, \boldsymbol{X}) = (\boldsymbol{\Sigma}\bar{\boldsymbol{Z}}, \boldsymbol{\Sigma X}) = (\sigma^2\bar{\boldsymbol{Z}} + \sigma_\delta^2 \boldsymbol{MM}'\bar{\boldsymbol{Z}}, \boldsymbol{\Sigma X}).$$

When the design is balanced in terms of whole plot size,

$$\begin{aligned}
\boldsymbol{MM}'\bar{\boldsymbol{Z}} =& \boldsymbol{MM}'(\boldsymbol{I} - \frac{1}{N}\mathbf{1}_N\mathbf{1}_N')\boldsymbol{Z} \\
=& \begin{pmatrix} \boldsymbol{J}_n & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{0} & \boldsymbol{J}_n & \cdots & \mathbf{0} \\ \cdots & \cdots & \cdots & \cdots \\ \mathbf{0} & \cdots & \cdots & \boldsymbol{J}_n \end{pmatrix} \begin{pmatrix} \mathbf{1}_{s_1} & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{0} & \mathbf{1}_{s_2} & \cdots & \mathbf{0} \\ \cdots & \cdots & \cdots & \cdots \\ \mathbf{0} & \cdots & \mathbf{0} & \mathbf{1}_{s_b} \end{pmatrix} - \frac{1}{N}(\boldsymbol{I}_m \bigotimes \boldsymbol{J}_n)(\boldsymbol{J}_m \bigotimes \boldsymbol{J}_n)\boldsymbol{Z} \\
=& \begin{pmatrix} n\mathbf{1}_{s_1} & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{0} & n\mathbf{1}_{s_2} & \cdots & \mathbf{0} \\ \cdots & \cdots & \cdots & \cdots \\ \mathbf{0} & \cdots & \mathbf{0} & n\mathbf{1}_{s_b} \end{pmatrix} - \frac{n}{N}(\boldsymbol{J}_m \bigotimes \boldsymbol{J}_n)\boldsymbol{Z} = n(\boldsymbol{I} - \frac{1}{N}\mathbf{1}_N\mathbf{1}_N')\boldsymbol{Z} = n\bar{\boldsymbol{Z}}.
\end{aligned}$$

Thus the The left side of Equation 5.2 becomes

$$(\sigma^2 \bar{\boldsymbol{Z}} + n\sigma_\delta^2 \bar{\boldsymbol{Z}}, \boldsymbol{\Sigma X}).$$

Let $\boldsymbol{F}^* = \begin{pmatrix} \boldsymbol{K}_{b\times b} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{F} \end{pmatrix}$, and the right side of Equation 5.2 becomes

$$\boldsymbol{U F}^* = (\bar{\boldsymbol{Z}}, \boldsymbol{X}) \begin{pmatrix} \boldsymbol{K} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{F} \end{pmatrix} = (\bar{\boldsymbol{Z}}\boldsymbol{K}, \boldsymbol{X F}).$$

Let $\boldsymbol{K} = \sigma^2 \boldsymbol{I}_{b\times b} + n\sigma_\delta^2 \boldsymbol{I}_{b\times b}$, both sides are equal. Therefore, a balanced OLS-GLS equivalent split-plot design with the addition of block effects is also OLS-GLS equivalent.

As a summary, we can partition the whole plots in available balanced OLS-GLS equivalent split-plot designs based on the orthogonal blocking condition $\bar{\boldsymbol{X}}'\bar{\boldsymbol{Z}} = 0$ to construct orthogonally blocked split-plot designs.

5.1.2 OLS-GLS Equivalent Split-Plot Designs

For a crossed split-plot design, which is called a *Cartesian product* design by Bisgaard (2000) and referred to by Taguchi as *product arrays*, Letsinger, Myers and Lentner (1996) show that the OLS estimates are equivalent to the GLS estimates. Vining, Kowalski and Montgomery (2005) (VKM) extend this result by showing that it is possible to construct second-order OLS-GLS equivalent non-crossed split-plot designs. The VKM designs have first-order orthogonal subplot designs within each whole plot. In addition, replication of the whole plots with overall center runs is highly recommended in order to obtain model independent pure-error estimates of the unknown variance components.

Parker, Kowalski, Vining (2005) (PKV) propose balanced minimum whole plot (MWP) OLS-GLS equivalent designs. These designs modify the VKM equivalent designs by reducing the number of the whole plots to the minimum number of whole plots required for fitting a second-order model. PKV's MWP designs have subplot center runs inside the whole plots containing subplot factorial runs and whole plot axial runs. In addition, the whole plots with only overall center runs is discarded to maintain the OLS-GLS equivalency. The VKM and MWP OLS-GLS equivalent split-plot designs provide candidates for constructing second-order orthogonally blocked split-plot designs.

In this Chapter we will use the orthogonality condition to discuss first-order orthogonally blocked split-plot designs in Section 2 and second-order orthogonally blocked split-plot design in Section 3. Two types of second-order orthogonally blocked split-plot designs will be discussed: the VKM design and the MWP design. We will show that by choosing appropriate parameters, these two types of designs can be orthogonally blocked. In Section 4, we illustrate the methodology with some examples. Finally, we conclude with a few comments in Section 5.

5.2 First-Order Orthogonally Blocked Split-Plot Designs

In split-plot designs, since the experimental runs are grouped into whole plots, the blocks now contain different whole plots instead of individual runs. Based on the number of whole plot factors and subplot factors, we can find the OLS-GLS crossed split-plot design first, then try to block the design using the orthogonality condition. Common first-order crossed

Table 5.1: A Crossed Split-Plot Design with Two Whole Plot and Two Subplot Factors

WP	z_1	z_2	x_1	x_2
1	-1	-1	-1	-1
	-1	-1	-1	1
	-1	-1	1	-1
	-1	-1	1	1
2	1	1	-1	-1
	1	1	-1	1
	1	1	1	-1
	1	1	1	1
3	-1	1	-1	-1
	-1	1	-1	1
	-1	1	1	-1
	-1	1	1	1
4	1	-1	-1	-1
	1	-1	-1	1
	1	-1	1	-1
	1	-1	1	1

split-plot designs include 2^k, 2^{k-p} and Plackett-Burman designs. For example, if we have two whole plot factors (z_1, z_2) and two subplot factors (x_1, x_2), one crossed first order split-plot design is given in Table 5.1. Because these designs are all first-order orthogonal, then for a first-order model or a first-order with interaction model, the orthogonal blocking condition can be automatically satisfied as long as we regroup the whole plots into different blocks so that the average of the columns within the block is zero.

Traditionally, when there is only one randomization, to take an example, $I = Z_1Z_2X_1X_2$ can be used as the defining equation to construct the blocks. However, in the split-plot case, this defining equation based on the overall interaction of the four factors will produce more whole plots. This is because the whole plot effect has to be the same in each whole plot. If we use $I = Z_1Z_2X_1X_2$ to construct blocks, then the design in Table 5.1 becomes the design shown in Table 5.2. Now, there are 8 whole plots instead of 4 whole plots. Since in most

Table 5.2: A Blocked Split-Plot Design Using $I = Z_1Z_2X_1X_2$ as the Defining Equation

Block	WP	z_1	z_2	x_1	x_2
Block 1	1	-1	-1	-1	-1
		-1	-1	1	1
	2	1	1	1	1
		1	1	-1	-1
	3	-1	1	-1	1
		-1	1	1	-1
	4	1	-1	1	-1
		1	-1	-1	1
Block 2	5	-1	-1	-1	1
		-1	-1	1	-1
	6	1	1	-1	1
		1	1	1	-1
	7	-1	1	-1	-1
		-1	1	1	1
	8	1	-1	-1	-1
		1	-1	1	1

split-plot designs, the whole plots cost significantly more than the subplots, this strategy is not recommended.

Consider a different strategy using $I = Z_1Z_2$ instead of $I = Z_1Z_2X_1X_2$ as the defining equation. In this way, the two-way whole plot interaction is confounded instead of the four-way overall interaction to construct blocks. Whole plots 1 and 2 form the first block, **B**1, and whole plots 3 and 4 form the second block, **B**2. The resulting design is given in Table 5.3. The block effect is confounded with the z_1z_2 effect, so the z_1z_2 interaction can not be estimated independently from the block effect. But the estimation of all the other effects is independent of the block effect. If the interaction between whole plot factors is negligible, the design is orthogonally blocked. Since many times in a split-plot design, the whole plot effects are less important than the subplot effects, it may be reasonable to sacrifice some higher order whole plot interactions. If there are more than 2 whole plot factors, then the

Table 5.3: A Blocked Split-Plot Design Using $I = Z_1 Z_2$ as the Defining Equation

Block	WP	z_1	z_2	x_1	x_2
Block 1	1	-1	-1	-1	-1
		-1	-1	-1	1
		-1	-1	1	-1
		-1	-1	1	1
	2	1	1	-1	-1
		1	1	-1	1
		1	1	1	-1
		1	1	1	1
Block 2	3	-1	1	-1	-1
		-1	1	-1	1
		-1	1	1	-1
		-1	1	1	1
	4	1	-1	-1	-1
		1	-1	-1	1
		1	-1	1	-1
		1	-1	1	1

highest order whole plot interaction can be chosen to confound with the block effect. Thus for a first-order or a first-order with interaction model, the resulting split-plot design is orthogonally blocked and all estimates of the effects in the model will be unaffected by the block effect.

5.3 Second-Order Orthogonally Blocked Split-Plot Designs

5.3.1 VKM Design Basics and Two Augmentation Strategies

VKM first partition the model matrix $\boldsymbol{X}$ as

$$\boldsymbol{X} = \begin{bmatrix} \mathbf{1}_1 & \boldsymbol{W}_1 & \boldsymbol{S}_{D_1} & \boldsymbol{S}_{O_1} \\ \mathbf{1}_2 & \boldsymbol{W}_2 & \boldsymbol{S}_{D_2} & \boldsymbol{S}_{O_2} \\ \vdots & \vdots & \vdots & \vdots \\ \mathbf{1}_m & \boldsymbol{W}_m & \boldsymbol{S}_{D_m} & \boldsymbol{S}_{O_m} \end{bmatrix}$$

where $\boldsymbol{W}_i$ is the whole plot model matrix including the WP first-order terms, the WP $\times$ WP interactions and the WP second-order terms, $\boldsymbol{S}_{D_i}$ is the subplot model matrix including the SP first-order terms, the SP $\times$ SP interactions and the SP $\times$ WP interactions, $\boldsymbol{S}_{O_i}$ is the subplot model matrix including the SP quadratic terms.

They show that if a design possesses the three properties below then it is a OLS-GLS equivalent design

1. the design is balanced
2. the sum of columns in each $\boldsymbol{S}_{D_i}$ is a constant vector $\boldsymbol{q}$
3. $\mathbf{1}\mathbf{1}'\boldsymbol{S}_{O_i} = \boldsymbol{S}_{O_i}\boldsymbol{G}$

where $\boldsymbol{G}$ is an appropriately chosen matrix which satisfies the third property above. As an example, for two whole plot factors and two subplot factors, the VKM equivalent design is

Table 5.4: The VKM CCD for Two Whole Plot and Two Subplot Factors

WP	z_1	z_2	x_1	x_2	WP	z_1	z_2	x_1	x_2
	-1	-1	-1	-1		0	$-\alpha$	0	0
1	-1	-1	-1	1	7	0	$-\alpha$	0	0
	-1	-1	1	-1		0	$-\alpha$	0	0
	-1	-1	1	1		0	$-\alpha$	0	0
	-1	1	-1	-1		0	α	0	0
2	-1	1	-1	1	8	0	α	0	0
	-1	1	1	-1		0	α	0	0
	-1	1	1	1		0	α	0	0
	1	-1	-1	-1	9	0	0	$-\beta$	0
3	1	-1	-1	1		0	0	β	0
	1	-1	1	-1		0	0	0	$-\beta$
	1	-1	1	1		0	0	0	β
	1	1	-1	-1	10	0	0	0	0
4	1	1	-1	1		0	0	0	0
	1	1	1	-1		0	0	0	0
	1	1	1	1		0	0	0	0
	$-\alpha$	0	0	0					
5	$-\alpha$	0	0	0					
	$-\alpha$	0	0	0					
	$-\alpha$	0	0	0					
	α	0	0	0					
6	α	0	0	0					
	α	0	0	0					
	α	0	0	0					

shown in Table 5.4. It is balanced and the sum of the columns in each $\boldsymbol{S}_{D_i}$ is zero, even though the split-plot designs within each whole plot are not the same.

