CONSTRUCTION OF ESTIMATION-EQUIVALENT SECOND-ORDER SPLIT-SPLIT-PLOT DESIGNS

by

FANG YUAN

MARCUS B. PERRY, COMMITTEE CHAIR
MICHAEL D. CONERLY
MICHAEL B. ADAMS
JUNSOO LEE
UZMA RAJA

A DISSERTATION

Submitted in partial fulfillment of the requirements
for the degree of Doctor of Philosophy in the
Department of Applied Statistics
in the Graduate School of
The University of Alabama

TUSCALOOSA, ALABAMA

2011

ABSTRACT

In many experimental settings, some experimental factors are very hard to change or very expensive to change, some factors are hard to change, and some factors are easy to change, which usually leads to a split-split-plot design. In such a case, there are randomization restrictions in our experiments. If the data is analyzed as if it were a completely randomized design, the results could be misleading. The analysis of split-split-plot designs is more complicated relative to the completely randomized design, as generalized least squares (GLS) is recommended for estimating the factor effects, and restricted maximum likelihood (REML) is recommended for estimating the variance components. As an alternative, one can consider estimation-equivalent designs, wherein ordinary least squares (OLS) and GLS estimates of the factor effects are equivalent. These designs provide practical benefits from the perspective of design selection and estimation and are consistent with traditional response surface methods. Although much work has been done with respect to estimation-equivalent second-order split-plot designs, less emphasis has been placed on split-split-plot (and higher strata) designs of this type. My research is to derive the general conditions for achieving OLS-GLS equivalence and use these conditions to construct balanced and unbalanced estimation-equivalent second-order split-split-plot designs from the central composite design (CCD).

LIST OF ABBREVIATIONS AND SYMBOLS

WP	Whole plot
SP	Subplot
SSP	Sub-subplot
OLS	Ordinary least square
GLS	Generalized least square
RSM	Response surface methodology
WPrep	Whole-plot replicates
DOE	Design of experiments
CRD	Completely randomized design
CCD	Central composite design
BBD	Box-Behnken design
VKM	Vining, Kowalski, and Montgomery
MWP	Minimum number of whole plots
SPD	Split-plot design
VTHC	Very-hard-to-change factor
HTC	Hard-to-change factor
ETC	Easy-to-change factor

REML	Restricted maximum likelihood
ML	Maximum likelihood
BLUE	Best linear unbiased estimates
Y	Vector of responses
X	Design matrix
β	Model parameters
Z_1	Indicator matrix for the whole-plot factors
Z_2	Indicator matrix for the subplot factors
ε	Vector of sub-subplot random errors
ν	Vector of subplot random errors
δ	Vector of whole-plot random errors
p	Number of model parameters
N	Total number of observations
w	Number of whole plots
m_i	Number of subplots in i^{th} whole plot
n_{ij}	Number of sub-subplots in j^{th} subplot of i^{th} whole plot
n_i	Number of sub-subplots in i^{th} whole plot
r_1	The variance ratios of whole plot to sub-subplot variance
r_2	The variance ratios of subplot to sub-subplot variance
Σ	The variance-covariance matrix

$\hat{\beta}_{OLS}$	The OLS model estimates
$\hat{\beta}_{GLS}$	The GLS model estimates
α	The distance between the whole-plot axial points to the center points
ϕ	The distance between the subplot axial points to the center points
γ	The distance between the sub-subplot axial points to the center points
W_{Dij}	The model sub matrix for the whole-plot main effect and two factor interaction terms contained in the j^{th} subplot of i^{th} whole plot
W_{Qij}	The model sub matrix for the whole-plot pure quadratic terms contained in the j^{th} subplot of i^{th} whole plot
S_{Dij}	The model sub matrix for the subplot main effect and two factor interaction terms between whole plot and subplot, subplot, and subplot interaction terms contained in the j^{th} subplot of i^{th} whole plot
S_{Qij}	The model submatrix for the subplot pure quadratic terms contained in the j^{th} subplot of i^{th} whole plot
SS_{Dij}	The model submatrix for the sub-subplot main effect and two factor interaction terms between whole plot and sub-subplot, subplot and sub-subplot, sub-subplot and sub-subplot interaction terms contained in the j^{th} subplot of i^{th} whole plot
SS_{Qij}	The model submatrix for the sub-subplot pure quadratic terms contained in the j^{th} subplot of i^{th} whole plot
a	The number of whole-plot factors
b	The number of subplot factors

l	The number of sub-subplot factors
Y	Vector of responses
n_w	The number of runs per whole plot
$q, v1, v2$	Constant vector
I_D, I_Q	Identity matrix
V_{SQ}	$b \times b$ matrix
V_{SSQ}	$l \times l$ matrix
G_{SSQ}	$l \times l$ matrix
I_{SD}, I_{SQ}	Identity matrix
M_{W0}	$a \times l$ matrix
M_{W1}	$a \times b$ matrix
M_{SSQ}	$l \times l$ matrix.
n_{nzf}	number of nonzero subplot factorial points at whole-plot high or low level
n_{nzsa}	number of nonzero subplot axial points at whole-plot center level
n_{nzssa}	number of nonzero sub-subplot axial points at whole-plot center level

ACKNOWLEDGMENTS

I am pleased to have this opportunity to express my sincere appreciation to my advisor, Dr. Marcus B. Perry, who introduced me into the field of Response Surface Methodology, for his guidance, strong support, and continuous encouragement during the past 3 years.

I really appreciate the great support of Dr. Michael Cornerly, Dr. B. Michael Adams, Dr. Junsoo Lee, and Dr. Uzma Raja, because their courses enhanced the knowledge and insights of my research.

I would like to thank Office of Institution Research and Assessment and the department of Applied Statistics for financial support. The professional assistance of Mr. Lorne Kuffle, Dr. Michael R. O'Real , Mr. Samual C. Strother, Ms. Julianna Proctor, Ms. Julia S. McAdams, Ms. Christine Kraft, Ms. Sharon Tidmore, Ms. Leticia Worthington and Mr. William W. Hughes is greatly appreciated.

Special thanks to Mrs. Dana for her professional assistance. And my classmates, Ms. Amanda Kaye McCracken, Dr. Yinaze (Herve) Dovoedo. It was a great pleasure to work with and to learn from them.

Finally, I wish to thank my Dad Senhang Yuan, my brother Yaodong Yuan, my husband Jinwen Wang, my son Winnie, and my daughter Camellia for their continuous love and support. I particularly dedicate this work to my husband, Jinwen Wang

CONTENTS

LIST OF TABLES

LIST OF FIGURES

CHAPTER 1

INTRODUCTION

1.1 Background

In statistics, design of experiments (DOE) or experimental design is a systematic process that helps us to characterize the variability in one or more response variables in terms of experimental factors. A common goal of experimental design is to collect data as parsimoniously as possible while providing sufficient information to accurately estimate model parameters. One important methodology in DOE is the response surface methodology (RSM) introduced by Box and Wilson (1951). The main idea of RSM is to use sequential experimentation to characterize and optimize a response that is affected by the levels of experimental factors.

When conducting a response surface design, researchers have recommended that the design points should be run in a completely randomized fashion, and this design can be called a completely randomized design (CRD). Constructing a CRD helps to eliminate any bias in the response variable due to lurking hidden variables. In addition, it provides a basis for modeling the response variable using only a single component of variance, which simplifies the analysis. However, in practice, it is often too expensive or too time consuming to conduct completely randomized designs (CRD). That is, it may be too difficult or costly to change levels of some experimental factors as many times as would be necessary. This results in a randomization restriction.

If there is one randomization restriction in the design, a split-plot design (SPD) is preferred. Two types of experimental factors are considered in a SPD: One type is time-consuming or hard-to-change (HTC) factors; the other is easy-to-change (ETC) factors. The randomization restriction is set in the HTC factors in order to reduce the number of times these variables are reset. If one instead considers three different types of experimental factors, that is, very hard to change (VHTC) factors, hard to change (HTC) factors, and easy to change (ETC) factors, then there are two restrictions on randomization. The first is associated with the VHTC factors, whereas the second is associated with the HTC factors. This leads to a split-split-plot design.

A split-split-plot design is a three stratum extension of a split-plot design. It contains three different sizes or types of experimental factors. The top stratum is for very-hard-to-change (VHTC) factors that are randomly assigned to the whole-plot experimental units; within each whole plot, the experimental subjects are divided further into additional units or the middle stratum, which is called subplots, containing the hard-to-change (HTC) factors. The subplots are additionally split into sub-subunits assigned randomly to another set of treatments or the lowest stratum. The factors in this stratum are called sub-subplot factors or easy-to-change (ETC) factors. Three randomization procedures result in three error sources: whole-plot error, subplot error, and sub-subplot error.

Tables 1-3 are constructed to illustrate a 2^3 full factorial design run as a CRD, split-plot, and split-split-plot design, respectively. Table 1 shows the CRD case where all three factors are assumed to be equivalent in terms of ease of manipulation. The total number of runs is eight. The

SPD is constructed in Table 2, in which one whole-plot factor is assigned to Factor A, and the other two subplot factors are assigned to Factor B and Factor C. This design gives two whole plots with four runs in each whole plot. One randomization restriction is in the whole plots. Table 3 shows the split-split-plot design in which Factor A represents the whole-plot factor, Factor B represents the subplot factor, and Factor C represents the sub-subplot factor. With two randomization restrictions in the whole-plot factors and subplot factors, one can see that the number of whole plots decreases to two with four runs in each whole plot. There are 2 subplots within each whole plot, and two runs in each subplot.

Table 1

Factorial Points in a Completely Randomized Design with Three Experimental Factors

Factor A	Factor B	Factor C
1	-1	1
-1	1	-1
1	-1	-1
-1	1	1
-1	-1	1
1	1	-1
-1	-1	-1

Table 2

Factorial Points in a Split-Plot Design with Three Experimental Factors

WP	Factor A	SP	Factor B	Factor C
1	1	1	-1	1
	1	2	1	-1
	1	3	1	1
	1	4	-1	-1
2	-1	5	-1	1
	-1	6	1	-1
	-1	7	-1	-1
	-1	8	1	1

Note. WP denotes whole plot, and SP denotes subplot.

Table 3

Factorial Points in a Split-Split-Plot Design with Three Experimental Factors

WP	Factor A	SP	Factor B	SSP	Factor C
1	1	1	1	1	1
	1		1	2	-1
	1	2	-1	3	1
	1		-1	4	-1
2	-1	3	1	5	1
	-1		1	6	-1
	-1	4	-1	7	1
	-1		-1	8	-1

Note. WP denotes whole plot, SP denotes subplot, and SSP denotes sub-subplot.

To better understand the restriction randomization designs, two figures are provided: Figure 1 graphically illustrates the treatment structure for a two-level split-plot design in four factors, with 2 HTCs (Factor A and Factor B) and 2 ETCs (Factor C and Factor D); Figure 2 illustrates graphically the treatment structure for a two-level split-split-plot design in six factors, with 2 VHTCs (Factor A and Factor B), 2 HTCs (Factor C and Factor D) and 2 ETCs (Factor E and Factor F).

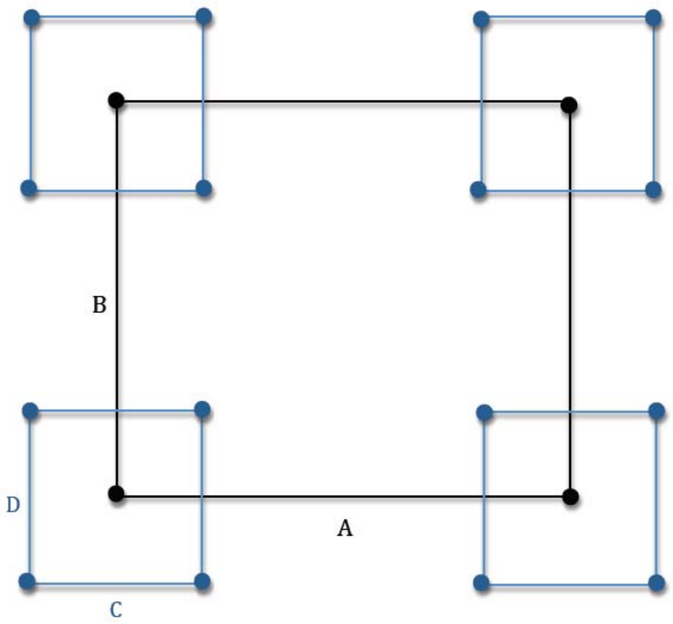

Figure 1. Two-level split-plot design with 2 HTCs and 2 ETCs.

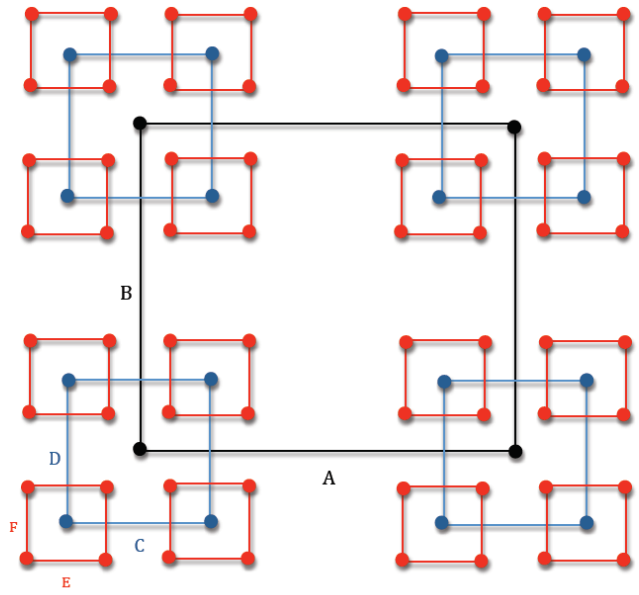

Figure 2. Two-level split-split-plot design with 2 VHTCs, 2 HTCs, and 2 ETCs.