In traditional second-order response surface designs, for example the CCD, the strategy to achieve orthogonal blocking is to put additional center runs in different blocks and then choose an appropriate value of the axial distance to satisfy the orthogonality condition. In the split-plot CCD case, we can implement a similar procedure. First, we can block the VKM CCD, then augment the design with additional center runs in each block and choose appropriate values of the axial distances to achieve orthogonal blocking.

In split-plot designs, we can define two types of center runs: the overall center run and the subplot center run. The overall center run has all whole plot and subplot factors at their center value, zero in coded units. The subplot center run has only the subplot factors at their center value. Both of these types of center runs need to be considered when augmenting in the split-plot case.

There are different augmentation strategies for VKM designs and MWP designs. To obtain an orthogonally blocked VKM design (OBVKM), whole plots with overall center runs are added into the blocks. For MWP designs, the strategy involves augmenting the whole plots containing subplot factorial runs and whole plot axial runs with subplot center runs, and adding overall center runs into the whole plots containing subplot axial runs. We will refer to the orthogonally blocked MWP designs as OBMWP.

5.3.2 The Orthogonally Blocked VKM Design

Two Blocks Case

In response surface methodology (RSM), experimenters tend to first run a screening experiment to identify important factors or variables. Follow-up experiments seek to improve the performance of the response. It is a dynamic, continuous learning process instead of a one-shot static strategy, hence, the important "sequential" nature of RSM. In constructing a CCD, experimenters initially run factorial designs with center runs and test for possible curvature. If the curvature at the center is significant, then axial runs and more center runs are augmented to the original design to form a CCD in order to optimize the response. This leads naturally to the two block situation.

In the two block split-plot CCD situation, the whole plots with overall center runs can be added into the block containing the whole plots with factorial runs, **B**1, and into the block containing the remaining whole plots with axial runs, **B**2. For example consider Table 5.4. Whole plots 1-4 make up $\mathbf{B}_1$ and whole plots 5-9 are in $\mathbf{B}_2$. For orthogonal blocking, we are trying to solve for the number of whole plot 10's to add into $\mathbf{B}_1$ and $\mathbf{B}_2$ as well as find the necessary values for α and β. It is important to note that this strategy provides degrees of freedom to test lack of fit and the ability to estimate model independent pure error (Box and Draper (1975)). Kowalski, Cornell and Vining (2002) discuss the advantage of pure error estimation for variance components in mixture designs with process variables run as a split-plot. Furthermore, Vining and Kowalski (2006) discuss using pure error estimates to provide exact inference for second-order response surface designs within a split-plot structure. To obtain more than 1 degree of freedom for the whole plot pure error variance estimate, it is desirable to run at least three whole plots with overall center runs.

Suppose we have k_1 whole plot factors and k_2 subplot factors, and we want to add n_{c1} overall center runs into **B**1 and n_{c2} overall center runs into **B**2. The resulting block sizes for **B**1 and **B**2 are s_1 and s_2, respectively. The design size is N. Extending the orthogonal blocking condition to an orthogonally blocked second-order VKM design gives

1. $\sum_{u=1}^{s_1} z_{ui}/s_1 = \sum_{u=1}^{s_2} z_{ui}/s_2 = \sum_{u=1}^{N} z_{ui}/N$ and $\sum_{u=1}^{s_1} x_{uj}/s_1 = \sum_{u=1}^{s_2} x_{uj}/s_2 = \sum_{u=1}^{N} x_{uj}/N$, $i = 1, \ldots, k_1$, $j = 1, \ldots, k_2$

2. $\sum_{u=1}^{s_1} z_{ui}x_{uj}/s_1 = \sum_{u=1}^{s_2} z_{ui}x_{uj}/s_2 = \sum_{u=1}^{N} z_{ui}x_{uj}/N, \quad i = 1, \ldots, k_1$ and $j = 1, \ldots, k_2$

3. $\sum_{u=1}^{s_1} z_{ui}^2/s_1 = \sum_{u=1}^{s_2} z_{ui}^2/s_2 = \sum_{u=1}^{N} z_{ui}^2/N$ and $\sum_{u=1}^{s_1} x_{ui}^2/s_1 = \sum_{u=1}^{s_2} x_{ui}^2/s_2 = \sum_{u=1}^{N} x_{ui}^2/N$,
$i = 1, \ldots, k_1$, $j = 1, \ldots, k_2$.

Since the subplot designs within each block of the VKM design are first order orthogonal, the first two conditions above are automatically satisfied.

To investigate the third condition above, define the whole plot axial distance as α and the subplot axial distance as β. Furthermore, let r be the number of $\pm\alpha$ that appear in the column for a whole plot factor in the design matrix and a be the number of $\pm\beta$ that appear in the column for a subplot factor in the design matrix. Let F be the sum of squares of the column in the whole plots with factorial runs. In **B**1, the average of the sum of squares for both whole plot and subplot factors is equal to $\frac{F}{F+n_{c1}}$ because the sum of squares for each column is F and the block size is $F + n_{c1}$. In **B**2, the average of the sum of squares for each whole plot factor column is $\frac{r\alpha^2}{k_1r+k_2a+n_{c2}}$ and the average of the sum of squares for each subplot factor column is $\frac{a\beta^2}{k_1r+k_2a+n_{c2}}$. To achieve orthogonal blocking, condition 3 becomes:

$$\begin{cases} \frac{r\alpha^2}{k_1r+k_2a+n_{c2}} & = \frac{F}{F+n_{c1}} = \frac{r\alpha^2+F}{k_1r+k_2a+n_{c2}+F+n_{c1}} \\ \frac{a\beta^2}{k_1r+k_2a+n_{c2}} & = \frac{F}{F+n_{c1}} = \frac{a\beta^2+F}{k_1r+k_2a+n_{c2}+F+n_{c1}} \end{cases}. \tag{5.3}$$

For a particular combination of k_1, k_2, r and a, the relationship in Equation 5.3 is a function of α, β, n_{c1}, and n_{c2}. Solving Equation 5.3 for α and β gives

$$\begin{cases} \alpha^2 & = \frac{(k_1r+k_2a+n_{c2})F}{r(F+n_{c1})} \\ \beta^2 & = \frac{(k_1r+k_2a+n_{c2})F}{a(F+n_{c1})} \end{cases}. \tag{5.4}$$

Since n_{c1} and n_{c2} have to be integers as well as a multiple of the whole plot size, α and β can not be chosen arbitrarily. There is a trade-off between the size of the design, the size of the blocks, and reasonable values for α and β. Box and Hunter (1957) choose the blocking strategy so that the orthogonal α is close to the rotatable α. Here we choose the blocking strategy to give some practical values for α and β. Tables 5.8 - 5.10 provide the values for α and β for different number of whole plot factors and subplot factors.

More than Two Blocks Case

In cases of more than two blocks, **B**1 can be further divided into additional blocks. However, **B**2 cannot be further divided because the axial runs for both the whole plot and the subplot factors have to be in the same block for the orthogonal blocking condition to be satisfied. If we further divide **B**1 into **B**11, **B**12, ...,**B**1b, the situation becomes that of blocking a factorial or fractional factorial split-plot design as shown in Section 2. We can augment n_{c11}, n_{c12}, ..., n_{c1b} overall center runs into these blocks respectively and n_{c2} into **B**2. Using the same strategy as Section 2 to block **B**1, we can construct a block design where the average of the first-order terms within each block is zero.

For two whole plot factors, if we use $I = Z_1Z_2$ as the defining equation, the average of z_1z_2 is not zero in **B**11, **B**12 but is zero in **B**2. Therefore, the orthogonal blocking condition can not be achieved in this case. Two blocks is recommended. When we have more than two whole plot factors, we can use the highest whole plot interaction as the defining equation. Let F_{1i} be the sum of squares of each column in **B**1i, the orthogonal blocking condition becomes

$$\begin{cases} \frac{r\alpha^2}{k_1r+k_2a+n_{c2}} &= \frac{F_{11}}{F_{11}+n_{c11}} = \ldots = \frac{F_{1b}}{F_{1b}+n_{c1b}} = \frac{r\alpha^2+F}{k_1r+k_2a+n_{c2}+F+n_{c11}+\ldots+n_{c1b}} \\ \frac{a\beta^2}{k_1r+k_2a+n_{c2}} &= \frac{F_{11}}{F_{11}+n_{c11}} = \ldots = \frac{F_{1b}}{F_{1b}+n_{c1b}} = \frac{a\beta^2+F}{k_1r+k_2a+n_{c2}+F+n_{c11}+\ldots+n_{c1b}} \end{cases}.$$

If $F_{11} = F_{12} = \ldots = F_{1b}$, which is the most common case in blocked factorial designs, we have $n_{c11} = n_{c12} = \ldots = n_{c1b}$ and

$$\begin{cases} \alpha^2 &= \frac{(k_1 r + k_2 a + n_{c2}) F_{11}}{r(F_{11} + n_{c11})} \\ \beta^2 &= \frac{(k_1 r + k_2 a + n_{c2}) F_{11}}{a(F_{11} + n_{c11})} \end{cases}.$$

5.3.3 The Orthogonally Blocked MWP Design

Two Blocks Case

As an alternative to the OBVKM CCD, we can construct OBMWP CCD based on Parker, Kowalski and Vining (2005) (PKV). A MWP design has the minimum number of whole plots necessary to fit a second-order model. Hence, it is highly cost effective. In these designs, there are no whole plots with only overall center runs. Instead, the overall center runs are in the whole plot with subplot axial runs. Subplot center runs appear in the other whole plots.

PKV show that the required condition to construct a balanced MWP design is $n_f = 2r_\alpha \beta^2 - \frac{k_1(2r_\alpha \beta^2)}{\alpha^2}$ where k_1 is the number of whole plot factors, n_f is the number of subplot factorial points contained in the whole plots with the whole plot level at ± 1, and r_α is the number of replicates of the subplot axial runs within one whole plot. Examining the condition, we can see that the constraint on α and β depends only on n_f, r_α, and k_1. Therefore, we can replicate the whole plot containing subplot axial runs t times without affecting the choice of α and β. The parameter r_α in this condition is closely related to the value a defined in Section 5.3.2. For example, suppose in a design, the whole plot with subplot axial runs is whole plot 9 from Table 5.5 and it is replicated to form whole plot 10, also shown in Table 5.5. Then $r_\alpha = 2$ since in each whole plot, the subplot axial runs are

Table 5.5: Two Possible Whole Plots for Showing the Relationship Between r_α and a

WP	z_1	z_2	x_1	x_2
9	0	0	$-\beta$	0
	0	0	β	0
	0	0	0	$-\beta$
	0	0	0	β
	0	0	$-\beta$	0
	0	0	β	0
	0	0	0	$-\beta$
	0	0	0	β
10	0	0	$-\beta$	0
	0	0	β	0
	0	0	0	$-\beta$
	0	0	0	β
	0	0	$-\beta$	0
	0	0	β	0
	0	0	0	$-\beta$
	0	0	0	β

replicated twice, $a = 8$ because a is the number of $\pm\beta$ in each column, and $a = 2r_\alpha t$, here $t = 2$.

The whole plots with factorial runs can still be considered as block 1, **B**1, and the whole plots with both whole plot and subplot axial runs can be considered as block 2, **B**2. We can examine directly whether the orthogonal blocking condition can be satisfied. Let F be the sum of squares of a whole plot factor column in **B**1 and F_s be the sum of squares of a subplot factor column in **B**1. Suppose there are b_1 whole plots in **B**1. Then for balanced MWP designs; $F = b_1 n$, $F_s = b_1 n_f$, thus, $\frac{F_s}{F} = \frac{n_f}{n}$. Also, we note that $r = 2n$ and $a = 2r_\alpha t$.