1.2 Example of Restricted Randomization in Split-Split-Plot Design

Suppose one is interested in studying the absorption times of a particular type of antibiotic capsule. There are two technicians, two dosage strengths, and four capsule wall thicknesses. The experiment is performed by assigning a unit of antibiotic to a technician who conducts the experiment on the two dosage strengths and the four capsule wall thicknesses. Once a particular dosage is formulated, all four wall thicknesses are tested at that strength. In this experiment, the technician corresponds to the whole-plot factor. The order in which the technicians are assigned the units of antibiotic is randomly determined. The dosage strength represents the subplot factor and may be randomly assigned by the technician. Within particular dosage strength, the four capsule wall thicknesses are tested randomly; the wall thicknesses are the sub-subplot factor. Note that for this experiment, there are two randomization restrictions: one associated with technician, and the other associated with dosage strength.

1.3 General form of Split-Split-Plot Model

The general form of split-split-plot model is expressed as:

$$Y = X\beta + Z_1\delta + Z_2\nu + \varepsilon, \qquad (1)$$

where

Y : $N \times 1$ vector of responses,

X : $N \times p$ known design matrix,

β : $p \times 1$ unknown vector of model parameters,

$Z_1 = blkdiag(1_{n_1}, 1_{n_2}, ..., 1_{n_w}) : N \times w$ known indicator matrix for the whole-plot factors (2)

$Z_2 = blkdiag(1_{n_{11}}, 1_{n_{12}}, ..., 1_{n_{1m1}}, ..., 1_{n_{21}}, 1_{n_{22}}, ..., 1_{n_{2m2}}, ..., 1_{n_{w1}}, 1_{n_{w2}}, ..., 1_{n_{wmw}})$: $N \times k$ known indicator matrix for subplot factors (3)

$\varepsilon \sim MVN(0_{Nx1}, \sigma_\varepsilon{}^2 I_{N\times N})$: $N \times 1$ random vector of sub-subplot errors,

$\nu \sim MVN(0_{kx1}, \sigma_\nu{}^2 I_{k\times k})$: $k \times 1$ random vector of subplot errors,

$\delta \sim MVN(0_{w\times 1}, \sigma_\delta{}^2 I_{w\times w})$: $w \times 1$ random vector of whole-plot errors,

δ, ν, ε are mutually independent.

p : number of model parameters,

$N = \sum_{i=1}^{w}\sum_{j=1}^{m_i} n_{ij} = total$ number of observations,

w : number of whole plots,

m_i : number of subplots in i^{th} whole plot,

n_{ij} : number of sub-subplots in j^{th} subplot of i^{th} whole plot,

$n_i = \sum_{j=1}^{m_i} n_{ij}$: number of sub-subplots in i^{th} whole plot.

The variance-covariance matrix is expressed as:

$$\text{var}(Y) = \Sigma = \sigma_\delta{}^2 Z_1 Z_1' + \sigma_\nu{}^2 Z_2 Z_2' + \sigma_\varepsilon{}^2 I_{N\times N} \quad (4)$$

It is convenient to define the variance ratios of whole plot to sub-subplot variance, subplot to sub-subplot variance as

$$r_1 = \frac{\sigma_\delta{}^2}{\sigma_\varepsilon{}^2},\ r_2 = \frac{\sigma_\nu{}^2}{\sigma_\varepsilon{}^2},$$

then the variance-covariance matrix can be expressed in terms of r_1 and r_2, as

$$\text{var}(Y) = \Sigma = \sigma_\varepsilon^{\;2}(I_{N\times N} + r_1 Z_1 Z_1' + r_2 Z_2 Z_2') \tag{5}$$

If r_1 and r_2 are equal to 0, then this model will be a completely randomized model, and the variance –covariance can be expressed as

$\text{var}(Y) = \Sigma = \sigma_\varepsilon^{\;2} I_{N\times N}$.

- If r_2 is equal to 0, this model reduces to the split-plot model, and the variance–covariance can be expressed as

$\text{var}(Y) = \Sigma = \sigma_\delta^{\;2} Z_1 Z_1' + \sigma_\varepsilon^{\;2} I_{N\times N}$

Note that the structures of $Z_1 Z_1'$ and $Z_2 Z_2'$ reveal that the experimental runs in different whole plots are independent, whereas the experimental runs within each whole plot are correlated; similarly, within a whole plot, sub-subplot observations contained in the same subplot are correlated further.

The ordinary least square (OLS) estimate of the model coefficients is expressed as

$\hat{\beta}_{OLS} = (X'X)^{-1} X'Y$,

and the variance-covariance matrix for $\hat{\beta}_{OLS}$ is

$\text{var}(\hat{\beta}_{OLS}) = (X'X)^{-1} X'\Sigma X(X'X)^{-1}$.

The generalized least square (GLS) estimate is expressed as

$\hat{\beta}_{GLS} = (X'\hat{\Sigma}^{-1}X)^{-1} X'\hat{\Sigma}^{-1} Y$,

and the variance-covariance matrix for $\hat{\beta}_{GLS}$ is

$\text{var}(\hat{\beta}_{GLS}) = (X'\hat{\Sigma}^{-1}X)^{-1} X'\hat{\Sigma}^{-1}\Sigma\hat{\Sigma}^{-1}X'(X'\hat{\Sigma}^{-1}X)^{-1}$.

Under the sufficient and necessary conditions of equivalent estimation,

$X'\hat{\Sigma}^{-1} = GX'$, where G is a nonsingular square matrix.

Then

$$\hat{\beta}_{GLS} = (X'\hat{\Sigma}^{-1}X)^{-1}X'\hat{\Sigma}^{-1}Y$$

$$= (GX'X)^{-1}GX'Y$$

$$= (X'X)^{-1}G^{-1}GX'Y$$

$$= (X'X)^{-1}X'Y$$

$$= \hat{\beta}_{OLS}$$

$$\mathrm{var}(\hat{\beta}_{GLS}) = (X'\hat{\Sigma}^{-1}X)^{-1}X'\hat{\Sigma}^{-1}\Sigma((X'\hat{\Sigma}^{-1}X)^{-1}X'\hat{\Sigma}^{-1})'$$

$$= (GX'X)^{-1}GX'\Sigma((GX'X)^{-1}GX')'$$

$$= (X'X)^{-1}G^{-1}GX'\Sigma((X'X)^{-1}G^{-1}GX')'$$

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

$$= \mathrm{var}(\hat{\beta}_{OLS})$$

Therefore, under estimation-equivalent conditions, if OLS estimates are equivalent to GLS estimates, then the variance–covariance matrix for the OLS estimates is the same as the variance–covariance matrix for the GLS estimates.

CHAPTER 2

LITERATURE REVIEW

Fisher (1925) proposed the split-plot design for use in agricultural experiments. Because there are always time-consuming or difficult to change processing factors between successive processing runs in agricultural and industrial experiments, split-plot designs have achieved much attention and application. There is a wide body of literature on the design and analysis of split-plot designs, see Box, Hunter & Hunter (2005), Jones & Nachtsheim (2009), Kowalski & Potcner (2003), Mather (1951). For the application of split-plot designs in industrial experiments, see Wooding (1973), Hahn (1978), Taguchi (1987) , Box (1996), and Simpson, Kowalski, and Landman (2004). Regarding the construction of split-plot designs, see Huang, Chen, and Voelkel (1998); Bingham and Sitter (1999a, 1999b, 2001, 2004), Bisgaard (2000), Goos (2006), Goos and Vandebroek, (2003), Langhans, Goos, and Vandebroek (2005), Goos (2006), and Goos and Vandebroek (2003).

In the situation where a completely randomized run order is planned, and the experimenter fails to change the setting before each run, Ganju and Lucas (1997, 1999) and Webb, Lucas, and Borkowski (2004) analyzed such experiments and illustrated that inappropriate operations could lead to incorrect inference about factor significance.

Letsinger, Myers, and Lentner (1996) investigated response analysis methods along with nested error variance and examined the efficiency of various second-order designs by conducting split-plot designs. The article is the first paper to fully focus on restriction randomizations in RSM. In their article, two model situations—first-order and second-order models—provided extreme evidence supporting the effects of a randomization scheme on RSM design efficiency over CRD. To get a better understanding of where to start the modification of the traditional RSM, they explored the deficiencies of traditional response surface techniques and the effects of using randomization designs. Draper and John (1998) discussed modifications of central composite designs (CCD) and Box-Behnken designs (BBD) to be run in a split-plot fashion. They examined two general types of designs, CUBE designs and STAR designs, and pointed out that rotatability is a more appropriate and useful criterion to be used if the experimental region and the model are unknown. Two review papers by Myers (1999), Myers, Montogomery, Vining (2004) emphasize the second-order split-plot designs in RSM.

If three strata in an experimental design exist, say, for example, via experimentation on processes with multi-stages or steps, and it is impossible or too difficult to re-order the experimental units between strata, this will lead to a split-split-plot design. Why is it necessary to conduct a split-split-plot design over a split-plot design when the experiment is run with two randomization restrictions? Castillo (2010) constructed split-split-plot design and split-plot designs in studying the high-throughput reactor. In his research, if a split-split-plot design was executed, then purge was assigned as a whole-plot factor; temperature and pressure were set as subplot factors; levels of catalyst type and catalyst concentration were allocated as the sub-subplot factors. If the experiments had been executed as a split-plot design, in which pressure and temperature were set as the whole-plot factors and levels of catalyst type and catalyst concentration were allocated as the subplot factors, the results for both types of designs would not be identical. Some factor effects that should be statistically significant would be missed. Therefore, it is vital to monitor how experiments are executed in order to perform an appropriate analysis and draw the correct conclusions.

Schoen (1999) constructed an orthogonal two-level split-split-plot design to experiment on a multistage cheese production process. The purpose of the experiment was to detect the significant factor effects that affect the quality characteristics of the cheeses. Milk storage was set to be the whole-plot factor, curd was assigned to the subplot factor, and individual cheese was set to the sub-subplot factor. Trinca and Gilmour (2001) derived a sequential strategy for designing multistratum designs based on a continuous protein extraction process. Jones and Goos (2007) derived D-optimal split-split-plot designs and applied their methods to the cheese experiments that were first analyzed by Schoen (1999). The Sensitivity to misspecification of the variance ratios has been studied. Moreover, considering that three-stratum processing will be more complicated when changing the sizes of whole plots, they made some recommendations on the choice of the number of whole plots. Comparing with the design of 128 runs in Schoen (1999), the design they approached reduced the total experiment runs to 32. Ferryanto and Tollefson (2010) applied a split-split-plot design for replicate testing to evaluate foil lidding for contact lens packages that should maintain a long-time integrity and be easy to open. Set temperature, seal pressure, and dwell time are considered the design factors at three levels each and are labeled whole-plot factor, subplot factor, and sub-subplot factor, respectively. By measuring continuous peel force and by classifying peel type as a categorical response, the quality of the package seal was evaluated.

Considering the methods of model estimation, Goos (2006) developed optimal experimental designs that are orthogonally blocked and equivalent estimation split-plot designs. Goos (2002) provided details of equivalence of OLS and GLS for saturated designs and orthogonally blocked designs. Those designs are crossed split-plot designs (experimental design in which every level of whole-plot factors occurs in combination with every level of subplot factors) and have homogeneous block sizes. Vining, Kowalski, and Montgomery (hereafter VKM) (2005) proposed a class of second-order split-plot designs for model estimation under the conditions that OLS is equal to GLS. They modified the standard central composite design by accommodating a split-plot structure. The design construction allows for OLS estimation of the model and pure-error estimates of the error variance terms. Moreover, they recognized that the cost of the split-plot experiment is primarily a function of the number of whole plots instead of the overall design runs.

Parker, Kowalski, and Vining (2007a, 2007b) proposed classes of equivalent estimation balanced and unbalanced second-order split-plot designs from CCD and BBD. They provided construction strategies for these designs that possess equivalent estimation optimality property. Regarding the unbalanced cases where the subplot cost approaches the whole-plot cost, minimal point designs are proposed with a split-plot Notz design (see Myers, Montgomery, & Anderson-cook, 2009). For balanced cases, design equivalent -estimation conditions and design construction strategies were provided for the VKM method and the minimum number of whole plots (hereafter MWP) method.

CHAPTER3

BALANCED DESIGN

In the literature review, I discussed much work related to split-plot first-order and second-order designs. In this chapter, I extend the work of Parker, Kowalski, and Vining (2007a, 2007b) to consider second-order split-split-plot designs.

In a split-split-plot design, three error terms need to be estimated. The traditional estimation methods for variance components such as restricted maximum likelihood (REML) or maximum likelihood (ML) are model dependent, that is, if the model is underspecified, the estimates of the variance components could be inflated. The designs I proposed in my research permit pure-error estimates of the variance. Moreover, the systematic design construction techniques for second-order split-split-plot equivalent estimation designs are explored in this study. The objective of this work was to develop some practical experimentation strategies for fitting second-order models in the presence of two randomization restrictions.

A balanced split-split-plot design is defined in this research as a design that has the same number of sub-subplots per subplot, and the same number of subplots per whole plot. Recall the two design construction criteria (VKM and MWP) introduced in chapter 2, second-order equivalent estimation designs are presented in Section 3.1. In Section 3.2, we explore the generalized equivalent conditions for split-split-plot designs. Section 3.3 shows the forms of two matrices to achieve estimation-equivalence for balanced split-split-plot designs for the VKM method. In Section 3.4, and the criteria for building an equivalent-estimation split-split-plot design for the VKM method are summarized and numerically demonstrated. Section 3.5 shows the forms of two matrices for achieving balanced estimation-equivalence second-order split-split-plot designs for the MWP method. The criteria for building an equivalent-estimation split-split-plot design for balanced split-split-plot designs for MWP method are summarized and numerically demonstrated in Section 3.6.