Combining the orthogonal blocking and the PKV conditions, we get

$$\begin{cases} \frac{r\alpha^2}{2k_1n+nt} & = \frac{F}{F} = 1 \\ \frac{a\beta^2}{2k_1n+nt} & = \frac{F_s}{F} \\ n_f & = 2r_\alpha\beta^2 - \frac{k_1(2r_\alpha\beta^2)}{\alpha^2}. \end{cases}$$

Solving for α and β gives

$$\begin{cases} \alpha^2 & = \frac{2k_1+t}{2} \\ \beta^2 & = \alpha^2 \cdot \frac{n_f}{r_\alpha t} \end{cases}. \tag{5.5}$$

Therefore for a given k_1 and k_2, we can always find the values of α and β to satisfy orthogonality and MWP OLS-GLS equivalency simultaneously. The values of α and β depend on the subplot factorial design nested within each whole plot, the number of whole plots factors, the number of replicates of a whole plot with subplot axial runs and the number of replicates of the subplot axial runs within a whole plot.

Sometimes, the required α and β values are too large and thus not very practical. In this case, we can replicate the whole plot with subplot axial runs (whole plot 9 in Table 5.5) to get more degrees of freedom to estimate pure error and to reduce the values of α and β. An example of this replication is given in the next Section.

More than Two Blocks Case

We can use a similar approach as shown in Section 5.3.2 to block **B**1. It is not necessary to add extra center runs to both blocks. It is important to notice that in Equation 5.5, the values of α and β do not depend on the size of **B**1 and **B**2. Therefore, adding more blocks based on defining equations does not change the necessary values of α and β.

5.4 Some Examples

5.4.1 Example: OBVKM(3,3) and OBMWP(3,3)

Suppose we have three whole plot factors and three subplot factors. The experimenters want to implement a second-order split-plot design in two days or three days. Because of the resource restriction, they can only run part of the experiment in one day. Also they don't want the estimation involving the six independent variables to be biased by the day effect. We can construct OBVKM and OBMWP designs with 2 blocks and 3 blocks. From the original VKM and MWP designs in Table 5.6 and Table 5.4.1, we can see that VKM has 3 whole plots for subplot axial runs and MWP has one. However, this VKM design allows exact inference of the subplot quadratic effects, see Vining and Kowalski (2006).

Two-Block OBVKM(3,3) Design

The original VKM(3,3) is listed in Table 5.6. In this example, $r = 8$, $a = 4$, $k_1 = 3$, $k_2 = 3$, $F = 32$. Using Equation 5.4, we have

$$\begin{cases} \alpha^2 & = \frac{(k_1 r + k_2 a + n_{c2})F}{r(F + n_{c1})} = \frac{(24+12+n_{c2})32}{8(32+n_{c1})} = \frac{4(36+n_{c2})}{(32+n_{c1})} \\ \beta^2 & = \frac{(k_1 r + k_2 a + n_{c2})F}{a(F + n_{c1})} = \frac{(24+12+n_{c2})32}{4(32+n_{c1})} = \frac{8(36+n_{c2})}{(32+n_{c1})} \end{cases}.$$

Suppose it is desired to have at least three whole plots with overall center runs to get pure error estimation, we can choose $n_{c1} = 8$ and $n_{c2} = 4$. Then $\alpha = 2$ and $\beta = \sqrt{8} = 2.828$. Compared with Box and Hunter (1957)'s rotatable $\alpha = 2.366$ for a completely randomized design with the same number of factorial points, our α is a little bit smaller and the β is a little bit larger. The **B**1 contains whole plots 1-8 and two augmented whole plots with overall center runs and **B**2 contains whole plots 9-17 and one augmented whole plot with

Table 5.6: The VKM CCD for Three Whole Plot Factors and Three Subplot Factors

WP	z_1	z_2	z_3	x_1	x_2	x_3	WP	z_1	z_2	z_3	x_1	x_2	x_3
1	-1	-1	-1	-1	-1	-1	10	α	0	0	0	0	0
	-1	-1	-1	1	1	-1		α	0	0	0	0	0
	-1	-1	-1	1	-1	1		α	0	0	0	0	0
	-1	-1	-1	-1	1	1		α	0	0	0	0	0
2	1	-1	-1	1	-1	-1	11	0	α	0	0	0	0
	1	-1	-1	-1	1	-1		0	α	0	0	0	0
	1	-1	-1	-1	-1	1		0	α	0	0	0	0
	1	-1	-1	1	1	1		0	α	0	0	0	0
3	-1	1	-1	1	-1	-1	12	0	$-\alpha$	0	0	0	0
	-1	1	-1	-1	1	-1		0	$-\alpha$	0	0	0	0
	-1	1	-1	-1	-1	1		0	$-\alpha$	0	0	0	0
	-1	1	-1	1	1	1		0	$-\alpha$	0	0	0	0
4	1	1	-1	-1	-1	-1	13	0	0	α	0	0	0
	1	1	-1	1	1	-1		0	0	α	0	0	0
	1	1	-1	1	-1	1		0	0	α	0	0	0
	1	1	-1	-1	1	1		0	0	α	0	0	0
5	-1	-1	1	1	-1	-1	14	0	0	$-\alpha$	0	0	0
	-1	-1	1	-1	1	-1		0	0	$-\alpha$	0	0	0
	-1	-1	1	-1	-1	1		0	0	$-\alpha$	0	0	0
	-1	-1	1	1	1	1		0	0	$-\alpha$	0	0	0
6	1	-1	1	-1	-1	-1	15	0	0	0	$-\beta$	0	0
	1	-1	1	1	1	-1		0	0	0	β	0	0
	1	-1	1	1	-1	1		0	0	0	$-\beta$	0	0
	1	-1	1	-1	1	1		0	0	0	β	0	0
7	-1	1	1	-1	-1	-1	16	0	0	0	0	$-\beta$	0
	-1	1	1	1	1	-1		0	0	0	0	β	0
	-1	1	1	1	-1	1		0	0	0	0	$-\beta$	0
	-1	1	1	-1	1	1		0	0	0	0	β	0
8	1	1	1	1	-1	-1	17	0	0	0	0	0	$-\beta$
	1	1	1	-1	1	-1		0	0	0	0	0	β
	1	1	1	-1	-1	1		0	0	0	0	0	$-\beta$
	1	1	1	1	1	1		0	0	0	0	0	β
9	$-\alpha$	0	0	0	0	0	18	0	0	0	0	0	0
	$-\alpha$	0	0	0	0	0		0	0	0	0	0	0
	$-\alpha$	0	0	0	0	0		0	0	0	0	0	0
	$-\alpha$	0	0	0	0	0		0	0	0	0	0	0

Table 5.7: MWP Design with Three WP Factors and Three Subplot Factors

WP	z_1	z_2	z_3	x_1	x_2	x_3	WP	z_1	z_2	z_3	x_1	x_2	x_3
1	-1	-1	-1	-1	-1	-1	9	$-\alpha$	0	0	0	0	0
	-1	-1	-1	-1	1	1		$-\alpha$	0	0	0	0	0
	-1	-1	-1	1	-1	1		$-\alpha$	0	0	0	0	0
	-1	-1	-1	1	1	-1		$-\alpha$	0	0	0	0	0
	-1	-1	-1	0	0	0		$-\alpha$	0	0	0	0	0
	-1	-1	-1	0	0	0		$-\alpha$	0	0	0	0	0
	-1	-1	-1	0	0	0		$-\alpha$	0	0	0	0	0
2	-1	-1	1	-1	-1	1	10	α	0	0	0	0	0
	-1	-1	1	-1	1	-1		α	0	0	0	0	0
	-1	-1	1	1	-1	-1		α	0	0	0	0	0
	-1	-1	1	1	1	1		α	0	0	0	0	0
	-1	-1	1	0	0	0		α	0	0	0	0	0
	-1	-1	1	0	0	0		α	0	0	0	0	0
	-1	-1	1	0	0	0		α	0	0	0	0	0
3	-1	1	-1	-1	-1	1	11	0	$-\alpha$	0	0	0	0
	-1	1	-1	-1	1	-1		0	$-\alpha$	0	0	0	0
	-1	1	-1	1	-1	-1		0	$-\alpha$	0	0	0	0
	-1	1	-1	1	1	1		0	$-\alpha$	0	0	0	0
	-1	1	-1	0	0	0		0	$-\alpha$	0	0	0	0
	-1	1	-1	0	0	0		0	$-\alpha$	0	0	0	0
	-1	1	-1	0	0	0		0	$-\alpha$	0	0	0	0
4	-1	1	1	-1	-1	-1	12	0	α	0	0	0	0
	-1	1	1	-1	1	1		0	α	0	0	0	0
	-1	1	1	1	-1	1		0	α	0	0	0	0
	-1	1	1	1	1	-1		0	α	0	0	0	0
	-1	1	1	0	0	0		0	α	0	0	0	0
	-1	1	1	0	0	0		0	α	0	0	0	0
	-1	1	1	0	0	0		0	α	0	0	0	0
5	1	-1	-1	-1	-1	1	13	0	0	$-\alpha$	0	0	0
	1	-1	-1	-1	1	-1		0	0	$-\alpha$	0	0	0
	1	-1	-1	1	-1	-1		0	0	$-\alpha$	0	0	0
	1	-1	-1	1	1	1		0	0	$-\alpha$	0	0	0
	1	-1	-1	0	0	0		0	0	$-\alpha$	0	0	0
	1	-1	-1	0	0	0		0	0	$-\alpha$	0	0	0
	1	-1	-1	0	0	0		0	0	$-\alpha$	0	0	0
6	1	-1	1	-1	-1	-1	14	0	0	α	0	0	0
	1	-1	1	-1	1	1		0	0	α	0	0	0
	1	-1	1	1	-1	1		0	0	α	0	0	0
	1	-1	1	1	1	-1		0	0	α	0	0	0
	1	-1	1	0	0	0		0	0	α	0	0	0
	1	-1	1	0	0	0		0	0	α	0	0	0
	1	-1	1	0	0	0		0	0	α	0	0	0
7	1	1	-1	-1	-1	-1	15	0	0	0	$-\beta$	0	0
	1	1	-1	-1	1	1		0	0	0	β	0	0
	1	1	-1	1	-1	1		0	0	0	0	$-\beta$	0
	1	1	-1	1	1	-1		0	0	0	0	β	0
	1	1	-1	0	0	0		0	0	0	0	0	$-\beta$
	1	1	-1	0	0	0		0	0	0	0	0	β
	1	1	-1	0	0	0		0	0	0	0	0	0
8	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							
	1	1	1	0	0	0							
	1	1	1	0	0	0							

overall center runs. Therefore the design has 20 whole plots, 10 in each block.

Three-Block OBVKM(3,3) Design

Using $I = Z_1 Z_2 Z_3$ to further block **B**1, the resulting **B**11 contains whole plots 1, 4, 6, 7, **B**12 contains whole plots 2, 3, 5, 8, and **B**2 still contains whole plots 9-17. Now $F_{11} = F_{12} = 16$. Therefore,

$$\begin{cases} \alpha^2 & = \frac{(24+12+n_{c2})16}{8(16+n_{c11})} = \frac{2(36+n_{c2})}{(16+n_{c11})} \\ \beta^2 & = \frac{(24+12+n_{c2})16}{4(16+n_{c11})} = \frac{4(36+n_{c2})}{(16+n_{c11})} \end{cases}.$$

If we still want the same α, β values from the two-block case for this design, we can choose $n_{c11} = 4$ and $n_{c2} = 4$. Therefore, the augmented **B**11 contains whole plots 1,4,6,7 and one whole plot with overall center runs and the augmented **B**12 contains 2, 3, 5, 8, and one whole plot with overall center runs. The augmented **B**2 contains whole plots 9-17 and one whole plot of overall center runs. Altogether, the design still has 20 whole plots.