3.1 Second-Order Equivalent Estimation Designs

Parker, Kowalski, and Vining (2007a, 2007b) summarized the benefits of general equivalent estimation designs as follows:

- Model parameter estimates are independent of the variance components and robust to the assumption of normality.
- Model parameter estimates are best linear unbiased estimates (BLUE).
- By using OLS instead of GLS, model parameter estimation is simplified, and it is available in all statistical software packages.
- Estimation equivalent designs can be constructed independent of any model assumption, that is, the designs support the model.
- Design selection is independent of variance components, that is, one does not need to have any knowledge of the variance components.

In the following sections, the central composite designs (CCD) have been regarded as the basis for constructing second-order equivalent-estimation split-split-plot designs. Two criteria proposed by Parker, Kowalski, and Vining (2007a, 2007b) for constructing a split-plot design are still applicable for constructing a split-split-plot design. One criterion is to employ an efficient allocation of resources in subplot designs and sub-subplot designs. In the presence of VHTC factors and HTC factors in the experiments, there is the minimum number of subplots and sub-subplots that should be included in the design. The other criterion is to use a minimum number of whole plots. The reason to construct a split-split-plot design is mainly to minimize the resetting times for the whole plot. Five-level designs are considered in this study : $-\alpha, -1, 0, 1, \alpha$ for VHTC factors; $-\phi, -1, 0, 1, \phi$ for HTC factors; and $-\gamma, -1, 0, 1, \gamma$ for ETC factors, where α , ϕ, and γ represent the distance between the whole plot axial points to the center points, the subplot axial points to the center points, and the sub-subplot axial points to the center points, respectively.

To construct a balanced estimation-equivalent split-split-plot design, one has to consider both the structures of whole plots and subplots. In the following section, I derive the generalized estimation-equivalence conditions for constructing a split-split-plot design.

3.2 Generalized Estimation-Equivalence Conditions

I started with the necessary and sufficient condition for equivalence from McElroy (1967), which can be expressed as

$$XK = \Sigma X. \tag{6}$$

Where X is an $N \times p$ model matrix with rank of *p*, and K is a $p \times p$ matrix. Σ is the $N \times N$ variance –covariance matrix.

Premultiplying X' on both sides of equation (6), the result is

$$X'XK = X'\Sigma X \tag{7}$$

Premultiplying $(X'X)^{-1}$ on both sides of equation (7), the result is

$$(X'X)^{-1}X'XK = (X'X)^{-1}X'\Sigma X \tag{8}$$

Therefore

$$K = (X'X)^{-1}X'\Sigma X \tag{9}$$

Recall from equation (4),

$$\Sigma = \sigma_\delta{}^2 Z_1Z_1' + \sigma_\nu{}^2 Z_2Z_2' + \sigma_\varepsilon{}^2 I_{N\times N}$$

Equation (9) can be rewritten as

$$K = (X'X)^{-1}X'(\sigma_\delta{}^2 Z_1Z_1' + \sigma_\nu{}^2 Z_2Z_2' + \sigma_\varepsilon{}^2 I_{N\times N})X$$

$$= \sigma_\varepsilon{}^2 I_{N\times N} + \sigma_\delta{}^2 (X'X)^{-1}X'Z_1Z_1'X + \sigma_\nu{}^2 (X'X)^{-1}X'Z_2Z_2'X$$

$$XK = \sigma_\varepsilon{}^2 X + \sigma_\delta{}^2 X(X'X)^{-1}X'Z_1Z_1'X + \sigma_\nu{}^2 X(X'X)^{-1}X'Z_2Z_2'X$$

$$X(X'X)^{-1}X' = H \tag{10}$$

$$K_1 = (X'X)^{-1}X'Z_1Z_1'X \tag{11}$$

$$K_2 = (X'X)^{-1}X'Z_2Z_2'X \tag{12}$$

then

$$XK = \sigma_\varepsilon{}^2 X + \sigma_\delta{}^2 XK_1 + \sigma_\nu{}^2 XK_2 \tag{13}$$

$$\Sigma X = \sigma_\varepsilon{}^2 X + \sigma_\delta{}^2 Z_1Z_1'X + \sigma_\nu{}^2 Z_2Z_2'X \tag{14}$$

Based on equation (13), (14), and equivalent-estimation condition in equation (6), by simplification and inspection, the general estimation-equivalent conditions for Ordinary Least Squares (OLS) and Generalized least Squares (GLS) must hold as:

$$\mathrm{XK}_1 = M_1 X \tag{15}$$

And

$$\mathrm{XK}_2 = M_2 X \tag{16}$$

where $\mathrm{M}_1 = \mathrm{Z}_1\mathrm{Z}_1'$, $\mathrm{M}_2 = \mathrm{Z}_2\mathrm{Z}_2'$, Z_1 and Z_2 are defined in expression (1.1) and (1.2).
From equation (11) and (12), the general form of K_1 and K_2 can be written as:

$$\mathrm{K}_1 = (X'X)^{-1} X' M_1 X \tag{17}$$

$$\mathrm{K}_2 = (X'X)^{-1} X' M_2 X \tag{18}$$

Note that even K matrix is non-singular, Matrices of K_1 and K_2 are singular. Equations (12) and (13) provide the ability to numerically evaluate K_1 and K_2 for any specific design.

Recall from chapter 2, Vining, Kowalski, and Montgomery (2005) modified the standard CCD by fitting a split-plot structure that permits the use of OLS estimates for the model and pure-error estimates for the error variance. I called this method the VKM method. In the next section, the forms of K_1 and K_2 for balanced estimation-equivalent split-split-plot designs for the VKM method are presented.

3.3 Balanced Forms of K_1 and K_2 Matrices for a Second-Order Split-Split-Plot Design for the VKM Method

In Section 1.3, I provided the general matrix form of a split-split-plot model in Equation (1). To illustrate all the terms in the model matrix, I expand as follows:

$$\begin{aligned} E(y) = \beta_0 &+ \sum_{o=1}^{a} \beta_i z_i + \sum_{o=1}^{a-1} \sum_{\iota=o+1}^{a} \beta_{o\iota} z_o z_\iota + \sum_{o=1}^{a} \beta_{oo} z_\iota^{\,2} \\ &+ \sum_{d=1}^{b} \theta_d x_d + \sum_{d=1}^{b-1} \sum_{e=d+1}^{b} \theta_{de} x_d x_e + \sum_{o=1}^{a} \sum_{d=1}^{b} \theta_{od} z_o x_d + \sum_{d=1}^{b} \theta_{dd} x_d^{\,2} \\ &+ \sum_{s=1}^{l} \psi_c g_c + \sum_{s=1}^{l-1} \sum_{v=s+1}^{l} \psi_{sv} g_s g_v + \sum_{o=1}^{a} \sum_{s=1}^{l} \psi_{os} z_o g_s + \sum_{d=1}^{b} \sum_{s=1}^{l} \psi_{ds} x_d g_s + \sum_{s=1}^{l} \psi_{ss} g_s^{\,2} \end{aligned}$$

where y is the response, z is a whole-plot factor, x is a subplot factor, and g is a sub-subplot factor. The β's are the regression coefficients at the whole-plot level, θ's are the regression coefficients at the subplot level , ψ's are the regression coefficients at the sub-subplot level. a denotes the number of whole-plot factors. b denotes the number of subplot factors. l denotes the number of sub-subplot factors. The total number of factors in the model is $f = a + b + l$. For a complete second-order model, including the intercept, one can express the total number of model terms, p as

$$p = 1 + 2f + \frac{f(f-1)}{2}.$$

Based on the structure of a split-split-plot design, I performed finer partitions of the design matrix X as follows:

$$X = \begin{bmatrix} 1 & W_{D1} & W_{Q1} & S_{D1} & S_{Q1} & SS_{D1} & SS_{Q1} \\ 1 & W_{D2} & W_{Q2} & S_{D2} & S_{Q2} & SS_{D2} & SS_{Q2} \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ 1 & W_{Dw} & W_{Qw} & S_{Dw} & S_{Qw} & SS_{Dw} & SS_{Qw} \end{bmatrix} X = \begin{bmatrix} 1 & W_{D11} & W_{Q11} & S_{D11} & S_{Q11} & SS_{D11} & SS_{Q11} \\ 1 & . & . & . & . & . & . \\ 1 & . & . & . & . & . & . \\ 1 & . & . & . & . & . & . \\ 1 & W_{D1m1} & W_{Q1m1} & S_{D1m1} & S_{Q1m1} & SS_{D1m1.} & SS_{Q1m1} \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ 1 & W_{Dwmw} & W_{Qwmw} & S_{Dwmw} & S_{Qwmw} & SS_{Dwmw} & SS_{Qwmw} \end{bmatrix}$$

where the first column of ones correspond to the intercept. w denotes the number of whole plots. W_{Di} denotes the model sub matrix for the whole-plot main effect and two factor interaction terms contained in the i^{th} whole plot, and W_{Qi} denotes the model sub matrix for the whole-plot pure quadratic terms contained in the i^{th} whole plot. Similarly, S_{Di} denotes the model submatrix for the subplot main effect and two factor interaction terms between whole plot and subplot, subplot and subplot interaction terms contained in the i^{th} whole plot, and S_{Qi} denotes the model sub matrix for the subplot pure quadratic terms contained in i^{th} whole plot. SS_{Di} denotes the model sub matrix for the sub-subplot main effect and two factor interaction terms between whole plot and sub-subplot, subplot and sub-subplot, sub-subplot and sub-subplot interaction terms contained in the i^{th} whole plot, and SS_{Qi} denotes the model sub matrix for the sub-subplot pure quadratic terms contained in the i^{th} whole plot. W_{Dij} denotes the model sub matrix for the whole-plot main effect and two factor interaction terms contained in the j^{th} subplot of i^{th} whole plot, and W_{Qij} denotes the model sub matrix for the whole-plot pure quadratic terms contained in the j^{th} subplot of i^{th} whole plot. Similarly, S_{Dij} denotes the model sub matrix for the subplot main effect and two factor interaction terms between whole plot and subplot, subplot and subplot interaction terms contained in the j^{th} subplot of i^{th} whole plot, and S_{Qij} denotes the model sub matrix for the subplot pure quadratic terms contained in the j^{th} subplot of i^{th} whole plot. SS_{Dij} denotes the model sub matrix for the sub-subplot main effect and two factor interaction terms between whole plot and sub-subplot, subplot and sub-subplot, sub-subplot and sub-subplot interaction terms contained in the j^{th} subplot of i^{th} whole plot, and SS_{Qij} denotes the model sub matrix for the sub-subplot pure quadratic terms contained in the j^{th} subplot of i^{th} whole plot.

Based on the equations (17) and (18), one can express K_1 and K_2 in matrix form as follows (see the details in Appendix A) :

$$K_1 = \begin{bmatrix} n_w & 0 & 0 & q' & 0 & v1' & 0 \\ 0 & n_w I_D & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & n_w I_Q & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & V_{SQ} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & V_{SSQ} \end{bmatrix} \quad K_2 = \begin{bmatrix} n_k & 0 & 0 & 0 & 0 & v2' & 0 \\ 0 & n_k\ I_D & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & n_k\ I_Q & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & n_k\ I_{SD} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & n_k I_{SQ} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & G_{SSQ} \end{bmatrix}$$

where n_w denotes the number of runs per whole plot, n_k denotes the number of runs per subplot, q is a constant vector with a length of $(b+ab+\frac{b(b-1)}{2})$, $v1$ and $v2$ are constant vectors with same length of $(l+al+bl+\frac{l(l-1)}{2})$. I_D and I_Q are $(a+\frac{a(a-1)}{2})\times(a+\frac{a(a-1)}{2})$ and $(a\times a)$ identity matrix. V_{SQ} is $(b\times b)$ matrix, and V_{SSQ} is $(l\times l)$ matrix. I_{SD} and I_{SQ} are $(b+ab+\frac{b(b-1)}{2})\times(b+ab+\frac{b(b-1)}{2})$ and $(b\times b)$ identity matrix. G_{SSQ} is $(l\times l)$ matrix.

In the following section, the technical criteria for constructing balanced estimation-equivalent CCD Second-order split-split-plot designs for the VKM method are numerically demonstrated.

3.4 Summary of the Equivalent Conditions for Balanced Second-Order Split-Split-Plot Designs for the VKM Method

With regard to the construction of a balanced estimation-equivalent second-order CCD split-split-plot design, based on the general estimation-equivalent conditions (15) and (16), I summarized the technical criteria as follows:

1. Criteria for Center points:

   All center points should be run in a separate whole plot.

2. Criteria for sub-subplot designs with each subplot , subplot designs within each whole plot:

   a. Within each whole plot, columns of subplot main effects, whole plot by subplot interactions, subplot by subplot interactions must sum to a constant. If you use orthogonal designs in the subplot factors within each whole plot, then you meet conditions.

b. Within each whole plot, columns of sub-subplot main effects, whole plot by sub-subplot interactions, subplot by sub-subplot interactions, sub-subplot by sub-subplot interactions must sum to a constant. If you use orthogonal designs in the sub-subplot factors within each whole plot, then you meet conditions.

c. Within each subplot, columns of sub-subplot main effects, whole plot by sub-subplot interactions, subplot by sub-subplot interactions, sub-subplot by sub-subplot interactions must sum to a constant. If you use orthogonal designs in the sub-subplot factors within each subplot, then you meet conditions.

3. Criteria for axial points (see details in Appendix A) :

Axial points for subplot factors and sub-subplot factors can be run in the following ways, which are dictated by whether or not the number of subplot factors is a power of two and whether or not the number of sub-subplot factors is a power of two. Recall from Section 1.3, n_w denotes the whole-plot size, and n_k denotes the subplot size within each whole plot.

a. If both the number of subplot factors and the number of sub-subplot factors are powers of two, then the axial points for all the subplot factors can be replicated evenly in the same whole plot, the axial points for all the sub-subplot factors can be replicated evenly in a separate whole plot. In this case,

$$V_{SQ} = \frac{n_w}{b} 1_b 1_b'.$$

$$V_{SSQ} = \frac{n_w}{l} 1_l 1_l'$$

$$G_{SSQ} = n_k I_l .$$

b. If the number of subplot factors is a power of two, but the number of sub-subplot factors is not a power of two, then the subplot axial points can be replicated evenly in a separate whole plot, different from the previous case (a), the sub-subplot axial points for each sub-subplot factor should be replicated in a separate whole plot. And this gives

$$V_{SQ} = \frac{n_w}{b} 1_b 1_b'$$

$$V_{SSQ} = n_w I_l$$

$$G_{SSQ} = n_k I_l$$

c. If the number of subplot factors is not a power of two, but the number of sub-subplot factors is a power of two, then the sub-subplot axial points can be replicated evenly in a separate whole plot, the subplot axial points for each subplot factor should be replicated in a separate whole plot. And this gives:

$$V_{SQ} = n_w I_b$$

$$V_{SSQ} = \frac{n_w}{l} 1_l 1_l'$$

$$G_{SSQ} = n_k I_l$$

d. If both the number of subplot factors and the sub-subplot factors are all not powers of two, the subplot axial points for each subplot factor should be replicated in a separate whole plot, and subplot axial points for each subplot factor should be replicated in a separate whole plot. And this gives

$$V_{SQ} = n_w\ I_b$$

$$V_{SSQ} = n_w I_l$$

$$G_{SSQ} = n_k I_l$$

Table 4 shows a balanced nonequivalent-estimation second-order CCD split-split-plot design with 1 VHTC, 2 HTCs, and 2 ETCs. This nonequivalent estimation design in Table 4 has six whole plots of size 16. Each whole plot has 4 subplots of size 4. With regard to the structure of the whole plot, the column sums of the whole-plot factor main effects and whole plot by whole-plot factor interactions are equal to zero. The column sums of the subplot factor main effects, two-way interactions between whole-plot factor and subplot factor are all equal to zero. The column sums of the sub-subplot factors main effects and two-way interactions between whole-plot factors and sub-subplot factors, subplot factors and sub-subplot factors, sub-subplot factors and sub-subplot factors are all equal to zero. However, as the center points are combined with sub-subplot axial points demonstrated in whole-plot 6, there are no changing levels for subplots, which breaks the structure of a split-split-plot design. Therefore this design does not satisfy the criteria described previously. It is not an equivalent-estimation split-split-plot design.

This split-split-plot design in Table 5 has seven whole plots of size 16. The first two whole plots contain the factorial points. Whole-plot 3-4 contains whole-plot axial points; subplot axial points have been included in whole-plot 5. Center points are included in whole-plot 7. The total experimental runs are 112, which is the same as that shown in Table 4. The structure of this design satisfies all the criteria for whole plots, subplots, and sub-subplots for an equivalent-estimation split-split-plot design, and it satisfies the criteria for OLS and GLS equivalent-estimation conditions. This design is a balanced equivalent-estimation second-order split-split-plot design.

Table 4

Balanced Second-Order CCD Split-Split-Plot Design with 1 VHTC, 2 HTCs, and 2 ETCs (Nonestim. Equiv. Design)

WP	SP	A	B	C	D	E	WP	SP	A	B	C	D	E
		Factor							Factor				
1	1	-1	-1	-1	-1	-1	5	17	0	-2.24	0	0	0
		-1	-1	-1	1	-1			0	-2.24	0	0	0
		-1	-1	-1	-1	1			0	-2.24	0	0	0
		-1	-1	-1	1	1			0	-2.24	0	0	0
	2	-1	-1	1	-1	-1		18	0	2.24	0	0	0
		-1	-1	1	1	-1			0	2.24	0	0	0
		-1	-1	1	-1	1			0	2.24	0	0	0
		-1	-1	1	1	1			0	2.24	0	0	0
	3	-1	1	-1	-1	-1		19	0	0	-2.24	0	0
		-1	1	-1	1	-1			0	0	-2.24	0	0
		-1	1	-1	-1	1			0	0	-2.24	0	0
		-1	1	-1	1	1			0	0	-2.24	0	0
	4	-1	1	1	-1	-1		20	0	0	2.24	0	0
		-1	1	1	1	-1			0	0	2.24	0	0
		-1	1	1	-1	1			0	0	2.24	0	0
		-1	1	1	1	1			0	0	2.24	0	0
2	5	1	-1	-1	-1	-1	6	21	0	0	0	-2.24	0
		1	-1	-1	1	-1			0	0	0	2.24	0
		1	-1	-1	-1	1			0	0	0	0	0
		1	-1	-1	1	1			0	0	0	0	0
	6	1	-1	1	-1	-1		22	0	0	0	0	-2.24
		1	-1	1	1	-1			0	0	0	0	2.24
		1	-1	1	-1	1			0	0	0	0	0
		1	-1	1	1	1			0	0	0	0	0
	7	1	1	-1	-1	-1		23	0	0	0	-2.24	0
		1	1	-1	1	-1			0	0	0	2.24	0
		1	1	-1	-1	1			0	0	0	0	0
		1	1	-1	1	1			0	0	0	0	0
	8	1	1	1	-1	-1		24	0	0	0	0	-2.24
		1	1	1	1	-1			0	0	0	0	2.24
		1	1	1	-1	1			0	0	0	0	0
		1	1	1	1	1			0	0	0	0	0
3	**9-12**	**-2.24**	**0**	**0**	**0**	**0**							
4	**13-16**	**2.24**	**0**	**0**	**0**	**0**							

Note. Whole-plot 3 and whole-plot 4 each contain 4 subplots and 16 sub-subplots.

In the previous design, $\alpha^2 = \phi^2 = \gamma^2 = 5$.

For K_1: $n_w = 16$; $V_{SSQ} = 0.7619(11'_2)$; $q = 0$; $\nu 1 = 0$;

For K_2: $n_k = 4$; $\nu 2 = 0$; $G_{SSQ} = \begin{bmatrix} 1.1905 & -0.8095 \\ -0.8095 & 1.1905 \end{bmatrix}$.

The matrix form of K_1 and K_2 are shown here:

$$K_1 = \begin{bmatrix} 16 & 0 & 0 & 0 & 0 & 0 & 20 \\ 0 & 16 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 16 & 0 & 0 & 0 & -3.8095 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 811'_2 & 0 & -3.218111'_2 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0.761911'_2 \end{bmatrix} \quad K_2 = \begin{bmatrix} 4 & 0 & 0 & 0 & 0 & 0 & 51_{1,2} \\ 0 & 4 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 4 & 0 & 0 & 0 & -0.95241_{1,2} \\ 0 & 0 & 0 & 4I_3 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 4I_2 & 0 & -0.80951_{1,2} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \begin{bmatrix} 1.1905 & -0.8095 \\ -0.8095 & 1.1905 \end{bmatrix} \end{bmatrix}$$

Table 5

Balanced Second-Order CCD Split-Split-Plot with 1 VHTC, 2 HTCs, and 2 ETCs (Est. Equiv. Design)

WP	SP	Factor					WP	SP	Factor				
		A	B	C	D	E			A	B	C	D	E
1	1	-1	-1	-1	-1	-1	5	17	0	-2.24	0	0	0
		-1	-1	-1	1	-1			0	-2.24	0	0	0
		-1	-1	-1	-1	1			0	-2.24	0	0	0
		-1	-1	-1	1	1			0	-2.24	0	0	0
	2	-1	-1	1	-1	-1		18	0	2.24	0	0	0
		-1	-1	1	1	-1			0	2.24	0	0	0
		-1	-1	1	-1	1			0	2.24	0	0	0
		-1	-1	1	1	1			0	2.24	0	0	0
	3	-1	1	-1	-1	-1		19	0	0	-2.24	0	0
		-1	1	-1	1	-1			0	0	-2.24	0	0
		-1	1	-1	-1	1			0	0	-2.24	0	0
		-1	1	-1	1	1			0	0	-2.24	0	0
	4	-1	1	1	-1	-1		20	0	0	2.24	0	0
		-1	1	1	1	-1			0	0	2.24	0	0
		-1	1	1	-1	1			0	0	2.24	0	0
		-1	1	1	1	1			0	0	2.24	0	0
2	5	1	-1	-1	-1	-1	6	21	0	0	0	-2.24	0
		1	-1	-1	1	-1			0	0	0	2.24	0
		1	-1	-1	-1	1			0	0	0	-2.24	0
		1	-1	-1	1	1			0	0	0	2.24	0
	6	1	-1	1	-1	-1		22	0	0	0	-2.24	0
		1	-1	1	1	-1			0	0	0	2.24	0
		1	-1	1	-1	1			0	0	0	-2.24	0
		1	-1	1	1	1			0	0	0	2.24	0
	7	1	1	-1	-1	-1		23	0	0	0	0	-2.24
		1	1	-1	1	-1			0	0	0	0	2.24
		1	1	-1	-1	1			0	0	0	0	-2.24
		1	1	-1	1	1			0	0	0	0	2.24
	8	1	1	1	-1	-1		24	0	0	0	0	-2.24
		1	1	1	1	-1			0	0	0	0	2.24
		1	1	1	-1	1			0	0	0	0	-2.24
		1	1	1	1	1			0	0	0	0	2.24
3	**9-12**	**-2.236**	**0**	**0**	**0**	**0**	**7**	**25-28**	**0**	**0**	**0**	**0**	**0**
4	**13-16**	**2.2361**	**0**	**0**	**0**	**0**							

Note. Whole-plot 3, whole-plot 4, and whole-plot 7 contain 4 subplots and 16 sub-subplots each.

In the previous design, $\alpha^2 = \phi^2 = \gamma^2 = 5$.

For K_1: $n_w = 16$; $V_{SQ} = 8(11')_2$; $V_{SSQ} = 8(11')_2$; $q = 0$; $\nu 1 = 0$;

For K_2: $n_k = 4$; $\nu 2 = 0$; $G_{SSQ} = 4I_2$.

The matrix form of K_1 and K_2 are shown below:

$$K_1 = \begin{bmatrix} 16 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 16 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 16 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 811'_2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 811'_2 \end{bmatrix} \qquad K_2 = \begin{bmatrix} 4 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 4 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 4 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 4I_5 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 4I_2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 4I_2 \end{bmatrix}.$$

Assuming a large proportion of experimental cost associated with the total number of whole plots, minimizing the total number of whole plots in a split-split-plot design will be more effective. In the following section, the balanced forms of K_1 and K_2 for the minimum number of the whole plots (MWP) method have been studied.

3.5 Balanced Form of K_1 and K_2 Matrices for the Minimum Number of Whole Plots (MWP) Method

Parker, Kowalski, and Vining (2007a, 2007b) proposed the MWP method for a split-plot design considering that cost for an experimental design is mainly a function of the number of whole plots, instead of the overall design size. In my research, I applied this method to construct a class of second-order CCD split-split-plot designs where the minimum number of whole plots was achieved.

To reduce the number of whole plots, I usually set the value of the whole-plot axial point α to the same value of the whole-plot factorial levels, such as 1 and -1 (i.e., points are placed on the face of the cube in the whole-plot design space). Thus, MWP designs are appropriate for cubodial regions in the whole-plot factors. In this study, I considered the case where the experimenter has only 1 VHTC factor. There are no restrictions for the settings of ϕ and γ. In my study, I chose ϕ and γ to be ± 1. By sorting the whole-plot column, there are only three levels for the whole-plot factors: high level, low level, and center. Therefore the total number of whole plots is reduced to three.

The general forms of K_1 and K_2 for MWP are given by the following (see detailed derivation in Appendix A):

$$K_1 = \begin{bmatrix} n_w & 0 & 0 & q' & t_1' & v1' & t_0' \\ 0 & n_w I_D & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & n_w I_Q & 0 & M_{W1} & 0 & M_{W0} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \quad K_2 = \begin{bmatrix} n_k & 0 & 0 & 0 & 0 & v2' & 0 \\ 0 & n_k I_D & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & n_k I_Q & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & n_k\ I_{SD} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & n_k\ I_{SQ} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & M_{SSQ} \end{bmatrix}$$

where n_w denotes the number of runs per whole plot, n_k denotes the number of runs per subplot, t_0 is a vector with length l, t_1 is a vector with length b, M_{W0} is $a \times l$ matrix, M_{W1} is $a \times b$ matrix, M_{SSQ} is $l \times l$ matrix, q, and $v1$ and $v2$ are constant vectors with the same length of $(l + al + bl + \frac{l(l-1)}{2})$.

Given the forms of K_1 and K_2, in the next section I summarize the criteria for building an equivalent-estimation design considering the structure of factorial points, axial points, and center points.

3.6 Summary of the Equivalent Conditions for Balanced Second-Order Split-Split-Plot Designs for the MWP method

In the previous section I proposed the forms of K_1 and K_2 for the balanced second-order CCD split-split-plot designs with minimal number of whole plots. I defined n_{nzf} as the number of nonzero subplot factorial points within the whole plot at high or low level, n_{nzsa} is the number of nonzero subplot axial points within the whole plot at center points, and n_{nzssa} is the number of nonzero sub-subplot axial points within the whole plot at center points.

n_k was already defined. The summarizations for this kind of designs are provided below:

1. Criteria for sub-subplot designs within each subplot, subplot designs within each whole plot are the following:

   a. Within each whole plot, columns of subplot factor main effects, columns of sub-subplot factor main effects , columns of whole-plot factor and subplot factors two-way interactions, columns of whole-plot factor and sub-subplot factors two-way interactions must sum to a constant. If you use orthogonal designs in the subplot factors within each whole plot, then you meet the conditions.

   b. Within each whole plot, in each subplot, columns of sub-subplot main effects, subplot by sub-subplot interactions, sub-subplot by sub-subplot interactions must sum to a constant. If you use orthogonal designs in the sub-subplot factors within each subplot, then you meet the conditions.