Two-Block OBMWP(3,3) Design

The original design is listed in Table 5.4.1. The whole plot size $n = 7$ and $t = 1$, then $r = 2n = 14$, $a = 2$ and $r_\alpha = 1$, $k_1 = 3$, $k_2 = 3$, $n_f = 4$. Using Equation 5.5, the condition becomes

$$\begin{cases} \alpha^2 = \frac{2k_1+t}{2} = \frac{2k_1+1}{2} = 3.5 \\ \beta^2 = \alpha^2 \cdot \frac{n_f}{r_\alpha t} = 4\alpha^2 = 14 \end{cases} \iff \begin{cases} \alpha = 1.871 \\ \beta = 3.742 \end{cases}.$$

B1 has whole plots 1-8 and **B**2 has whole plots 9-15. Altogether the two-block OBMWP(3,3) has 15 whole plots, which is the same number of whole plots as the original MWP design. The value for β is quite large and may not be practical. We can reduce the required value of β by replicating whole plot 15 in Table 5.4.1 t times. For example, if we replicate whole plot 15 $t = 4$ times, the resulting values of $\alpha = \sqrt{5} = 2.24$ and $\beta = \sqrt{5} = 2.24$ are more practical. However, the resulting design has 18 whole plots and is now closer to the size of the OBVKM(3,3) design. Clearly there is a tradeoff between the size of the design and obtaining reasonable values for α and β.

Three-Block OBMWP(3,3) Design

Using $I = Z_1Z_2Z_3$, the resulting **B**11 has whole plots 1, 4, 6, 7 and **B**12 has whole plots 2, 3, 5, 8. **B**2 has whole plots 9-15. The values for α and β are the same. If we replicate whole plot 15 four times, we still get $\alpha = \sqrt{5} = 2.24$ and $\beta = \sqrt{5} = 2.24$. For OBMWP designs, the number of factorial blocks will not affect the values of α and β. This gives the practitioner more flexibility in choosing the number of blocks in the design.

5.5 Conclusion

To achieve orthogonal blocking in an OLS-GLS equivalent split-plot design, the whole plot size has to be the same. A block contains several whole plots instead of individual runs. For a first-order crossed split-plot design, a defining equation based on the combination of whole plot factors and subplot factors increases the number of whole plots and thus, is not desirable. It is better to construct orthogonal blocks by scarifying some higher-order whole plot interaction involving only whole plot effects.

For a VKM second-order design, extra overall center runs have to be added to achieve orthogonal blocking. The choice of the axial distances depends on the block size and the number of center runs. For a MWP second-order design, no additional runs are required for the design to achieve orthogonal blocking. The allocation of overall center runs and subplot center runs automatically allows orthogonal blocking with the appropriate choice of the axial distances. In addition, the choice of the axial distances remain the same when increasing the number of blocks for the whole plot factorial portion of the design.

OBVKM designs have the ability to estimate model independent whole plot pure error while OBMWP designs do not. However OBMWP designs use the minimum number of whole plots, which is cost efficient. Often in OBMWP designs, the values of α and β are not practical, but the whole plot with subplot axial runs can be replicated several times to get more reasonable values for α and β. A disadvantage of this replication is that the design size is increased. As with any experimental design situation, there are tradeoffs between competing design criteria and cost. In this case, the tradeoffs are between orthogonal blocking, design size and practical values for α and β. Practitioners will need to make their own decision about the tradeoffs for their particular design situation.

5.6 Catalogs of α and β in OBVKM and OBMWP for 1-3 whole plot factors and 1-4 subplot factors

Table 5.8: The Catalog of α and β for OBMWP CCD with Two Blocks

Block	(k_1, k_2)	(1,1)	(1,2)	(1,3)	(1,4)	(2,1)	(2,2)	(2,3)	(2,4)	(3,1)	(3,2)	(3,3)	(3,4)
Factorial	F	15	25	40	45	27	45	63	81	45	75	105	135
Block	Block Number	1	1	1	1	1	1	1	1	1	1	1	1
	Total WP	5	5	5	5	9	9	9	9	15	15	15	15
Axial	Orthogonal α t=1	1.225	1.225	1.225	1.225	1.581	1.581	1.581	1.581	1.871	1.871	1.871	1.871
Block	Orthogonal α t=2	1.414	1.414	1.414	1.414	1.732	1.732	1.732	1.732	2.000	2.000	2.000	2.000
	Orthogonal α t=3	1.581	1.581	1.581	1.581	1.871	1.871	1.871	1.871	2.121	2.121	2.121	2.121
	Orthogonal α t=4	1.732	1.732	1.732	1.732	2.000	2.000	2.000	2.000	2.236	2.236	2.236	2.236
	Orthogonal β t=1	1.732	2.449	3.464	3.464	2.236	3.162	3.162	4.472	2.646	3.742	3.742	5.292
	Orthogonal β t=2	1.414	2.000	2.828	2.828	1.732	2.449	2.449	3.464	2.000	2.828	2.828	4.000
	Orthogonal β t=3	1.291	1.826	2.582	2.582	1.528	2.160	2.160	3.055	1.732	2.449	2.449	3.464
	Orthogonal β t=4	1.225	1.732	2.449	2.449	1.414	2.000	2.000	2.828	1.581	2.236	2.236	3.162
	$\sqrt{k_1 + k_2}$	1.414	1.732	2	2.236	1.732	2	2.236	2.449	2	2.236	2.449	2.646

Table 5.9: The Catalog of α and β for OBVKM CCD with Two Blocks

Block	(k_1, k_2)	(1,1)	(1,2)	(1,3)	(1,4)	(2,1)	(2,2)	(2,3)	(2,4)	(3,1)	(3,2)	(3,3)	(3,4)
	F	4	8	16	16	8	16	16	32	16	32	32	64
Factorial	Block Number	1	1	1	1	1	1	1	1	1	1	1	1
Block	n_c1	4	8	24	8	4	8	4	0	2	4	8	8
	WP added	2	2	3	1	2	2	1	0	1	1	2	1
	n_c2	2	8	0	24	2	4	12	24	4	8	4	16
Axial	WP added	1	2	0	3	1	1	3	3	2	2	1	2
Block	Total WP	8	9	10	9	12	12	15	12	18	18	20	18
	Orthogonal α	1	1.414	1	1.414	1.414	1.414	2	1.414	2	2	2	2
	Orthogonal β	1.414	2	1.414	4	2	2.828	2.828	4	2.828	4	2.828	5.657
	$\sqrt{k_1 + k_2}$	1.414	1.732	2	2.236	1.732	2	2.236	2.449	2	2.236	2.449	2.646

Table 5.10: The Catalog of α and β for OBVKM CCD with Three Blocks

Block	(k_1, k_2)	(3,1)	(3,2)	(3,3)	(3,4)
	F	8	16	16	32
Factorial	Block Number	2	2	2	2
Block	n_c1	6	4	4	24
	WP added	3	1	1	3
	n_c2	0	12	4	0
Axial	WP added	0	3	1	0
Block	Total WP	21	20	20	21
	Orthogonal α	2	2	2	1.414
	Orthogonal β	2.828	4	2.828	4
	$\sqrt{k_1 + k_2}$	2	2.236	2.449	2.646

Chapter 6

Summary and Future Research

The primary goal of this research is to make recommendations for the design parameter α in a central composite design with a split-plot structure. In the completely randomized case, Box and Hunter (1957) provide two recommendations: rotatable values for α and orthogonal blocking values for α. In this research, we modify the idea of rotatability for two-strata rotatability and make two recommendations as well: two-strata rotatable values for α and orthogonal blocking values for α.

A rotatable design ensures the prediction variance is a function of the overall distance. Chapter 3 discusses the rotatable condition in split-plot central composite designs. Since rotatability cannot be achieved in the split-plot case, we propose two-strata rotatable designs where the prediction variance is a function of whole plot distance and subplot distance separately. We provide the condition to achieve two-strata rotatability for four types of reasonable split-plot central composite designs. We further show that the completely randomized rotatable central composite design can be constructed by using the two-strata rotatability condition since rotatability is a special case of two-strata rotatability. Since the idea of two-strata rotatability is similar to rotatability, they share similar properties and limitations. We further discuss the alias structure, model dependency, and center runs in two-strata rotatable split-plot central composite designs.

Since the construction of two-strata rotatable designs depends on the unknown variance component ratio d, in Chapter 4, we discuss several approaches to deal with the situation when d is unknown. One approach is to use historical data and estimate d. Another approach is to use the "sequential nature" of central composite designs to estimate d in factorial and center runs. If the curvature is significant, then axial runs can be added to the design based on the estimated sequential value for d. From the design point of view, we discuss the robustness of a two-strata rotatable design. We propose two methods to evaluate robustness. One method is a numerical measure to compare the moment matrix of the non two-strata rotatable design and the two-strata rotatable design. The other method is to draw contour plots in both the whole plot and the subplot spaces. Scaling is discussed and scaling by $1 + d$ is recommended. A simulation study shows that the two methods agree with each other pretty well. Two-strata rotatable designs are fairly robust as long as d is reasonably estimated.

An orthogonal blocking strategy minimizes the impact of block effect on model estimations. In the completely randomized case, the condition to achieve orthogonal blocking is given by Box and Hunter (1957). In split-plot designs, a generalized least square estimate is used instead of an ordinary least square estimate. Therefore, unknown variance components are involved in estimation of the model. To eliminate the effect of the variance components, we find that the orthogonal blocking condition can be achieved in OLS-GLS equivalent split-plot designs. As long as the OLS estimate is equivalent to GLS estimate, by assigning different values to axial runs of whole plot and subplot, orthogonal blocking can be achieved. We provide the conditions to achieve orthogonal blocking in OLS-GLS equivalent designs, especially the VKM (2005) design and Parker's MWP design (2006). In addition, we provide catalogs of axial runs for different number of whole plot factors and subplot factors. This provides another reasonable recommendation for α for the practitioners.

Two-strata rotatability is a property that can be used not only in split-plot central composite designs but also in all kinds of split-plot second-order designs. We can expand the research to other type of second-order response surface designs with a split-plot structure, for example: Box-Behnken designs, Hoke saturated designs and Notz saturated designs. The moment matrix for these different designs may have a different form and separate conditions may be derived. It would be an ideal case if we can summarize all of the conditions into one general moment condition, similar to Box and Hunter (1957).

The issue of scaling may be further studied not only for the contour plots but also for the evaluation of two-strata rotatable designs. We simply suggested a reasonable approach but an optimum approach may exist.

Chapter 7

Appendix

7.1 The Relationship Between Scalars in Q and Q^{-1}

We can write $\boldsymbol{Q}$ as

$$\begin{pmatrix} A & B\mathbf{1}' & C\mathbf{1}' \\ B\mathbf{1} & M\boldsymbol{I} + G\boldsymbol{J}_{k_1} & G\boldsymbol{J}_{k_1 \times k_2} \\ C\mathbf{1} & G\boldsymbol{J}_{k_2 \times k_1} & T\boldsymbol{I} + G\boldsymbol{J}_{k_2} \end{pmatrix}.$$

Theoretically, the format of $\boldsymbol{Q}^{-1}$ is the same as $\boldsymbol{Q}$. If we write the $\boldsymbol{Q}^{-1}$ as,

$$\begin{pmatrix} a & b\mathbf{1}' & c\mathbf{1}' \\ b\mathbf{1} & m\boldsymbol{I} + e\boldsymbol{J}_{k_1} & g\boldsymbol{J}_{k_1 \times k_2} \\ c\mathbf{1} & g\boldsymbol{J}_{k_1 \times k_2} & t\boldsymbol{I} + h\boldsymbol{J}_{k_2} \end{pmatrix}$$

then, we have

$$\begin{pmatrix} A & B\mathbf{1}' & C\mathbf{1}' \\ B\mathbf{1} & M\boldsymbol{I}+G\boldsymbol{J}_{k_1} & G\boldsymbol{J}_{k_1\times k_2} \\ C\mathbf{1} & G\boldsymbol{J}_{k_2\times k_1} & T\boldsymbol{I}+G\boldsymbol{J}_{k_2} \end{pmatrix} \begin{pmatrix} a & b\mathbf{1}' & c\mathbf{1}' \\ b\mathbf{1} & m\boldsymbol{I}+e\boldsymbol{J}_{k_1} & g\boldsymbol{J}_{k_1\times k_2} \\ c\mathbf{1} & g\boldsymbol{J}_{k_2\times k_1} & t\boldsymbol{I}+h\boldsymbol{J}_{k_2} \end{pmatrix} = \begin{pmatrix} 1 & \mathbf{0}' & \mathbf{0}' \\ \mathbf{0} & \boldsymbol{I} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \boldsymbol{I} \end{pmatrix}.$$