2. Criteria for center points and axial points:

   a. To obtain a balanced split-split-plot design, subplot and sub-subplot center points will be added within each whole plot, and may be added one-subplot-by-one-subplot to the whole plots.

b. Depending on whether the number of subplot factors is a power of two, or the number of sub-subplot factors is a power of two, the subplot axial points and sub-subplot axial points can be run as follows:

(i) If both the number of subplot factors and the number of sub-subplot factors are powers of two, then the axial points for all the subplot factors can be replicated in successive subplots, where the number of subplots required depends on the number of subplot factors. For example, if there are two subplot factors, then running subplot axial points requires at least two additional subplots. The axial points for all the sub-subplot factors can be replicated evenly in a separate subplot. In this case,

$$n_{nzsa=} \frac{n_{nzf}}{b},$$

$$n_{nzssa=} \frac{n_k}{l}$$

$$t_1' = \frac{n_{nzf}}{b} \phi^2 1_b',$$

$$M_{W1} = (n_{nzf} - \frac{n_{nzf}}{b} \phi^2) 1_b',$$

$$t_0' = \frac{n_k}{l} \gamma^2 1_l',$$

$$M_{W0} = (n_{nzf} - \frac{n_k}{l} \gamma^2) 1_l',$$

$$M_{SSQ} = \frac{n_k}{l} (11')_l .$$

(ii) If the number of subplot factors is a power of two, but the number of sub-subplot factors is not a power of two, then the axial points for all the subplot factors can be replicated at the corresponding level in successive subplots and the number of subplots required depends on the number of subplot factors. The axial points for all the sub-subplot factors can be replicated in a separate subplot. In this case,

$$n_{nzsa=} \frac{n_{nzf}}{b},$$

$$n_{nzssa=} n_k$$

$$t_1' = \frac{n_{nzf}}{b} \phi^2 1_b',$$

$$M_{W1} = (n_{nzf} - \frac{n_{nzf}}{b} \phi^2) 1_b',$$

$$t_0' = n_k \gamma^2 1_l',$$

$$M_{W0} = (n_{nzf} - n_k \gamma^2) 1_l',$$

$$M_{SSQ} = n_k (11')_l$$

(iii) If the number of subplot factors is not a power of two, but the number of sub-subplot factors is a power of two, then axial points for subplot factors need to be run in separate subplots, while the axial points for all the sub-subplot factors can be replicated evenly in a separate subplot. In this case,

$$n_{nzsa} = n_{nzf},$$

$$n_{nzssa=} \frac{n_k}{l}$$

$$t_1' = n_{nzf} \phi^2 1_b',$$

$$M_{W1} = (n_{nzf} - n_{nzf} \phi^2) 1_b',$$

$$t_0' = \frac{n_k}{l}\gamma^2 1_l',$$

$$M_{W0} = (n_{nzf} - \frac{n_k}{l}\gamma^2)1_l',$$

$$M_{SSQ} = \frac{n_k}{l}(11')_l.$$

(iv) If both the number of subplot factors and the number of sub-subplot factors are not powers of two, then axial points for subplot factors need to be run in separate subplots, and the axial points for all the sub-subplot factors can be run in a separate subplot. In this case,

$$n_{nzsa=}n_{nzf},$$

$$n_{nzssa=}n_k$$

$$t_1' = n_{nzf}\phi^2 1_l',$$

$$M_{W1} = (n_{nzf} - n_{nzf}\phi^2)1_b',$$

$$t_0' = n_k\gamma^2 1_l',$$

$$M_{W0} = (n_{nzf} - n_k\gamma^2)1_l',$$

$$M_{SSQ} = n_k I_l.$$

In general, with only 1 VHTC factor for MWP method, to construct a balanced equivalent-estimation split-split-plot design, I combined the whole-plot axial points with whole-plot factorial points at the same level: The whole-plot axial points at high level are required to be combined with whole-plot factorial points at high level. The whole-plot axial points at low level are required to be combined with whole-plot factorial points at low. Moreover, to keep balance, the way to add the whole-plot axial points into the whole-plot at factorial level depends on the size of whole plot at center level.

Numerical verifications have been presented in the following tables. First, an estimation-equivalent split-split-plot design with 1 VHTC , 1 HTC, and 2 ETCs is presented in Table 6. Note that there does not exist a whole plot that contains all the whole-plot center points, subplot center points, and sub-subplot center points. Whole-plot 3 contains 3 subplots. Subplot 7 and 8 contains subplot axial points. Subplot 9 contains sub-subplot axial points. Two axial subplots for whole-plot factors at low level have been added in whole-plot 1. Similarly, two axial subplots for whole-plot factors at the high level have been added in whole-plot 2. More examples are shown in Tables 7-12.

In general, in regard to a balanced estimation-equivalent second-order split-split-plot design for MWP method with one whole-plot factor, the design contains three whole plots: whole plot at high level, whole plot at low level, and whole plot at center. An estimation-equivalent design is achieved if the sub-subplot axial points are replicated within each subplot.

This design in Table 6 contains one subplot factor and two sub-subplot factors. Three whole plots of size 12 have been included. Each whole plot contains 3 subplots. Each subplot contains 4 sub-subplots. The total runs of this design are 36 runs. In whole-plot 3 represented by wp3, sp7 and sp8 contains the subplot axial points. Sub-subplot axial points have been included in sp9. The nonzero subplot factorial points in whole-plot 1 at high level is 8, and the nonzero subplot axial points in the whole plot at center level is 8. The nonzero sub-subplot axial points in the whole plot at center level is 2.

The design in Table 7 contains one subplot factor and three sub-subplot factors. Three whole plots of size 40 have been included in this design. Each whole plot contains 5 subplots. Each subplot contains 8 sub-subplots. There are 120 runs included in this design. Subplot 11 and subplot 12 contain the subplot axial points. Sub-subplot axial points have been included in subplots 13-15. The nonzero subplot factorial points in whole-plot 1 at low level is 16. The nonzero subplot axial points in the whole plot at center level is 16. The nonzero sub-subplot axial points in whole plot at center level is 8.

Table 6

MWP Method –CCD ($\alpha = \phi = \gamma = 1$) for 1 VHTC,1 HTC, and 2 ETCs

(Equivalent Estimation Design)

WP	SP	A	B	C	D	WP	SP	A	B	C	D	WP	SP	A	B	C	D
1	1	-1	-1	-1	-1	2	4	1	-1	-1	-1	3	7	0	-1	0	0
		-1	-1	1	-1			1	-1	1	-1			0	-1	0	0
		-1	-1	-1	1			1	-1	-1	1			0	-1	0	0
		-1	-1	1	1			1	-1	1	1			0	-1	0	0
	2	-1	1	-1	-1		5	1	1	-1	-1		8	0	1	0	0
		-1	1	1	-1			1	1	1	-1			0	1	0	0
		-1	1	-1	1			1	1	-1	1			0	1	0	0
		-1	1	1	1			1	1	1	1			0	1	0	0
	3	-1	0	0	0		6	1	0	0	0		9	0	0	-1	0
		-1	0	0	0			1	0	0	0			0	0	1	0
		-1	0	0	0			1	0	0	0			0	0	0	-1
		-1	0	0	0			1	0	0	0			0	0	0	1

For K_1:

$n_w = 12;\ q = v1 = 0;$

$t_1' = 8;\quad M_{W1} = 0; t_0' = [2,2]; M_{W0} = [6,6].$

For K_2:

$n_k = 4 \quad v2 = 0;$

$M_{SSQ} = 2(11')_2.$

The matrix form of K_1 and K_2 are shown below:

$$K_1 = \begin{bmatrix} 12 & 0 & 0 & 0 & 8 & 0 & 2(1_{1,3}) \\ 0 & 12 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 12 & 0 & 0 & 0 & 6(1_{1,3}) \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \qquad K_2 = \begin{bmatrix} 4 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 4 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 4 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 4I_2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 4 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 2(11')_2 \end{bmatrix}$$

Table 7

MWP Method–CCD ($\alpha = \phi = \gamma = 1$) for 1 VHTC,1 HTC, and 3 ETCs (Equiv. Est. Design)

WP	SP	Factor A	B	C	D	E
1	1	-1	-1	-1	-1	-1
		-1	-1	1	-1	-1
		-1	-1	-1	1	-1
		-1	-1	1	1	-1
		-1	-1	-1	-1	1
		-1	-1	1	-1	1
		-1	-1	-1	1	1
		-1	-1	1	1	1
	2	-1	1	-1	-1	-1
		-1	1	1	-1	-1
		-1	1	-1	1	-1
		-1	1	1	1	-1
		-1	1	-1	-1	1
		-1	1	1	-1	1
		-1	1	-1	1	1
		-1	1	1	1	1
	3-5	**-1**	**0**	**0**	**0**	**0**
2	6	1	-1	-1	-1	-1
		1	-1	1	-1	-1
		1	-1	-1	1	-1
		1	-1	1	1	-1
		1	-1	-1	-1	1
		1	-1	1	-1	1
		1	-1	-1	1	1
		1	-1	1	1	1
	7	1	1	-1	-1	-1
		1	1	1	-1	-1
		1	1	-1	1	-1
		1	1	1	1	-1
		1	1	-1	-1	1
		1	1	1	-1	1
		1	1	-1	1	1
		1	1	1	1	1
	8-10	**1**	**0**	**0**	**0**	**0**
3	**11**	**0**	**-1**	**0**	**0**	**0**
	12	**0**	**1**	**0**	**0**	**0**
	13	0	0	-1	0	0
		0	0	1	0	0
		0	0	-1	0	0
		0	0	1	0	0
		0	0	-1	0	0
		0	0	1	0	0
		0	0	-1	0	0
		0	0	1	0	0
	14	0	0	0	-1	0
		0	0	0	1	0
		0	0	0	-1	0
		0	0	0	1	0
		0	0	0	-1	0
		0	0	0	1	0
		0	0	0	-1	0
		0	0	0	1	0
	15	0	0	0	0	-1
		0	0	0	0	1
		0	0	0	0	-1
		0	0	0	0	1
		0	0	0	0	-1
		0	0	0	0	1
		0	0	0	0	-1
		0	0	0	0	1

Note. Subplot 3-5 in whole-plot 1, subplot 8-10 in whole-plot 2, subplot 11 and subplot 12 in whole-plot 3 contain 8 sub-subplots each.

For K_1: $n_w = 40;\ q = v1 = 0;$

$t_1' = 16;\ M_{W1} = 0;\ t_0' = [8,8,8];\ M_{W0} = [8,8,8]$

For K_2: $n_k = 8;\ v2 = 0;$

$M_{SSQ} = 8I_3$.

The matrix form of K_1 and K_2 are shown below:

$$K_1 = \begin{bmatrix} 40 & 0 & 0 & 0 & 16 & 0 & 8(1_{1,3}) \\ 0 & 40 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 40 & 0 & 0 & 0 & 8(1_{1,3}) \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \qquad K_2 = \begin{bmatrix} 8 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 8 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 8 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 8I_3 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 8I_3 \end{bmatrix}$$

This nonequivalent estimation design in Table 8 contains three whole plots of size 24. Each whole plot contains 3 subplots. Each subplot contains 8 sub-subplots. In whole-plot 3, subplot 7 and 8 contain the subplot axial points. The sub-subplot axial points and center points have been included in subplot 9. As the center points have not been run in a separate subplot, and the sub-subplot axial points have not replicated within a separate subplot, the structure of this design is not matched with the criteria for building an equivalent-estimation design. This design is a nonequivalent estimation design.

The design in Table 9 contains two subplot factors and two sub-subplot factors. Three whole plots of size 20 have been included in this design. Each whole plot contains 5 subplots. Each subplot contains 4 sub-subplots. This design contains 60 runs. Subplots 11 -14 contain the subplot axial points. Sub-subplot axial points have been included in subplot 15. The nonzero subplot factorial points in whole-plot 1 at low level is 16. The nonzero subplot axial points in the whole plot at center level is 8. The nonzero sub-subplot axial points in whole plot at center level is 2.

Table 8

MWP method –CCD ($\alpha = \phi = \gamma = 1$ *) for 1 VHTC,1 HTC, and 3 ETCs*

(Nonequivalent Estimation Design)

WP	SP	Factor					WP	SP	Factor					WP	SP	Factor				
		A	B	C	D	E			A	B	C	D	E			A	B	C	D	E
		-1	-1	-1	-1	-1			1	-1	-1	-1	-1			0	-1	0	0	0
		-1	-1	1	-1	-1			1	-1	1	-1	-1			0	-1	0	0	0
		-1	-1	-1	1	-1			1	-1	-1	1	-1			0	-1	0	0	0
	1	-1	-1	1	1	-1		4	1	-1	1	1	-1		7	0	-1	0	0	0
		-1	-1	-1	-1	1			1	-1	-1	-1	1			0	-1	0	0	0
		-1	-1	1	-1	1			1	-1	1	-1	1			0	-1	0	0	0
		-1	-1	-1	1	1			1	-1	-1	1	1			0	-1	0	0	0
		-1	-1	1	1	1			1	-1	1	1	1			0	-1	0	0	0
		-1	1	-1	-1	-1			1	1	-1	-1	-1			0	1	0	0	0
		-1	1	1	-1	-1			1	1	1	-1	-1			0	1	0	0	0
		-1	1	-1	1	-1			1	1	-1	1	-1			0	1	0	0	0
1	2	-1	1	1	1	-1	2	5	1	1	1	1	-1	3	8	0	1	0	0	0
		-1	1	-1	-1	1			1	1	-1	-1	1			0	1	0	0	0
		-1	1	1	-1	1			1	1	1	-1	1			0	1	0	0	0
		-1	1	-1	1	1			1	1	-1	1	1			0	1	0	0	0
		-1	1	1	1	1			1	1	1	1	1			0	1	0	0	0
		-1	0	0	0	0			1	0	0	0	0			0	0	-1	0	0
		-1	0	0	0	0			1	0	0	0	0			0	0	1	0	0
		-1	0	0	0	0			1	0	0	0	0			0	0	0	-1	0
	3	-1	0	0	0	0		6	1	0	0	0	0		9	0	0	0	1	0
		-1	0	0	0	0			1	0	0	0	0			0	0	0	0	-1
		-1	0	0	0	0			1	0	0	0	0			0	0	0	0	1
		-1	0	0	0	0			1	0	0	0	0			0	0	0	0	0
		-1	0	0	0	0			1	0	0	0	0			0	0	0	0	0

For K_1:

$n_w = 24$; $q = v1 = 0$;

$t_1' = 16$; $M_{W1} = 0$; $t_0' = [2,2,2]$; $M_W = [14,14,14]$

For K_2:

$n_k = 8$; $v2 = 0$; $M_{SSQ} = 2.589(11')_3$.

And there are a few nonzeros appear in the last column.

The matrix form of K_1 and K_2 are shown below:

$$K_1 = \begin{bmatrix} 24 & 0 & 0 & 0 & 16 & 0 & 2(1_{1,3}) \\ 0 & 24 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 24 & 0 & 0 & 0 & 14(1_{1,3}) \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \qquad K_2 = \begin{bmatrix} 8 & 0 & 0 & 0 & 0 & 0 & -0.0712(1_{1,3}) \\ 0 & 8 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 8 & 0 & 0 & 0 & 0.1359(1_{1,3}) \\ 0 & 0 & 0 & 8I_3 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0.1359(1_{1,3}) \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 2.5890(11')_3 \end{bmatrix}$$

Table 9

MWP Method–CCD ($\alpha = \phi = \gamma = 1$) for 1 VHTC, 2 HTCs, and 2 ETCs

(Equivalent Estimation Design)

WP	SP	A	B	C	D	E	WP	SP	A	B	C	D	E	WP	SP	A	B	C	D	E
1	1	-1	-1	-1	-1	-1	2	6	1	-1	-1	-1	-1	3	11	0	-1	0	0	0
		-1	-1	-1	1	-1			1	-1	-1	1	-1			0	-1	0	0	0
		-1	-1	-1	-1	1			1	-1	-1	-1	1			0	-1	0	0	0
		-1	-1	-1	1	1			1	-1	-1	1	1			0	-1	0	0	0
	2	-1	-1	1	-1	-1		7	1	-1	1	-1	-1		12	0	1	0	0	0
		-1	-1	1	1	-1			1	-1	1	1	-1			0	1	0	0	0
		-1	-1	1	-1	1			1	-1	1	-1	1			0	1	0	0	0
		-1	-1	1	1	1			1	-1	1	1	1			0	1	0	0	0
	3	-1	1	-1	-1	-1		8	1	1	-1	-1	-1		13	0	0	-1	0	0
		-1	1	-1	1	-1			1	1	-1	1	-1			0	0	-1	0	0
		-1	1	-1	-1	1			1	1	-1	-1	1			0	0	-1	0	0
		-1	1	-1	1	1			1	1	-1	1	1			0	0	-1	0	0
	4	-1	1	1	-1	-1		9	1	1	1	-1	-1		14	0	0	1	0	0
		-1	1	1	1	-1			1	1	1	1	-1			0	0	1	0	0
		-1	1	1	-1	1			1	1	1	-1	1			0	0	1	0	0
		-1	1	1	1	1			1	1	1	1	1			0	0	1	0	0
	5	-1	0	0	0	0		10	1	0	0	0	0		15	0	0	0	1	0
		-1	0	0	0	0			1	0	0	0	0			0	0	0	-1	0
		-1	0	0	0	0			1	0	0	0	0			0	0	0	0	1
		-1	0	0	0	0			1	0	0	0	0			0	0	0	0	-1

For K_1:

$n_w = 20$; $q = v1 = 0$;

$t_1' = [8,8]$; $M_{W1} = [8,8]$; $t_0' = [2,2]$; $M_{W0} = [14,14]$

For K_2:

$n_k = 4$; $v2 = 0$; $M_{SSQ} = 2(11')_2$.

The matrix form of K_1 and K_2 are shown here:

$$K_1 = \begin{bmatrix} 20 & 0 & 0 & 0 & 8(1_{1,2}) & 0 & 2(1_{1,3}) \\ 0 & 20 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 20 & 0 & 8(1_{1,2}) & 0 & 14(1_{1,2}) \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \qquad K_2 = \begin{bmatrix} 4 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 4 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 4 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 4I_3 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 2(11')_2 \end{bmatrix}$$

This design in Table 10 contains three subplot factors and two sub-subplot factors. Three whole plots of size 36 have been included in this design. Each whole plot contains 9 subplots. Each subplot contains 4 sub-subplots. The total runs of this design are 108. Subplots 19-24 contain the subplot axial points. Sub-subplot axial points have been included in subplot 25. Center points have been run in two separate subplots 26 and 27. The nonzero subplot factorial points in whole-plot 1 at high and low levels is 32. The nonzero subplot axial points in the whole plot at center level is 8; the nonzero sub-subplot axial points in whole plot at center level is 2.

Table 10

MWP Method–CCD ($\alpha = \phi = \gamma = 1$) for 1 VHTC, 3 HTCs and 2 ETCs (Equivalent Estimation Design)

WP	SP	Factor						WP	SP	Factor						WP	SP	Factor					
		A	B	C	D	E	F			A	B	C	D	E	F			A	B	C	D	E	F
		1	1	1	1	1	1			-1	1	1	1	1	1			0	1	0	0	0	0
	1	1	1	1	1	-1	-1		10	-1	1	1	1	-1	-1		19	0	1	0	0	0	0
		1	1	1	1	1	-1			-1	1	1	1	1	-1			0	1	0	0	0	0
		1	1	1	1	-1	1			-1	1	1	1	-1	1			0	1	0	0	0	0
		1	-1	1	1	1	1			-1	-1	1	1	1	1			0	-1	0	0	0	0
	2	1	-1	1	1	-1	-1		11	-1	-1	1	1	-1	-1		20	0	-1	0	0	0	0
		1	-1	1	1	1	-1			-1	-1	1	1	1	-1			0	-1	0	0	0	0
		1	-1	1	1	-1	1			-1	-1	1	1	-1	1			0	-1	0	0	0	0
		1	1	-1	1	1	1			-1	1	-1	1	1	1			0	0	1	0	0	0
	3	1	1	-1	1	-1	-1		12	-1	1	-1	1	-1	-1		21	0	0	1	0	0	0
		1	1	-1	1	1	-1			-1	1	-1	1	1	-1			0	0	1	0	0	0
		1	1	-1	1	-1	1			-1	1	-1	1	-1	1			0	0	1	0	0	0
		1	-1	-1	1	1	1			-1	-1	-1	1	1	1			0	0	-1	0	0	0
	4	1	-1	-1	1	-1	-1		13	-1	-1	-1	1	-1	-1		22	0	0	-1	0	0	0
		1	-1	-1	1	1	-1			-1	-1	-1	1	1	-1			0	0	-1	0	0	0
		1	-1	-1	1	-1	1			-1	-1	-1	1	-1	1			0	0	-1	0	0	0
		1	1	1	-1	1	1			-1	1	1	-1	1	1			0	0	0	1	0	0
1	5	1	1	1	-1	-1	-1	2	14	-1	1	1	-1	-1	-1	3	23	0	0	0	1	0	0
		1	1	1	-1	1	-1			-1	1	1	-1	1	-1			0	0	0	1	0	0
		1	1	1	-1	-1	1			-1	1	1	-1	-1	1			0	0	0	1	0	0
		1	-1	1	-1	1	1			-1	-1	1	-1	1	1			0	0	0	-1	0	0
	6	1	-1	1	-1	-1	-1		15	-1	-1	1	-1	-1	-1		24	0	0	0	-1	0	0
		1	-1	1	-1	1	-1			-1	-1	1	-1	1	-1			0	0	0	-1	0	0
		1	-1	1	-1	-1	1			-1	-1	1	-1	-1	1			0	0	0	-1	0	0
		1	1	-1	-1	1	1			-1	1	-1	-1	1	1			0	0	0	0	1	0
	7	1	1	-1	-1	-1	-1		16	-1	1	-1	-1	-1	-1		25	0	0	0	0	-1	0
		1	1	-1	-1	1	-1			-1	1	-1	-1	1	-1			0	0	0	0	0	1
		1	1	-1	-1	-1	1			-1	1	-1	-1	-1	1			0	0	0	0	0	-1
		1	-1	-1	-1	1	1			-1	-1	-1	-1	1	1			0	0	0	0	0	0
	8	1	-1	-1	-1	-1	-1		17	-1	-1	-1	-1	-1	-1		26	0	0	0	0	0	0
		1	-1	-1	-1	1	-1			-1	-1	-1	-1	1	-1			0	0	0	0	0	0
		1	-1	-1	-1	-1	1			-1	-1	-1	-1	-1	1			0	0	0	0	0	0
		1	0	0	0	0	0			-1	0	0	0	0	0			0	0	0	0	0	0
	9	1	0	0	0	0	0		18	-1	0	0	0	0	0		27	0	0	0	0	0	0
		1	0	0	0	0	0			-1	0	0	0	0	0			0	0	0	0	0	0
		1	0	0	0	0	0			-1	0	0	0	0	0			0	0	0	0	0	0

For K_1:

$n_w = 36$; q = $v1 = 0$;

$t_1' = [8,8,8]$; $M_{W1} = [24,24,24]$; $t_0' = [2,2]$; $M_{W0} = [30,30]$.

For K_2:

$v2 = 0$;

$n_k = 4$; $M_{SSQ} = 2(11')_2$.

The matrix form of K_1 and K_2 are shown below:

$$K_1 = \begin{bmatrix} 36 & 0 & 0 & 0 & 8(1_{1,3}) & 0 & 2(1_{1,2}) \\ 0 & 36 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 36 & 0 & 24(1_{1,3}) & 0 & 30(1_{1,2}) \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \qquad K_2 = \begin{bmatrix} 4 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 4 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 4 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 4I_3 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 2(11')_2 \end{bmatrix}$$

The design in Table 11 contains three subplot factors and three sub-subplot factors. Three whole plots of size 72 have been included in this design. Each whole plot contains 9 subplots. Each subplot contains 8 sub-subplots. Subplots 19-24 contain the subplot axial points; sub-subplot axial points have been included in subplot 25-27. The nonzero subplot factorial points in whole-plot 1 at high and low level is 64; the nonzero subplot axial points in the whole plot at center level is 16; the nonzero sub-subplot axial points in whole plot at center level is 8.

Table 11

MWP Method –CCD ($\alpha = \phi = \gamma = 1$) for 1 VHTC, 3 HTCs and 3 ETCs

(Equivalent Estimation Design)