The unknown parameters are a, b, c, m, e, g, t, h. The first step in solving for these parameters is to multiply the three block-rows in $\boldsymbol{Q}$ by the first column of $\boldsymbol{Q}^{-1}$. This yields

$$\begin{pmatrix} a \\ b \\ c \end{pmatrix} = \begin{pmatrix} A & k_1B & k_2C \\ B & M+k_1G & k_2G \\ C & k_1G & T+k_2G \end{pmatrix}^{-1} \begin{pmatrix} 1 \\ \mathbf{0} \\ \mathbf{0} \end{pmatrix}.$$

If we write $\begin{pmatrix} A & k_1B & k_2C \\ B & M+k_1G & k_2G \\ C & k_1G & T+k_2G \end{pmatrix}^{-1}$ as Den^{-1} and we can have $|Den| = k_1k_2(2BCG - B^2G - C^2G) + k_1(ATG - B^2T) + k_2(AMG - C^2M) + AMT$, then

$$a = \frac{MT + k_2MG + Tk_1G}{|Den|} \tag{7.1}$$

$$b = \frac{k_2(CG - BG) - BT}{|Den|} \tag{7.2}$$

$$c = \frac{k_1(BG - CG) - CM}{|Den|}. \tag{7.3}$$

Next, multiply the three block-rows in $\boldsymbol{Q}$ by the second column of $\boldsymbol{Q}^{-1}$, we can get four equations:

$$\begin{aligned}
Ab + Bm + k_1Be + k_2Cg &= 0 \\
Bb + Mm + Me + Gm + k_1Ge + k_2Gh &= 1 \\
Bb + +Me + Gm + k_1Ge + k_2Gh &= 0 \\
Cb + Gm + k_1Ge + Tg + k_2Gg &= 0.
\end{aligned}$$

Simplifying these equations gives

$$m = \frac{1}{M}$$
$$\begin{pmatrix} e \\ g \end{pmatrix} = \begin{pmatrix} k_1B & k_2C \\ k_1G & T + k_2G \end{pmatrix}^{-1} \begin{pmatrix} -Ab - Bm \\ -Cb - Gm \end{pmatrix}.$$

Therefore, we have

$$e = \frac{-TAb - BT/M - k_2GAb - k_2GB/M + k_2C^2b + k_2CG/M}{k_1BT + k_1k_2BG - k_1k_2GC} \tag{7.4}$$
$$g = \frac{k_1GAb + k_1GB/M - k_1BCb - k_1BG/M}{k_1BT + k_1k_2BG - k_1k_2GC}. \tag{7.5}$$

Finally, multiplying the three block-rows in $\boldsymbol{Q}$ by the third column of $\boldsymbol{Q}^{-1}$, gives

$$\begin{aligned}
Ac + k_1Bg + Ct + k_2Ch &= 0 \\
Bc + Mg + k_1Gg + Gt + k_2Gh &= 0 \\
Cc + k_1Gg + Tt + Th + Gt + k_2Gh &= 1 \\
Cc + k_1Gg + Th + Gt + k_2Gh &= 0.
\end{aligned}$$

Therefore we get

$$t = \frac{1}{T} \tag{7.6}$$

$$h = \frac{1}{k_2 C}(Ac - k_1 Bg - C/T). \tag{7.7}$$

As a summary, when we have k_1 whole plot factors and k_2 sub-plot factors, $\boldsymbol{Q}^{-1}$ can be written as:

$$\begin{pmatrix} a & b\mathbf{1}' & c\mathbf{1}' \\ b\mathbf{1} & m\boldsymbol{I} + e\boldsymbol{J}_{k_1} & g\boldsymbol{J}_{k_1 \times k_2} \\ c\mathbf{1} & g\boldsymbol{J}_{k_2 \times k_1} & t\boldsymbol{I} + h\boldsymbol{J}_{k_2} \end{pmatrix}$$

where

$$a = \frac{MT + k_2 MG + Tk_1 G}{|Q|}$$

$$b = \frac{k_2(CG - BG) - BT}{|Q|}$$

$$c = \frac{k_1(BG - CG) - CM}{|Q|}$$

$$m = \frac{1}{M}$$

$$e = \frac{-TAb - BT/M - k_2 GAb - k_2 GB/M + k_2 C^2 b + k_2 CG/M}{k_1 BT + k_1 k_2 BG - k_1 k_2 GC}$$

$$g = \frac{k_1 GAb + k_1 GB/M - k_1 BCb - k_1 BG/M}{k_1 BT + k_1 k_2 BG - k_1 k_2 GC}$$

$$t = \frac{1}{T}$$

$$h = \frac{1}{k_2 C}(Ac - k_1 Bg - C/T).$$

and $|Den| = k_1 k_2(2BCG - B^2 G - C^2 G) + k_1(ATG - B^2 T) + k_2(AMG - C^2 M) + AMT$

7.2 Moment Matrices for Different Split-Plot Central Composite Designs

7.2.1 Balanced and S_O is a subset of WP effects

In the design in Table 3.3, $G = F$, $P = F + 2n\alpha^4$ and $E = F + n\beta^4$. Therefore, (3.10) becomes $2(\frac{1}{-2n\alpha^4}) + \frac{1}{F} = 0$ and $(1 + nd)2\frac{1}{(-n\beta^4)} + \frac{1}{F} = 0$. Furthermore, our condition for this design is:

$$\begin{cases} \alpha = \sqrt[4]{\frac{F}{n}}, \\ \beta = \sqrt[4]{\frac{2(1+nd)F}{n}} \end{cases} \tag{7.8}$$

7.2.2 Balanced and S_O is not a subset of WP effects

The designs in Table 3.1 and Table 3.2 are examples in this scenario. Since $\boldsymbol{S}_O$ is not effectively a subset of the WP effects, then $\boldsymbol{W}_i^* \neq \mathbf{1}_n \boldsymbol{w}_i'$. Now $\boldsymbol{X}'\boldsymbol{\Sigma}^{-1}\boldsymbol{X}$ becomes

$$\boldsymbol{X}'\boldsymbol{\Sigma}^{-1}\boldsymbol{X} = \frac{1}{\sigma^2}\boldsymbol{X}'\boldsymbol{X} - \frac{\sigma_\delta^2}{\sigma^2(\sigma^2 + n\sigma_\delta^2)}\boldsymbol{X}'\boldsymbol{M}\boldsymbol{M}'\boldsymbol{X}. \tag{7.9}$$

Since $\boldsymbol{X} = [\boldsymbol{T}, \boldsymbol{W}_F, \boldsymbol{S}_D]$, then

$$\begin{aligned}
\boldsymbol{X}'\boldsymbol{X} &= \begin{pmatrix} \boldsymbol{T}' \\ \boldsymbol{W}_F' \\ \boldsymbol{S}_D' \end{pmatrix} \begin{pmatrix} \boldsymbol{T} & \boldsymbol{W}_F & \boldsymbol{S}_D \end{pmatrix} \\
&= \begin{pmatrix} \boldsymbol{T}'\boldsymbol{T} & \boldsymbol{T}'\boldsymbol{W}_F & \boldsymbol{T}'\boldsymbol{S}_D \\ \boldsymbol{W}_F'\boldsymbol{T} & \boldsymbol{W}_F'\boldsymbol{W}_F & \boldsymbol{W}_F'\boldsymbol{S}_D \\ \boldsymbol{S}_D'\boldsymbol{T} & \boldsymbol{S}_D'\boldsymbol{W}_F & \boldsymbol{S}_D'\boldsymbol{S}_D \end{pmatrix}.
\end{aligned}$$

Moreover, $\boldsymbol{S}_D'\mathbf{1} = \mathbf{0}$; $\boldsymbol{S}_D'\boldsymbol{W}_F = \mathbf{0}$; and $\boldsymbol{T}'\boldsymbol{W}_F = \mathbf{0}$. As a result,

$$\boldsymbol{X}'\boldsymbol{X} = \begin{pmatrix} \boldsymbol{T}'\boldsymbol{T} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \boldsymbol{W}_F'\boldsymbol{W}_F & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \boldsymbol{S}_D'\boldsymbol{S}_D \end{pmatrix}$$

Note that

$$\begin{aligned}
\boldsymbol{X}'\boldsymbol{M}\boldsymbol{M}'\boldsymbol{X} &= \begin{pmatrix} \boldsymbol{T}' \\ \boldsymbol{W}_F' \\ \boldsymbol{S}_D' \end{pmatrix} \boldsymbol{M}\boldsymbol{M}' \begin{pmatrix} \boldsymbol{T} & \boldsymbol{W}_F & \boldsymbol{S}_D \end{pmatrix} \\
&= \begin{pmatrix} \boldsymbol{T}'\boldsymbol{M}\boldsymbol{M}'\boldsymbol{T} & \boldsymbol{T}'\boldsymbol{M}\boldsymbol{M}'\boldsymbol{W}_F & \boldsymbol{T}'\boldsymbol{M}\boldsymbol{M}'\boldsymbol{S}_D \\ \boldsymbol{W}_F'\boldsymbol{M}\boldsymbol{M}'\boldsymbol{T} & \boldsymbol{W}_F'\boldsymbol{M}\boldsymbol{M}'\boldsymbol{W}_F & \boldsymbol{W}_F'\boldsymbol{M}\boldsymbol{M}'\boldsymbol{S}_D \\ \boldsymbol{S}_D'\boldsymbol{M}\boldsymbol{M}'\boldsymbol{T} & \boldsymbol{S}_D'\boldsymbol{M}\boldsymbol{M}'\boldsymbol{W}_F & \boldsymbol{S}_D'\boldsymbol{M}\boldsymbol{M}'\boldsymbol{S}_D \end{pmatrix}.
\end{aligned}$$

However, $\boldsymbol{MM'1} = n\boldsymbol{1}$, $\boldsymbol{MM'W}_F = n\boldsymbol{W}_F$, and $\boldsymbol{MM'S}_D = \boldsymbol{0}$, Thus,

$$\boldsymbol{X'MM'X} = \begin{pmatrix} \boldsymbol{T'} \\ \boldsymbol{W}'_F \\ \boldsymbol{S}'_D \end{pmatrix} \boldsymbol{MM'} \begin{pmatrix} \boldsymbol{T} & \boldsymbol{W}_F & \boldsymbol{S}_D \end{pmatrix}$$
$$= \begin{pmatrix} \boldsymbol{T'MM'T} & \boldsymbol{0} & \boldsymbol{0} \\ \boldsymbol{0} & n\boldsymbol{W}'_F\boldsymbol{W}_F & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{0} & \boldsymbol{0} \end{pmatrix}$$

and

$$\frac{1}{\sigma^2}\boldsymbol{X'X} - \frac{\sigma_\delta^2}{\sigma^2(\sigma^2+n\sigma_\delta^2)}\boldsymbol{X'MM'X}$$
$$= \frac{1}{\sigma^2}\left(\begin{bmatrix} \boldsymbol{T'T} & \boldsymbol{0} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{W}'_F\boldsymbol{W}_F & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{0} & \boldsymbol{S}'_D\boldsymbol{S}_D \end{bmatrix} - \frac{d}{1+nd} \begin{bmatrix} \boldsymbol{T'MM'T} & \boldsymbol{0} & \boldsymbol{0} \\ \boldsymbol{0} & n\boldsymbol{W}'_F\boldsymbol{W}_F & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{0} & \boldsymbol{0} \end{bmatrix} \right)$$
$$= \frac{1}{\sigma^2} \begin{bmatrix} \boldsymbol{T'T} - \frac{d}{1+nd}\boldsymbol{T'MM'T} & \boldsymbol{0} & \boldsymbol{0} \\ \boldsymbol{0} & \frac{1}{1+nd}\boldsymbol{W}'_F\boldsymbol{W}_F & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{0} & \boldsymbol{S}'_D\boldsymbol{S}_D \end{bmatrix}$$

Since $\boldsymbol{T} = [\boldsymbol{1}, \boldsymbol{W}_Q, \boldsymbol{S}_O]$, we have

$$\boldsymbol{T'T} - \frac{d}{1+nd}\boldsymbol{T'MM'T}$$
$$= \begin{bmatrix} \boldsymbol{1'1} - \frac{d}{1+nd}\boldsymbol{1'MM'1} & \boldsymbol{1'W}_Q - \frac{d}{1+nd}\boldsymbol{1'MM'W}_Q & \boldsymbol{1'S}_O - \frac{d}{1+nd}\boldsymbol{1'MM'S}_O \\ \boldsymbol{W}'_Q\boldsymbol{1} - \frac{d}{1+nd}\boldsymbol{W}'_Q\boldsymbol{MM'1} & \boldsymbol{W}'_Q\boldsymbol{W}_Q - \frac{d}{1+nd}\boldsymbol{W}'_Q\boldsymbol{MM'W}_Q & \boldsymbol{W}'_Q\boldsymbol{S}_O - \frac{d}{1+nd}\boldsymbol{W}'_Q\boldsymbol{MM'S}_O \\ \boldsymbol{S}'_O\boldsymbol{1} - \frac{d}{1+nd}\boldsymbol{S}'_O\boldsymbol{MM'1} & \boldsymbol{S}'_O\boldsymbol{W}_Q - \frac{d}{1+nd}\boldsymbol{S}'_O\boldsymbol{MM'W}_Q & \boldsymbol{S}'_O\boldsymbol{S}_O - \frac{d}{1+nd}\boldsymbol{S}'_O\boldsymbol{MM'S}_O \end{bmatrix}.$$

Because $\boldsymbol{MM}'\mathbf{1} = n\mathbf{1}$ and $\boldsymbol{MM}'\boldsymbol{W}_Q = n\boldsymbol{W}_Q$, with some algebra, the above equation can be further reduced to

$$= \begin{bmatrix} \frac{1}{1+nd}\mathbf{1}'\mathbf{1} & \frac{1}{1+nd}\mathbf{1}'\boldsymbol{W}_Q & \frac{1}{1+nd}\mathbf{1}'\boldsymbol{S}_O \\ \frac{1}{1+nd}\boldsymbol{W}'_Q\mathbf{1} & \frac{1}{1+nd}\boldsymbol{W}'_Q\boldsymbol{W}_Q & \frac{1}{1+nd}\boldsymbol{W}'_Q\boldsymbol{S}_O \\ \frac{1}{1+nd}\mathbf{1}'\boldsymbol{S}_Q & \frac{1}{1+nd}\boldsymbol{S}'_O\boldsymbol{W}_Q & \boldsymbol{S}'_O\boldsymbol{S}_O - \frac{d}{1+nd}\boldsymbol{S}'_O\boldsymbol{MM}'\boldsymbol{S}_O \end{bmatrix}.$$

Specifically,

$$\boldsymbol{S}'_O\boldsymbol{S}_O - \frac{d}{1+nd}\boldsymbol{S}'_O\boldsymbol{MM}'\boldsymbol{S}_O = \begin{bmatrix} F + \frac{n}{2}\beta^4 & F \\ F & F + \frac{n}{2}\beta^4 \end{bmatrix} - \frac{nd}{1+nd}\begin{bmatrix} F+\beta^4 & F+\beta^4 \\ F+\beta^4 & F+\beta^4 \end{bmatrix}$$
$$= \begin{bmatrix} \frac{F-nd\beta^4}{1+nd} + \frac{n}{2}\beta^4 & \frac{F-nd\beta^4}{1+nd} \\ \frac{F-nd\beta^4}{1+nd} & \frac{F-nd\beta^4}{1+nd} + \frac{n}{2}\beta^4 \end{bmatrix}$$

Now the off-diagonal elements in $\boldsymbol{S}'_O\boldsymbol{S}_O$ are no longer F anymore. We get $G = F$ and $P = F + 2n\alpha^4$, $H = \frac{1}{\sigma^2}(\frac{F-nd\beta^4}{1+nd})$ and $E = \frac{1}{\sigma^2}(\frac{F-nd\beta^4}{1+nd} + \frac{n}{2}\beta^4)$, $F_w^* = F$ and $F_s = F$.

The condition (3.10) becomes

$$\begin{cases} \frac{2}{-2n\alpha^4} + \frac{1}{F} = 0, \\ -\frac{4\sigma^2}{n\beta^4} + (\sigma^2)\frac{1}{F} = 0 \end{cases} \tag{7.10}$$

and for this scenario, we get

$$\begin{cases} \alpha = \sqrt[4]{\frac{F}{n}} \\ \beta = \sqrt[4]{\frac{4F}{n}} \end{cases} \tag{7.11}$$

7.2.3 Unbalanced and S_O is a subset of WP effects

We observe that $\boldsymbol{\Sigma}^{-1} = \frac{1}{\sigma^2}\boldsymbol{I}_N - Diag(\frac{\sigma_\delta^2}{\sigma^2(\sigma^2+n_i\sigma_\delta^2)}\boldsymbol{I}_{n_i})\boldsymbol{M}\boldsymbol{M}'$. As a result,

$$\boldsymbol{X}'\boldsymbol{\Sigma}^{-1}\boldsymbol{X} = \frac{1}{\sigma^2}\boldsymbol{X}'\boldsymbol{X} - \boldsymbol{X}'Diag(\frac{\sigma_\delta^2}{\sigma^2(\sigma^2+n_i\sigma_\delta^2)}\boldsymbol{I}_{n_i})\boldsymbol{M}\boldsymbol{M}'\boldsymbol{X}$$

Let $\boldsymbol{W}^* = [\boldsymbol{T}, \boldsymbol{W}_F]$, thus $\boldsymbol{X} = [\boldsymbol{W}^*, \boldsymbol{S}_D]$, and

$$\begin{aligned}
\boldsymbol{X}'\boldsymbol{\Sigma}^{-1}\boldsymbol{X} =& \frac{1}{\sigma^2}\boldsymbol{X}'\boldsymbol{X} - \boldsymbol{X}'Diag(\frac{\sigma_\delta^2}{\sigma^2(\sigma^2+n_i\sigma_\delta^2)}\boldsymbol{I}_{n_i})\boldsymbol{M}\boldsymbol{M}'(\boldsymbol{W}^*, \boldsymbol{S}_D) \\
=& \frac{1}{\sigma^2}\boldsymbol{X}'\boldsymbol{X} - \boldsymbol{X}'Diag(\frac{n_i\sigma_\delta^2}{\sigma^2(\sigma^2+n_i\sigma_\delta^2)}\boldsymbol{I}_{n_i})(\boldsymbol{W}^*, \boldsymbol{0}) \\
=& \frac{1}{\sigma^2}\begin{pmatrix}\boldsymbol{W}^{*'} \\ \boldsymbol{S}_D\end{pmatrix}\begin{pmatrix}\boldsymbol{W}^* & \boldsymbol{S}_D\end{pmatrix} - \begin{pmatrix}\boldsymbol{W}^{*'} \\ \boldsymbol{S}_D'\end{pmatrix} Diag(\frac{n_i\sigma_\delta^2}{\sigma^2(\sigma^2+n_i\sigma_\delta^2)}\boldsymbol{I}_{n_i})(\boldsymbol{W}^*, \boldsymbol{0}) \\
=& \frac{1}{\sigma^2}\begin{pmatrix}\boldsymbol{W}^{*'}\boldsymbol{W}^* & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{S}_D'\boldsymbol{S}_D\end{pmatrix} - \begin{pmatrix}\boldsymbol{W}^{*'}Diag(\frac{n_i\sigma_\delta^2}{\sigma^2(\sigma^2+n_i\sigma_\delta^2)}\boldsymbol{I}_{n_i})\boldsymbol{W}^* & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{0}\end{pmatrix}.
\end{aligned}$$

Since

$$\begin{aligned}
& \boldsymbol{W}^{*'}\boldsymbol{W}^* - \boldsymbol{W}^{*'}Diag(\frac{n_i\sigma_\delta^2}{\sigma^2+n_i\sigma_\delta^2}\boldsymbol{I}_{n_i})\boldsymbol{W}^* \\
=& \boldsymbol{W}^{*'}(\boldsymbol{I}_N - Diag(\frac{n_i\sigma_\delta^2}{\sigma^2+n_i\sigma_\delta^2}\boldsymbol{I}_{n_i}))\boldsymbol{W}^* \\
=& \boldsymbol{W}^{*'}Diag(\frac{\sigma^2}{\sigma^2+n_i\sigma_\delta^2}\boldsymbol{I}_{n_i})\boldsymbol{W}^*
\end{aligned}$$

then

$$\boldsymbol{X}'\boldsymbol{\Sigma}^{-1}\boldsymbol{X} = \begin{pmatrix}\boldsymbol{W}'Diag(\frac{1}{\sigma^2+n_i\sigma_\delta^2}\boldsymbol{I}_{n_i})\boldsymbol{W} & \boldsymbol{0} \\ \boldsymbol{0} & \frac{1}{\sigma^2}\boldsymbol{S}_D'\boldsymbol{S}_D\end{pmatrix}.$$

Let $\boldsymbol{W}^* = (\boldsymbol{T}, \boldsymbol{W}_F) = \begin{pmatrix} \mathbf{1}_1 & \boldsymbol{W}_{Q_1} & \boldsymbol{S}_{O_1} & \boldsymbol{W}_{F_1} \\ \vdots & \vdots & \vdots & \vdots \\ \mathbf{1}_m & \boldsymbol{W}_{Q_m} & \boldsymbol{S}_{O_m} & \boldsymbol{W}_{F_m} \end{pmatrix}$ then $\boldsymbol{W}' Diag(\frac{1}{\sigma^2+n_i\sigma_\delta^2}\boldsymbol{I}_{n_i})\boldsymbol{W}$ is

$$\begin{pmatrix} \boldsymbol{T}' Diag(\frac{1}{\sigma^2+n_i\sigma_\delta^2}\boldsymbol{I}_{n_i})\boldsymbol{T} & \boldsymbol{T}' Diag(\frac{1}{\sigma^2+n_i\sigma_\delta^2}\boldsymbol{I}_{n_i})\boldsymbol{W}_F \\ \boldsymbol{T}' Diag(\frac{1}{\sigma^2+n_i\sigma_\delta^2}\boldsymbol{I}_{n_i})\boldsymbol{W}_F & \boldsymbol{W}_F' Diag(\frac{1}{\sigma^2+n_i\sigma_\delta^2}\boldsymbol{I}_{n_i})\boldsymbol{W}_F \end{pmatrix}$$