wp	sp	A	B	C	D	E	F	G
1	1	1	1	-1	1	-1	-1	-1
		1	1	-1	1	1	-1	-1
		1	1	-1	1	-1	1	-1
		1	1	-1	1	1	1	-1
		1	1	-1	1	-1	-1	1
		1	1	-1	1	1	-1	1
		1	1	-1	1	-1	1	1
		1	1	-1	1	1	1	1
	2	1	1	1	1	-1	-1	-1
		1	1	1	1	1	-1	-1
		1	1	1	1	-1	1	-1
		1	1	1	1	1	1	-1
		1	1	1	1	-1	-1	1
		1	1	1	1	1	-1	1
		1	1	1	1	-1	1	1
		1	1	1	1	1	1	1
	3	1	-1	1	1	-1	-1	-1
		1	-1	1	1	1	-1	-1
		1	-1	1	1	-1	1	-1
		1	-1	1	1	1	1	-1
		1	-1	1	1	-1	-1	1
		1	-1	1	1	1	-1	1
		1	-1	1	1	-1	1	1
		1	-1	1	1	1	1	1
	4	1	-1	-1	1	-1	-1	-1
		1	-1	-1	1	1	-1	-1
		1	-1	-1	1	-1	1	-1
		1	-1	-1	1	1	1	-1
		1	-1	-1	1	-1	-1	1
		1	-1	-1	1	1	-1	1
		1	-1	-1	1	-1	1	1
		1	-1	-1	1	1	1	1
	5	1	1	-1	-1	-1	-1	-1
		1	1	-1	-1	1	-1	-1
		1	1	-1	-1	-1	1	-1
		1	1	-1	-1	1	1	-1
		1	1	-1	-1	-1	-1	1
		1	1	-1	-1	1	-1	1
		1	1	-1	-1	-1	1	1
		1	1	-1	-1	1	1	1
	6	1	1	1	-1	-1	-1	-1
		1	1	1	-1	1	-1	-1
		1	1	1	-1	-1	1	-1
		1	1	1	-1	1	1	-1
		1	1	1	-1	-1	-1	1
		1	1	1	-1	1	-1	1
		1	1	1	-1	-1	1	1
		1	1	1	-1	1	1	1
	7	1	-1	1	-1	-1	-1	-1
		1	-1	1	-1	1	-1	-1
		1	-1	1	-1	-1	1	-1
		1	-1	1	-1	1	1	-1
		1	-1	1	-1	-1	-1	1
		1	-1	1	-1	1	-1	1
		1	-1	1	-1	-1	1	1
		1	-1	1	-1	1	1	1
	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	-1
		1	-1	-1	-1	-1	-1	1
		1	-1	-1	-1	1	-1	1
		1	-1	-1	-1	-1	1	1
		1	-1	-1	-1	1	1	1
	9	1	0	0	0	0	0	0
		1	0	0	0	0	0	0
		1	0	0	0	0	0	0
		1	0	0	0	0	0	0
		1	0	0	0	0	0	0
		1	0	0	0	0	0	0
		1	0	0	0	0	0	0
		1	0	0	0	0	0	0
2	10	-1	1	-1	1	-1	-1	-1
		-1	1	-1	1	1	-1	-1
		-1	1	-1	1	-1	1	-1
		-1	1	-1	1	1	1	-1
		-1	1	-1	1	-1	-1	1
		-1	1	-1	1	1	-1	1
		-1	1	-1	1	-1	1	1
		-1	1	-1	1	1	1	1
	11	-1	1	1	1	-1	-1	-1
		-1	1	1	1	1	-1	-1
		-1	1	1	1	-1	1	-1
		-1	1	1	1	1	1	-1
		-1	1	1	1	-1	-1	1
		-1	1	1	1	1	-1	1
		-1	1	1	1	-1	1	1
		-1	1	1	1	1	1	1
	12	-1	-1	1	1	-1	-1	-1
		-1	-1	1	1	1	-1	-1
		-1	-1	1	1	-1	1	-1
		-1	-1	1	1	1	1	-1
		-1	-1	1	1	-1	-1	1
		-1	-1	1	1	1	-1	1
		-1	-1	1	1	-1	1	1
		-1	-1	1	1	1	1	1
	13	-1	-1	-1	1	-1	-1	-1
		-1	-1	-1	1	1	-1	-1
		-1	-1	-1	1	-1	1	-1
		-1	-1	-1	1	1	1	-1
		-1	-1	-1	1	-1	-1	1
		-1	-1	-1	1	1	-1	1
		-1	-1	-1	1	-1	1	1
		-1	-1	-1	1	1	1	1
	14	-1	1	-1	-1	-1	-1	-1
		-1	1	-1	-1	1	-1	-1
		-1	1	-1	-1	-1	1	-1
		-1	1	-1	-1	1	1	-1
		-1	1	-1	-1	-1	-1	1
		-1	1	-1	-1	1	-1	1
		-1	1	-1	-1	-1	1	1
		-1	1	-1	-1	1	1	1
	15	-1	1	1	-1	-1	-1	-1
		-1	1	1	-1	1	-1	-1
		-1	1	1	-1	-1	1	-1
		-1	1	1	-1	1	1	-1
		-1	1	1	-1	-1	-1	1
		-1	1	1	-1	1	-1	1
		-1	1	1	-1	-1	1	1
		-1	1	1	-1	1	1	1
	16	-1	-1	1	-1	-1	-1	-1
		-1	-1	1	-1	1	-1	-1
		-1	-1	1	-1	-1	1	-1
		-1	-1	1	-1	1	1	-1
		-1	-1	1	-1	-1	-1	1
		-1	-1	1	-1	1	-1	1
		-1	-1	1	-1	-1	1	1
		-1	-1	1	-1	1	1	1
	17	-1	-1	-1	-1	-1	-1	-1
		-1	-1	-1	-1	1	-1	-1
		-1	-1	-1	-1	-1	1	-1
		-1	-1	-1	-1	1	1	-1
		-1	-1	-1	-1	-1	-1	1
		-1	-1	-1	-1	1	-1	1
		-1	-1	-1	-1	-1	1	1
		-1	-1	-1	-1	1	1	1
	18	-1	0	0	0	0	0	0
		-1	0	0	0	0	0	0
		-1	0	0	0	0	0	0
		-1	0	0	0	0	0	0
		-1	0	0	0	0	0	0
		-1	0	0	0	0	0	0
		-1	0	0	0	0	0	0
		-1	0	0	0	0	0	0
3	19	0	1	0	0	0	0	0
		0	1	0	0	0	0	0
		0	1	0	0	0	0	0
		0	1	0	0	0	0	0
		0	1	0	0	0	0	0
		0	1	0	0	0	0	0
		0	1	0	0	0	0	0
		0	1	0	0	0	0	0
	20	0	-1	0	0	0	0	0
		0	-1	0	0	0	0	0
		0	-1	0	0	0	0	0
		0	-1	0	0	0	0	0
		0	-1	0	0	0	0	0
		0	-1	0	0	0	0	0
		0	-1	0	0	0	0	0
		0	-1	0	0	0	0	0
	21	0	0	1	0	0	0	0
		0	0	1	0	0	0	0
		0	0	1	0	0	0	0
		0	0	1	0	0	0	0
		0	0	1	0	0	0	0
		0	0	1	0	0	0	0
		0	0	1	0	0	0	0
		0	0	1	0	0	0	0
	22	0	0	-1	0	0	0	0
		0	0	-1	0	0	0	0
		0	0	-1	0	0	0	0
		0	0	-1	0	0	0	0
		0	0	-1	0	0	0	0
		0	0	-1	0	0	0	0
		0	0	-1	0	0	0	0
		0	0	-1	0	0	0	0
	23	0	0	0	1	0	0	0
		0	0	0	1	0	0	0
		0	0	0	1	0	0	0
		0	0	0	1	0	0	0
		0	0	0	1	0	0	0
		0	0	0	1	0	0	0
		0	0	0	1	0	0	0
		0	0	0	1	0	0	0
	24	0	0	0	-1	0	0	0
		0	0	0	-1	0	0	0
		0	0	0	-1	0	0	0
		0	0	0	-1	0	0	0
		0	0	0	-1	0	0	0
		0	0	0	-1	0	0	0
		0	0	0	-1	0	0	0
		0	0	0	-1	0	0	0
	25	0	0	0	0	1	0	0
		0	0	0	0	-1	0	0
		0	0	0	0	1	0	0
		0	0	0	0	-1	0	0
		0	0	0	0	1	0	0
		0	0	0	0	-1	0	0
		0	0	0	0	1	0	0
		0	0	0	0	-1	0	0
	26	0	0	0	0	0	1	0
		0	0	0	0	0	-1	0
		0	0	0	0	0	1	0
		0	0	0	0	0	-1	0
		0	0	0	0	0	1	0
		0	0	0	0	0	-1	0
		0	0	0	0	0	1	0
		0	0	0	0	0	-1	0
	27	0	0	0	0	0	0	1
		0	0	0	0	0	0	-1
		0	0	0	0	0	0	1
		0	0	0	0	0	0	-1
		0	0	0	0	0	0	1
		0	0	0	0	0	0	-1
		0	0	0	0	0	0	1
		0	0	0	0	0	0	-1

For K_1:

$n_w = 72;\ q = v1 = 0;$

$t_1' = [16,16,16];\ M_{W1} = [48,48,48];\ t_0' = [8,8,8];\ M_{W0} = [56,56,56]$

For K_2:

$n_k = 8;\ v2 = 0;$

$M_{SSQ} = 8I_3.$

The matrix form of K_1 and K_2 are shown below:

$$K_1 = \begin{bmatrix} 72 & 0 & 0 & 0 & 16(1_{1,3}) & 0 & 8(1_{1,2}) \\ 0 & 72 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 72 & 0 & 48(1_{1,3}) & 0 & 56(1_{1,2}) \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \qquad K_2 = \begin{bmatrix} 8 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 8 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 8 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 8I_3 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 8I_3 \end{bmatrix}$$

In summary, I analyzed balanced estimation-equivalent second-order split-split-plot designs for MWP method with one whole-plot factor. We can see that this method for the design with 1 VHTC has the restriction that the values of α have to be set to the same level of the whole-plot factor main effects. As a structure of this kind of design allows for subplot center points to be added one-by-one to each whole plot, it is flexible.

Due to cost constraints, there are often times where balanced designs are not feasible. In a split-split-plot design, the unbalance can occur in whole plots, or subplots, or sub-subplots, therefore there will be a variety of unbalanced designs. In the following chapter, I explore a kind of unbalance that is expected to occur frequently in practice.

CHAPTER 4

UNBALANCED DESIGN

In chapter 3, I considered the construction of balanced equivalent-estimation split-split-plot CCDs using the VKM construction method, as well as the MWP construction method when there is a single VHTC factor. Note that the center points are replicated one by one to keep balance within each subplot and each whole plot. If there is a cost issue, one has to cut the running times for center points, and the design will become an unbalanced design. In this chapter, I begin with an unbalanced second-order CCD split-split-plot design for the VKM method where the size of the whole plot at center level is smaller than the sizes of the whole plots at factorial level and axial level. Clearly there are unbalanced MWP split-split-plot designs that might arise in practice too. The conditions for that catalog of unbalanced MWP equivalent-estimation designs are quite involved. I will leave this idea for future research.

There are two sections in this chapter. Section 4.1 provides the forms of K_1 and K_2 for unbalanced second-order split-split-plot designs. The estimation-equivalent conditions are summarized in Section 4.2.

4.1 Unbalanced Forms of K_1 and K_2 Matrices for Estimation-Equivalent Second-Order Split-Split-Plot Designs for the VKM Method

Recall the definitions of variable a, b, l in section 3.3. The general forms of K_1 and K_2 for an unbalanced design are proposed as follows:

$$K_1 = \begin{bmatrix} n_0 & 0 & 0 & q' & 0 & v1' & 0 \\ 0 & n_w I_D & 0 & 0 & 0 & 0 & 0 \\ U_{W1} & 0 & n_w\ I_Q & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ U_{k1} & 0 & 0 & 0 & V_{SQ} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ U_{S1} & 0 & 0 & 0 & 0 & 0 & V_{SSQ} \end{bmatrix} \quad K_2 = \begin{bmatrix} n_0 & 0 & 0 & 0 & 0 & v2' & 0 \\ 0 & n_k I_D & 0 & 0 & 0 & 0 & 0 \\ U_{W2} & 0 & n_k I_Q & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & n_k I_{SD} & 0 & 0 & 0 \\ U_{k2} & 0 & 0 & 0 & n_k I_{SQ} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ U_{S2} & 0 & 0 & 0 & 0 & 0 & G_{SSQ} \end{bmatrix}$$

where n_0 denotes the center points. n_w denotes the number of runs per whole plot, n_k denotes the number of runs per subplot, U_{W1}, U_{W2} are vectors of length a. U_{k1}, U_{k2} are vectors of length b. U_{s1}, U_{s2} are vectors of length l. q is a constant vector with length of $(b + ab + \frac{b(b-1)}{2})$, $v1$ and $v2$ are constant vectors with same length of $(l + al + bl + \frac{l(l-1)}{2})$. I_D and I_Q are $(a + \frac{a(a-1)}{2}) \times (a + \frac{a(a-1)}{2})$ and $(a \times a)$ identity matrix. V_{SQ} is $(b \times b)$ matrix, and V_{SSQ} is $(l \times l)$ matrix. I_{SD} and I_{SQ} are $(b + ab + \frac{b(b-1)}{2}) \times (b + ab + \frac{b(b-1)}{2})$ and $(b \times b)$ identity matrices, respectively. G_{SSQ} is $(l \times l)$ matrix.

Compared with balanced designs, I proposed six new elements in both K_1 and K_2 matrices. U_{W1}, U_{W2} are associated with whole-plot factor quadratic terms. U_{k1}, U_{k2} are associated with subplot factor quadratic terms. U_{s1}, U_{s2} are associated with sub-subplot factor quadratic terms. These new elements will be defined in this chapter. One can see that a little change in a sub-subplot that results in an unbalance split-split-plot design will bring significant changes in the matrices of K_1 and K_2.

Table 12 shows the structure of this kind of unbalanced equivalent-estimation design for the VKM method. WP denotes whole plots, SP denotes subplots, and SSP denotes sub-subplots. n_h represents five cases of the quadratic terms of WP, SP and SSP . Letter n_c denotes center points . n_w denotes the number of runs within each whole plot at factorial level and axial level. n_k denotes the number of runs within each subplot at factorial level and axial level. Under i^{th} whole plot, within j^{th} subplot, the r^{th} row of the model matrix for the whole plot, subplot and sub-subplot quadratic terms represented as W_{Qijr}, S_{Qijr}, SS_{Qijr}, respectively.

Table 12

Unbalanced Estimation-Equivalent Second-Order Split-Split-Plot Design for the VKM Method (Unbalances in Center Points)

WP, SP, and SSP Type	W_{Qijr}	S_{Qijr}	SS_{Qijr}
All centers	$[0 \quad . \quad . \quad . \quad 0]_a$	$[0 \quad . \quad . \quad . \quad 0]_b$	$[0 \quad . \quad . \quad . \quad 0]_l$
WP axials, SP centers, SSP centers	$[\alpha^2 \quad 0 \quad . \quad . \quad 0]_a$	$[0 \quad . \quad . \quad . \quad 0]_b$	$[0 \quad . \quad . \quad . \quad 0]_l$
WP centers, SP axials, SSP centers	$[0 \quad . \quad . \quad . \quad 0]_a$	$[\phi^2 \quad 0 \quad . \quad . \quad 0]_b$	$[0 \quad . \quad . \quad . \quad 0]_l$
WP centers, SP centers, SSP axials	$[0 \quad . \quad . \quad . \quad 0]_a$	$[0 \quad . \quad . \quad . \quad 0]_b$	$[\gamma^2 \quad 0 \quad . \quad . \quad 0]_l$
All factorials	$[1 \quad . \quad . \quad . \quad 1]_a$	$[1 \quad . \quad . \quad . \quad 1]_b$	$[1 \quad . \quad . \quad . \quad 1]_l$

Based on the equations (15) and (16), the conditions to satisfy are

$$n_h = n_0 + W_{Q_{ijr}} U_{W1} + S_{Q_{ijr}} U_{k1} + SS_{Q_{ijr}} \mathrm{U}_{S1} \qquad \forall \mathrm{i}. \tag{19}$$

Let $U_{W1}, U_{W2}, U_{k1}, U_{k2}$ and U_{S1}, U_{S2} be defined as $\lambda_1 1_a$, $\lambda_2 1_a$, $\rho_1 1_b$, $\rho_2 1_b$, $\varsigma_1 1_l$, $\varsigma_2 1_l$ respectively, where λ_1, λ_2, ρ_1, ρ_2, ς_1, ς_2 are appropriate real numbers. 1_a, 1_b, 1_l are vectors of ones.