and it can be further reduced to

$$\begin{pmatrix} \sum_{i=1}^m \mathbf{1}_i'(\frac{1}{\sigma^2+n_i\sigma_\delta^2}\boldsymbol{I}_{n_i})\mathbf{1}_i & \sum_{i=1}^m \mathbf{1}_i'(\frac{1}{\sigma^2+n_i\sigma_\delta^2}\boldsymbol{I}_{n_i})\boldsymbol{W}_{Q_i} & \sum_{i=1}^m \mathbf{1}_i'(\frac{1}{\sigma^2+n_i\sigma_\delta^2}\boldsymbol{I}_{n_i})\boldsymbol{S}_{O_i} & \sum_{i=1}^m \mathbf{1}_i'(\frac{1}{\sigma^2+n_i\sigma_\delta^2}\boldsymbol{I}_{n_i})\boldsymbol{W}_{F_i} \\ \sum_{i=1}^m \boldsymbol{W}_{Q_i}'(\frac{1}{\sigma^2+n_i\sigma_\delta^2}\boldsymbol{I}_{n_i})\mathbf{1}_i & \sum_{i=1}^m \boldsymbol{W}_{Q_i}'(\frac{1}{\sigma^2+n_i\sigma_\delta^2}\boldsymbol{I}_{n_i})\boldsymbol{W}_{Q_i} & \sum_{i=1}^m \boldsymbol{W}_{Q_i}'(\frac{1}{\sigma^2+n_i\sigma_\delta^2}\boldsymbol{I}_{n_i})\boldsymbol{S}_{O_i} & \sum_{i=1}^m \boldsymbol{W}_{Q_i}'(\frac{1}{\sigma^2+n_i\sigma_\delta^2}\boldsymbol{I}_{n_i})\boldsymbol{W}_{F_i} \\ \sum_{i=1}^m \boldsymbol{S}_{O_i}'(\frac{1}{\sigma^2+n_i\sigma_\delta^2}\boldsymbol{I}_{n_i})\mathbf{1}_i & \sum_{i=1}^m \boldsymbol{S}_{O_i}'(\frac{1}{\sigma^2+n_i\sigma_\delta^2}\boldsymbol{I}_{n_i})\boldsymbol{W}_{Q_i} & \sum_{i=1}^m \boldsymbol{S}_{O_i}'(\frac{1}{\sigma^2+n_i\sigma_\delta^2}\boldsymbol{I}_{n_i})\boldsymbol{S}_{O_i} & \sum_{i=1}^m \boldsymbol{S}_{O_i}'(\frac{1}{\sigma^2+n_i\sigma_\delta^2}\boldsymbol{I}_{n_i})\boldsymbol{W}_{F_i} \\ \sum_{i=1}^m \boldsymbol{W}_{F_i}'(\frac{1}{\sigma^2+n_i\sigma_\delta^2}\boldsymbol{I}_{n_i})\mathbf{1}_i & \sum_{i=1}^m \boldsymbol{W}_{F_i}'(\frac{1}{\sigma^2+n_i\sigma_\delta^2}\boldsymbol{I}_{n_i})\boldsymbol{W}_{Q_i} & \sum_{i=1}^m \boldsymbol{W}_{F_i}'(\frac{1}{\sigma^2+n_i\sigma_\delta^2}\boldsymbol{I}_{n_i})\boldsymbol{S}_{O_i} & \sum_{i=1}^m \boldsymbol{W}_{F_i}'(\frac{1}{\sigma^2+n_i\sigma_\delta^2}\boldsymbol{I}_{n_i})\boldsymbol{W}_{F_i} \end{pmatrix}.$$

We observe that

$$\begin{aligned} \mathbf{1}_i'(\frac{1}{\sigma^2+n_i\sigma_\delta^2}\boldsymbol{I}_{n_i})\boldsymbol{W}_{F_i} &= \frac{1}{\sigma^2+n_i\sigma_\delta^2}\mathbf{1}_i'\boldsymbol{I}_{n_i}\boldsymbol{W}_{F_i} = \mathbf{0} \\ \boldsymbol{W}_{Q_i}'(\frac{1}{\sigma^2+n_i\sigma_\delta^2}\boldsymbol{I}_{n_i})\boldsymbol{W}_{F_i} &= \frac{1}{\sigma^2+n_i\sigma_\delta^2}\boldsymbol{W}_{Q_i}'\boldsymbol{W}_{F_i} = \mathbf{0} \\ \boldsymbol{S}_{O_i}'(\frac{1}{\sigma^2+n_i\sigma_\delta^2}\boldsymbol{I}_{n_i})\boldsymbol{W}_{F_i} &= \frac{1}{\sigma^2+n_i\sigma_\delta^2}\boldsymbol{S}_{O_i}'\boldsymbol{W}_{F_i} = \mathbf{0} \end{aligned}$$

As a result, $\boldsymbol{W}' Diag(\frac{1}{\sigma^2+n_i\sigma_\delta^2}\boldsymbol{I}_{n_i})\boldsymbol{W}$ becomes

$$\begin{pmatrix} \boldsymbol{T}' Diag(\frac{1}{\sigma^2+n_i\sigma_\delta^2}\boldsymbol{I}_{n_i})\boldsymbol{T} & \mathbf{0} \\ \mathbf{0} & \boldsymbol{W}_F' Diag(\frac{1}{\sigma^2+n_i\sigma_\delta^2}\boldsymbol{I}_{n_i})\boldsymbol{W}_F \end{pmatrix}$$

=

$$\begin{pmatrix} \sum_{i=1}^m \mathbf{1}'_{n_i}(\frac{1}{\sigma^2+n_i\sigma_\delta^2}\boldsymbol{I}_{n_i})\mathbf{1}_{n_i} & \sum_{i=1}^m \mathbf{1}'_{n_i}(\frac{1}{\sigma^2+n_i\sigma_\delta^2}\boldsymbol{I}_{n_i})\boldsymbol{W}_{Q_i} & \sum_{i=1}^m \mathbf{1}'_{n_i}(\frac{1}{\sigma^2+n_i\sigma_\delta^2}\boldsymbol{I}_{n_i})\boldsymbol{S}_{O_i} & \mathbf{0} \\ \sum_{i=1}^m \boldsymbol{W}'_{Q_i}(\frac{1}{\sigma^2+n_i\sigma_\delta^2}\boldsymbol{I}_{n_i})\mathbf{1}_{n_i} & \sum_{i=1}^m \boldsymbol{W}'_{Q_i}(\frac{1}{\sigma^2+n_i\sigma_\delta^2}\boldsymbol{I}_{n_i})\boldsymbol{W}_{Q_i} & \sum_{i=1}^m \boldsymbol{W}'_{Q_i}(\frac{1}{\sigma^2+n_i\sigma_\delta^2}\boldsymbol{I}_{n_i})\boldsymbol{S}_{O_i} & \mathbf{0} \\ \sum_{i=1}^m \boldsymbol{S}'_{O_i}(\frac{1}{\sigma^2+n_i\sigma_\delta^2}\boldsymbol{I}_{n_i})\mathbf{1}_{n_i} & \sum_{i=1}^m \boldsymbol{S}'_{O_i}(\frac{1}{\sigma^2+n_i\sigma_\delta^2}\boldsymbol{I}_{n_i})\boldsymbol{W}_{Q_i} & \sum_{i=1}^m \boldsymbol{S}'_{O_i}(\frac{1}{\sigma^2+n_i\sigma_\delta^2}\boldsymbol{I}_{n_i})\boldsymbol{S}_{O_i} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \sum_{i=1}^m \boldsymbol{W}'_{F_i}(\frac{1}{\sigma^2+n_i\sigma_\delta^2}\boldsymbol{I}_{n_i})\boldsymbol{W}_{F_i} \end{pmatrix}.$$

There are many possible allocation schemes for putting observations in the WPs. Therefore, there are infinite numbers of n_is. A reasonable and common scheme would be to:

let the WP size for WP factorial runs be the same, noted as n_{WF};

let the WP size for WP axial runs be the same, noted as n_{WA};

let the WP size for SP axial runs be the same, noted as n_{SA}.

Then we can define three coefficients $C_1 = \frac{1}{\sigma^2+n_{WF}\sigma_\delta^2}$, $C_2 = \frac{1}{\sigma^2+n_{WA}\sigma_\delta^2}$ and $C_3 = \frac{1}{\sigma^2+n_{SA}\sigma_\delta^2}$. Furthermore, we define the number of the axial runs appeared in the column for each WP factor as r and the number of the axial runs for each SP factor as a. In the split-plot experiment with no replicate of WP axial runs, the number of axial runs for each WP factor is 2. However, when we calculate the conditions for rotatability, we have to use the number of αs and $-\alpha$s appearing in each column for the corresponding WP factor. Effectively, $r = 2n_{WA}$ here. For example, for the design in Table 3.4, r=6 and a=2; for the design in Table 3.3, r=8 and a=4.

In general the elements in $(\boldsymbol{T}'Diag(\frac{1}{\sigma^2+n_i\sigma_\delta^2}\boldsymbol{I}_{n_i})\boldsymbol{T})$ are

$$\sum_{i=1}^{m}\mathbf{1}_i'(\frac{1}{\sigma^2+n_i\sigma_\delta^2}\boldsymbol{I}_{n_i})\mathbf{1}_i = C_1F + C_2rk_1 + C_3ak_2$$
$$\sum_{i=1}^{m}\mathbf{1}_i'(\frac{1}{\sigma^2+n_i\sigma_\delta^2}\boldsymbol{I}_{n_i})\boldsymbol{W}_{Q_i} = (C_1F + C_2r\alpha^2, ..., C_1F + C_2r\alpha^2)'$$
$$\sum_{i=1}^{m}\mathbf{1}_i'(\frac{1}{\sigma^2+n_i\sigma_\delta^2}\boldsymbol{I}_{n_i})\boldsymbol{S}_{O_i} = (C_1F + C_3a\beta^2, ..., C_1F + C_3a\beta^2)'$$

$$\begin{pmatrix} \sum_{i=1}^m \boldsymbol{W}_{Q_i}'(\frac{1}{\sigma^2+n_i\sigma_\delta^2}\boldsymbol{I}_{n_i})\boldsymbol{W}_{Q_i} & \sum_{i=1}^m \boldsymbol{W}_{Q_i}'(\frac{1}{\sigma^2+n_i\sigma_\delta^2}\boldsymbol{I}_{n_i})\boldsymbol{S}_{O_i} \\ \sum_{i=1}^m \boldsymbol{S}_{O_i}'(\frac{1}{\sigma^2+n_i\sigma_\delta^2}\boldsymbol{I}_{n_i})\boldsymbol{W}_{Q_i} & \sum_{i=1}^m \boldsymbol{S}_{O_i}'(\frac{1}{\sigma^2+n_i\sigma_\delta^2}\boldsymbol{I}_{n_i})\boldsymbol{S}_{O_i} \end{pmatrix} =$$

$$\begin{pmatrix} C_1F+C_2r\alpha^4 & C_1F & \cdots & C_1F & C_1F & \cdots & C_1F \\ C_1F & C_1F+C_2r\alpha^4 & \cdots & C_1F & C_1F & \cdots & C_1F \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ C_1F & C_1F & \cdots & C_1F+C_2r\alpha^4 & C_1F & \cdots & C_1F \\ C_1F & C_1F & \cdots & C_1F & C_1F+C_3a\beta^4 & \cdots & C_1F \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ C_1F & C_1F & \cdots & C_1F & C_1F & \cdots & C_1F+C_3a\beta^4 \end{pmatrix}.$$

Now we can see that $(\boldsymbol{T}'Diag(\frac{1}{\sigma^2+n_i\sigma_\delta^2}\boldsymbol{I}_{n_i})\boldsymbol{T})$ becomes

$$\begin{pmatrix} C_1F+C_2rk_1+C_3ak_2 & C_1F+C_2r\alpha^2 & C_1F+C_2r\alpha^2 & \cdots & C_1F+C_2r\alpha^2 & C_1F+C_3a\beta^2 & \cdots & C_1F+C_3a\beta^2 \\ C_1F+C_2r\alpha^2 & C_1F+C_2r\alpha^4 & C_1F & \cdots & C_1F & C_1F & \cdots & C_1F \\ C_1F+C_2r\alpha^2 & C_1F & C_1F+C_2r\alpha^4 & \cdots & C_1F & C_1F & \cdots & C_1F \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ C_1F+C_2r\alpha^2 & C_1F & C_1F & \cdots & C_1F+C_2r\alpha^4 & C_1F & \cdots & C_1F \\ C_1F+C_3a\beta^2 & C_1F & C_1F & \cdots & C_1F & C_1F+C_3a\beta^4 & \cdots & C_1F \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ C_1F+C_3a\beta^2 & C_1F & C_1F & \cdots & C_1F & C_1F & \cdots & C_1F+C_3a\beta^4 \end{pmatrix}$$

and

$$\sum_{i=1}^{b} \boldsymbol{W'}_{F_i}(\frac{1}{\sigma^2+n_i\sigma_\delta^2}\boldsymbol{I}_{n_i})\boldsymbol{W}_{F_i} = \begin{pmatrix} C_1F+a\alpha^2 & \cdots & \mathbf{0} & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{0} & \cdots & \mathbf{0} & \mathbf{0} & \cdots & \mathbf{0} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \mathbf{0} & \cdots & C_1F+a\alpha^2 & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{0} & \cdots & \mathbf{0} & C_1F & \cdots & \mathbf{0} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \mathbf{0} & \cdots & \mathbf{0} & \mathbf{0} & \cdots & C_1F \end{pmatrix}.$$

Notice that $(\boldsymbol{T'}Diag(\frac{1}{\sigma^2+n_i\sigma_\delta^2}\boldsymbol{I}_{n_i})\boldsymbol{T})$ is still of the matrix form in Appendix A1. Now $H = G = C_1F$, P=$C_1F + C_2r\alpha^2$ and E=$C_1F + C_3a\beta^2$. $F_w^* = C_1F$ instead of F and $F_s = F$. So the condition (3.10) becomes

$$\begin{cases} \frac{2}{-C_2r\alpha^2} + \frac{1}{C_1F} = 0, \\ \frac{2}{-C_3a\beta^4} + (\sigma^2)\frac{1}{F} = 0, \end{cases}$$
$$\Longleftrightarrow \begin{cases} \alpha = \sqrt[4]{\frac{2C_1F}{rC_2}} = \sqrt[4]{\frac{2F(1+n_{WA}d)}{r(1+n_{WF}d)}} \\ \beta = \sqrt[4]{\frac{2F}{a\sigma^2C_3}} = \sqrt[4]{\frac{2F(1+n_{SA}d)}{a}} \end{cases} \qquad (7.12)$$

7.2.4 Unbalanced and S_O is not a subset of WP effects

We observe that $\boldsymbol{\Sigma}^{-1} = \frac{1}{\sigma^2}\boldsymbol{I}_N - Diag(\frac{\sigma_\delta^2}{\sigma^2(\sigma^2+n_i\sigma_\delta^2)}\boldsymbol{I}_{n_i})\boldsymbol{MM'}$. As a result,

$$\boldsymbol{X'\Sigma}^{-1}\boldsymbol{X} = \frac{1}{\sigma^2}\boldsymbol{X'X} - \boldsymbol{X'}Diag(\frac{\sigma_\delta^2}{\sigma^2(\sigma^2+n_i\sigma_\delta^2)}\boldsymbol{I}_{n_i})\boldsymbol{MM'X}$$

Let $\boldsymbol{X} = [\boldsymbol{T}, \boldsymbol{W}_F, \boldsymbol{S}_D]$, thus,

$$\begin{aligned}
\boldsymbol{X}'\boldsymbol{\Sigma}^{-1}\boldsymbol{X} =& \frac{1}{\sigma^2}\boldsymbol{X}'\boldsymbol{X} - \boldsymbol{X}' Diag(\frac{\sigma_\delta^2}{\sigma^2(\sigma^2 + n_i\sigma_\delta^2)}\boldsymbol{I}_{n_i})\boldsymbol{M}\boldsymbol{M}'\boldsymbol{X} \\
=& \frac{1}{\sigma^2}\begin{pmatrix} \boldsymbol{T}' \\ \boldsymbol{W}_F' \\ \boldsymbol{S}_D' \end{pmatrix}\begin{pmatrix} \boldsymbol{T} & \boldsymbol{W}_F & \boldsymbol{S}_D \end{pmatrix} - \begin{pmatrix} \boldsymbol{T}' \\ \boldsymbol{W}_F' \\ \boldsymbol{S}_D' \end{pmatrix} Diag(\frac{\sigma_\delta^2}{\sigma^2(\sigma^2 + n_i\sigma_\delta^2)}\boldsymbol{I}_{n_i})\boldsymbol{M}\boldsymbol{M}'\begin{pmatrix} \boldsymbol{T} & \boldsymbol{W}_F & \boldsymbol{S}_D \end{pmatrix} \\
=& \frac{1}{\sigma^2}\begin{pmatrix} \boldsymbol{T}'\boldsymbol{T} & \boldsymbol{0} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{W}_F'\boldsymbol{W}_F & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{0} & \boldsymbol{S}_D'\boldsymbol{S}_D \end{pmatrix} \\
&- \begin{pmatrix} \boldsymbol{T}' Diag(\frac{\sigma_\delta^2}{\sigma^2(\sigma^2+n_i\sigma_\delta^2)}\boldsymbol{I}_{n_i})\boldsymbol{M}\boldsymbol{M}'\boldsymbol{T} & \boldsymbol{0} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{W}_F' Diag(\frac{n_i\sigma_\delta^2}{\sigma^2(\sigma^2+n_i\sigma_\delta^2)}\boldsymbol{I}_{n_i})\boldsymbol{W}_F & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{0} & \boldsymbol{0} \end{pmatrix} \\
=& \begin{pmatrix} \frac{1}{\sigma^2}\boldsymbol{T}'\boldsymbol{T} - \boldsymbol{T}' Diag(\frac{\sigma_\delta^2}{\sigma^2(\sigma^2+n_i\sigma_\delta^2)}\boldsymbol{I}_{n_i})\boldsymbol{M}\boldsymbol{M}'\boldsymbol{T} & \boldsymbol{0} & \boldsymbol{0} \\ \boldsymbol{0} & \sum_{i=1}^m \frac{1}{\sigma^2+n_i\sigma_\delta^2}\boldsymbol{W}_{F_i}'\boldsymbol{W}_{F_i} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{0} & \boldsymbol{S}_D'\boldsymbol{S}_D \end{pmatrix}.
\end{aligned}$$

We observe that

$$\begin{aligned}
&\frac{1}{\sigma^2}\boldsymbol{T}'\boldsymbol{T} - \boldsymbol{T}' Diag(\frac{\sigma_\delta^2}{\sigma^2(\sigma^2 + n_i\sigma_\delta^2)}\boldsymbol{I}_{n_i})\boldsymbol{M}\boldsymbol{M}'\boldsymbol{T} \\
=& \begin{pmatrix} \sum_{i=1}^m \boldsymbol{1}_i'(\frac{1}{\sigma^2+n_i\sigma_\delta^2}\boldsymbol{I}_{n_i})\boldsymbol{1}_i & \sum_{i=1}^m \boldsymbol{1}_i'(\frac{1}{\sigma^2+n_i\sigma_\delta^2}\boldsymbol{I}_{n_i})\boldsymbol{W}_{Q_i} & \sum_{i=1}^m \boldsymbol{1}_i'(\frac{1}{\sigma^2+n_i\sigma_\delta^2}\boldsymbol{I}_{n_i})\boldsymbol{S}_{O_i} \\ \sum_{i=1}^m \boldsymbol{W}_{Q_i}'(\frac{1}{\sigma^2+n_i\sigma_\delta^2}\boldsymbol{I}_{n_i})\boldsymbol{1}_i & \sum_{i=1}^m \boldsymbol{W}_{Q_i}'(\frac{1}{\sigma^2+n_i\sigma_\delta^2}\boldsymbol{I}_{n_i})\boldsymbol{W}_{Q_i} & \sum_{i=1}^m \boldsymbol{W}_{Q_i}'(\frac{1}{\sigma^2+n_i\sigma_\delta^2}\boldsymbol{I}_{n_i})\boldsymbol{S}_{O_i} \\ \sum_{i=1}^m \boldsymbol{S}_{O_i}'(\frac{1}{\sigma^2+n_i\sigma_\delta^2}\boldsymbol{I}_{n_i})\boldsymbol{1}_i & \sum_{i=1}^m \boldsymbol{S}_{O_i}'(\frac{1}{\sigma^2+n_i\sigma_\delta^2}\boldsymbol{I}_{n_i})\boldsymbol{W}_{Q_i} & \frac{1}{\sigma^2}\boldsymbol{S}_O'\boldsymbol{S}_O - \boldsymbol{S}_O'(Diag(\frac{\sigma_\delta^2}{\sigma^2(\sigma^2+n_i\sigma_\delta^2)}\boldsymbol{I}_{n_i})\boldsymbol{M}\boldsymbol{M}')\boldsymbol{S}_O \end{pmatrix}
\end{aligned}$$

we still have

$$\sum_{i=1}^{m}\frac{1}{\sigma^2+n_i\sigma_\delta^2}\boldsymbol{W}'_{F_i}\boldsymbol{W}_{F_i}=\begin{pmatrix} C_1F+a\alpha^2 & \cdots & \mathbf{0} & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{0} & \cdots & \mathbf{0} & \mathbf{0} & \cdots & \mathbf{0} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \mathbf{0} & \cdots & C_1F+a\alpha^2 & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{0} & \cdots & \mathbf{0} & C_1F & \cdots & \mathbf{0} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \mathbf{0} & \cdots & \mathbf{0} & \mathbf{0} & \cdots & C_1F \end{pmatrix}.$$

All the elements in $\frac{1}{\sigma^2}\boldsymbol{T}'\boldsymbol{T}-\boldsymbol{T}'Diag(\frac{\sigma_\delta^2}{\sigma^2(\sigma^2+n_i\sigma_\delta^2)}\boldsymbol{I}_{n_i})\boldsymbol{M}\boldsymbol{M}'\boldsymbol{T}$ are the same as in Appendix B3 except the lower-right block matrix which is $\frac{1}{\sigma^2}\boldsymbol{S}'_O\boldsymbol{S}_O-\boldsymbol{S}'_O(Diag(\frac{\sigma_\delta^2}{\sigma^2(\sigma^2+n_i\sigma_\delta^2)}\boldsymbol{I}_{n_i})\boldsymbol{M}\boldsymbol{M}')\boldsymbol{S}_O$. Let $m-t$ be the number of whole plots with factorial runs, then

$$\begin{aligned}
&\frac{1}{\sigma^2}\boldsymbol{S}'_O\boldsymbol{S}_O-\boldsymbol{S}'_O(Diag(\frac{\sigma_\delta^2}{\sigma^2(\sigma^2+n_i\sigma_\delta^2)}\boldsymbol{I}_{n_i})\boldsymbol{M}\boldsymbol{M}')\boldsymbol{S}_O\\
=&\frac{1}{\sigma^2}(\sum_{i=1}^{m-t}\boldsymbol{S}'_{O_i}\boldsymbol{S}_{O_i}-\sum_{i=1}^{m-t}\frac{n_{WF}\sigma_\delta^2}{\sigma^2+n_{WF}\sigma_\delta^2}\boldsymbol{S}'_{O_i}\boldsymbol{S}_{O_i})\\
+&\frac{1}{\sigma^2}(\sum_{i=m-t+1}^{m}\boldsymbol{S}'_{O_i}\boldsymbol{S}_{O_i}-\sum_{i=m-t+1}^{m}\frac{n_{SA}\sigma_\delta^2}{\sigma^2+n_{SA}\sigma_\delta^2}\boldsymbol{S}'_{O_i}\boldsymbol{M}\boldsymbol{M}'\boldsymbol{S}_{O_i})\\
=&C_1FJ_k+\frac{1}{\sigma^2}\left[\begin{pmatrix} a\beta^4 & \mathbf{0} \\ \mathbf{0} & a\beta^4\end{pmatrix}-\frac{n_{SA}\sigma_\delta^2}{\sigma^2+n_{SA}\sigma_\delta^2}\begin{pmatrix} 2a\beta^4 & 2a\beta^4 \\ 2a\beta^4 & 2a\beta^4\end{pmatrix}\right]\\
=&\begin{pmatrix} C_1F-C_32adn_{SA}\beta^4+\frac{1}{\sigma^2}a\beta^4 & C_1F-C_32adn_{SA}\beta^4 \\ C_1F-C_32adn_{SA}\beta^4 & C_1F-C_32adn_{SA}\beta^4+\frac{1}{\sigma^2}a\beta^4\end{pmatrix}.
\end{aligned}$$

Note that $G=C_1F$, $P=C_1F+C_2r\alpha^2$, $H=C_1F-C_32adn_{SA}\beta^4$ and $E=C_1F-$

$C_3 2adn_{SA}\beta^4 + \frac{1}{\sigma^2}a\beta^4$. Therefore, the condition (3.10) becomes

$$\begin{cases} \frac{2}{-C_2 r\alpha^2} + \frac{1}{C_1 F} = 0 \\ \frac{2\sigma^2}{a\beta^4} + \frac{\sigma^2}{F} = 0 \end{cases}$$
$$\Longleftrightarrow \begin{cases} \alpha = \sqrt[4]{\frac{2C_1 F}{rC_2}} = \sqrt[4]{\frac{2F(1+n_{WA}d)}{r(1+n_{WF}d)}} \\ \beta = \sqrt[4]{\frac{2F}{a}} \end{cases} . \tag{7.13}$$

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Vita

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