Then the condition in equation (19) can be rewriten as:

$$n_h = n_0 + \lambda_1 W_{Q_{ijr}} 1_a + \rho_1 S_{Q_{ijr}} 1_b + \varsigma_1 SS_{Q_{ijr}} 1_l \quad \forall \text{ i}; \forall \text{j}; \ r = 1,\ 2,\ ...,\ \text{n}_{\text{w}} \tag{20}$$

The derivation for K_1 and K_2 matrices are shown as follows:

For K_1,

When all the factors are at center level, $W_{Q_{ijr}}, S_{Q_{ijr}}, SS_{Q_{ijr}}$ are equal to zero vector. Plugging into equation (20), the result is

$$n_h = n_c = n_0 \quad ,$$

When whole-plot factors are at axial level,

$$W_{Q_{ijr}} = [\alpha^2 \quad 0 \quad . \quad . \quad 0]_a,\ S_{Q_{ijr}} = [0 \quad 0 \quad . \quad . \quad 0]_b,\ SS_{Q_{ijr}} = [0 \quad 0 \quad . \quad . \quad 0]_l,$$

Plugging into equation (20), the result is

$$n_h = n_w = n_c + \lambda_1 \alpha^2$$

When subplot factors are at axial level,

$$W_{Q_{ijr}} = [0 \quad 0 \quad . \quad . \quad 0]_a,\ S_{Q_{ijr}} = [\phi^2 \quad 0 \quad . \quad . \quad 0]_b,\ SS_{Q_{ijr}} = [0 \quad 0 \quad . \quad . \quad 0]_l,$$

Plugging into equation (20), the result is

$$n_w = n_c + \rho_1 \phi^2$$

When sub-subplot factors are at axial level,

$$W_{Q_{ijr}} = [0 \quad 0 \quad . \quad . \quad 0]_a,\ S_{Q_{ijr}} = [0 \quad 0 \quad . \quad . \quad 0]_b,\ SS_{Q_{ijr}} = [\phi^2 \quad 0 \quad . \quad . \quad 0]_l,$$

Plugging into equation (20), the result is

$$n_w = n_c + \varsigma_1 \gamma^2$$

At factorial level,

$$n_h = n_w$$

$$W_{Q_{ijr}} = [1 \quad 1 \quad . \quad . \quad 1]_a,\ S_{Q_{ijr}} = [1 \quad 1 \quad . \quad . \quad 1]_b,\ SS_{Q_{ijr}} = [1 \quad 1 \quad . \quad . \quad 1]_l,$$

Plugging into equation (20), the result is

$$n_w = n_c + \lambda_1 a + \rho_1 b + \varsigma_1 l \qquad (21)$$

Therefore,

$$\lambda_1 = \frac{n_w - n_c}{\alpha^2},\ \rho_1 = \frac{n_w - n_c}{\phi^2},\ \varsigma_1 = \frac{n_w - n_c}{\gamma^2}$$

Plugging into Equation (21), by simplification,

$$(4.9) \quad \frac{a}{\alpha^2} + \frac{b}{\phi^2} + \frac{l}{\gamma^2} = 1$$

If $\alpha^2 = \phi^2 = \gamma^2$,

Then

$$a + b + l = \alpha^2 = \phi^2 = \gamma^2 \qquad (22)$$

and

$$\lambda_1 = \rho_1 = \varsigma = \frac{n_w - n_c}{a + b + l} \qquad (23)$$

For K_2,

In a similar way,

$$\lambda_2 = \rho_2 = \varsigma_2 = \frac{n_k - n_c}{a + b + l}.$$

In the next Section, the equivalent-estimation conditions for the unbalanced second-order split-split-plot designs for the VKM method are summarized and numerically demonstrated.

4.2 Summary of the Equivalent Conditions for the Unbalanced Second-Order Split-Split-Plot Designs for the VKM Method

With regard to the construction of the previously mentioned unbalanced second-order CCD split-split-plot designs, except center points, all other criteria are same as that for balanced second-order CCD split-split-plot designs summarized in chapter 3. The criterion for center points is shown below:

- Criteria for center points:

With respect to the center points, I reduced the whole-plot runs at center level. The center points still need to be run in their own whole plot.

For example, Table 13 shows an unbalanced estimation-equivalent second-order split-split-plot design with 1 VHTC, 2 HTCs, and 2 ETCs. This design contains 7 whole plots. Two center points have been included in subplot 25 within whole-plot 7. Within each whole plot, the column sums of the subplot factor main effects and all two-way interactions between whole-plot factors and subplot factors are all equal to zero. The column sums of the sub-subplot factors main effects and all two-way interactions are all equal to zero. Except center points, each subplot contains 4 sub-subplots. $\lambda_1, \rho_1, \varsigma_1$ are equal to each other. $\lambda_2, \rho_2, \varsigma_2$ are equal to each other. The form of G_{SSQ} is met with the form of an estimation-equivalent split-split-plot design.

Table 13

Unbalanced Second-Order CCD Split-Split-Plot Design with 1 VHTC, 2HTCs, and 2 ETCs (Equivalent Estimation Design)

WP	SP	Factor A	B	C	D	E	WP	SP	Factor A	B	C	D	E
1	1	-1	-1	-1	-1	-1	**3**	**9-12**	**-2.24**	**0**	**0**	**0**	**0**
		-1	-1	-1	1	-1	**4**	**13-16**	**2.24**	**0**	**0**	**0**	**0**
		-1	-1	-1	-1	1	**5**	**17**	**0**	**-2.24**	**0**	**0**	**0**
		-1	-1	-1	1	1		**18**	**0**	**2.24**	**0**	**0**	**0**
	2	-1	-1	1	-1	-1		**19**	**0**	**0**	**-2.24**	**0**	**0**
		-1	-1	1	1	-1		**20**	**0**	**0**	**2.24**	**0**	**0**
		-1	-1	1	-1	1	6	21	0	0	0	-2.24	0
		-1	-1	1	1	1			0	0	0	2.24	0
	3	-1	1	-1	-1	-1			0	0	0	-2.24	0
		-1	1	-1	1	-1			0	0	0	2.24	0
		-1	1	-1	-1	1		22	0	0	0	-2.24	0
		-1	1	-1	1	1			0	0	0	2.24	0
	4	-1	1	1	-1	-1			0	0	0	-2.24	0
		-1	1	1	1	-1			0	0	0	2.24	0
		-1	1	1	-1	1		23	0	0	0	0	-2.24
		-1	1	1	1	1			0	0	0	0	2.24
2	5	1	-1	-1	-1	-1			0	0	0	0	-2.24
		1	-1	-1	1	-1			0	0	0	0	2.24
		1	-1	-1	-1	1		24	0	0	0	0	-2.24
		1	-1	-1	1	1			0	0	0	0	2.24
	6	1	-1	1	-1	-1			0	0	0	0	-2.24
		1	-1	1	1	-1			0	0	0	0	2.24
		1	-1	1	-1	1	7	25	0	0	0	0	0
		1	-1	1	1	1			0	0	0	0	0
	7	1	1	-1	-1	-1							
		1	1	-1	1	-1							
		1	1	-1	-1	1							
		1	1	-1	1	1							
	8	1	1	1	-1	-1							
		1	1	1	1	-1							
		1	1	1	-1	1							
		1	1	1	1	1							

Note. Whole plot 3 and whole plot 4 each contain 4 subplots and 16 sub-subplots, and whole plot 5 contains 4 subplots, each containing 4 sub-subplots.

In the above design: $\alpha^2 = \phi^2 = \gamma^2 = 5$

For K_1:

$n_c = 2$; $\mathrm{n_w} = 16$; $q = v1 = 0$;

$\lambda_1 = \rho_1 = \varsigma_1 = 2.8$;

$U_{W1} = 2.8$; $U_{k1} = [2.8, 2.8]'$; $U_{S1} = [2.8, 2.8]'$;

$V_{\mathrm{SSQ}} = 8(11')_2$.

For K_2:

$n_c = 2; n_w = 4$; $v2 = 0$;

$\lambda_1 = \rho_1 = \varsigma_1 = 0.4$;

$U_{W2} = 0.4; U_{k2} = [0.4, 0.4]'; U_{S2} = [0.4, 0.4]'$;

$G_{\mathrm{SSQ}} = 4I_2$.

The matrix forms of K_1 and K_2 are shown below:

$$K_1 = \begin{bmatrix} 2 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 16 & 0 & 0 & 0 & 0 & 0 \\ 2.8 & 0 & 16 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 2.8(1_{2,1}) & 0 & 0 & 0 & 811'_2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 2.8(1_{2,1}) & 0 & 0 & 0 & 0 & 0 & 8(11')_2 \end{bmatrix} \quad K_2 = \begin{bmatrix} 2 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 4 & 0 & 0 & 0 & 0 & 0 \\ 0.4 & 0 & 4 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 4 & 0 & 0 & 0 \\ 0.4(1_{2,1}) & 0 & 0 & 0 & 4 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0.4(1_{2,1}) & 0 & 0 & 0 & 0 & 0 & 4I_2 \end{bmatrix}$$

Table 14 shows an unbalanced nonequivalent estimation second-order split-split-plot design with 1 VHTC, 2 HTCs, and 2 ETCs. Each whole plot at factorial level and axial level contains 4 subplots. In whole-plot 6, subplots 22 and 23 contain two sub-subplots each. All other subplots except center points in this design contain 4 sub-subplots. This construction is not permissible to achieve equivalence.

Table 14

Unbalanced Second-Order CCD Split-Split-Plot Design with 1 VHTC, 2HTCs, and 2 ETCs (Nonequivalent Estimation Design)

WP	SP	Factor					WP	SP	Factor				
		A	B	C	D	E			A	B	C	D	E
1	1	-1	-1	-1	-1	-1	**3**	**9-12**	**-2.24**	**0**	**0**	**0**	**0**
		-1	-1	-1	1	-1	**4**	**13-16**	**2.24**	**0**	**0**	**0**	**0**
		-1	-1	-1	-1	1	5	17	0	-2.24	0	0	0
		-1	-1	-1	1	1			0	-2.24	0	0	0
	2	-1	-1	1	-1	-1			0	-2.24	0	0	0
		-1	-1	1	1	-1			0	-2.24	0	0	0
		-1	-1	1	-1	1		18	0	2.24	0	0	0
		-1	-1	1	1	1			0	2.24	0	0	0
	3	-1	1	-1	-1	-1			0	2.24	0	0	0
		-1	1	-1	1	-1			0	2.24	0	0	0
		-1	1	-1	-1	1		19	0	0	-2.24	0	0
		-1	1	-1	1	1			0	0	-2.24	0	0
	4	-1	1	1	-1	-1			0	0	-2.24	0	0
		-1	1	1	1	-1			0	0	-2.24	0	0
		-1	1	1	-1	1		20	0	0	2.24	0	0
		-1	1	1	1	1			0	0	2.24	0	0
2	5	1	-1	-1	-1	-1			0	0	2.24	0	0
		1	-1	-1	1	-1			0	0	2.24	0	0
		1	-1	-1	-1	1	6	21	0	0	0	-2.24	0
		1	-1	-1	1	1			0	0	0	2.24	0
	6	1	-1	1	-1	-1			0	0	0	-2.24	0
		1	-1	1	1	-1			0	0	0	2.24	0
		1	-1	1	-1	1		22	0	0	0	-2.24	0
		1	-1	1	1	1			0	0	0	2.24	0
	7	1	1	-1	-1	-1		23	0	0	0	0	-2.24
		1	1	-1	1	-1			0	0	0	0	2.24
		1	1	-1	-1	1		24	0	0	0	0	-2.24
		1	1	-1	1	1			0	0	0	0	2.24
	8	1	1	1	-1	-1			0	0	0	0	-2.24
		1	1	1	1	-1			0	0	0	0	2.24
		1	1	1	-1	1	7	25	0	0	0	0	0
		1	1	1	1	1			0	0	0	0	0

Note. Whole plot 3 and whole plot 4 each contain 4 subplots and 16 sub-subplots.

In the above design: $\alpha^2 = \phi^2 = \gamma^2 = 5$

For K_1:

$n_c = 2$; $\mathrm{n_w} = 16$; $q = v1 = 0$;

$\lambda_1 = 2.8358$; $\rho_1 = 2.9433$; $\varsigma_1 = 2.1910$;

$U_{W1} = 2.8358$; $U_{k1} = [2.9433, 2.9433]'$; $U_{S1} = [2.1910, 2.1910]'$;

$\mathrm{V_{SSQ}} = 6.4776(11'_2)$;

For K_2:

$\mathrm{n_k} = 4$; $v2 = 0$;

$\lambda_2 = 0.4060$; $\rho_2 = 0.4239$; $\varsigma_2 = 0.2985$;

$U_{W_2} = 0.4060$; $U_{\mathrm{k2}} = [0.4239, 0.4239]'$; $U_{\mathrm{S2}} = [0.2985, 0.2985]'$

$$G_{SSQ} = \begin{bmatrix} 3.4129 & 0.0796 \\ 0.0796 & 3.4129 \end{bmatrix}.$$

There are nonzero elements shown in the last column of K_1 and K_2.

The matrix forms of K_1 and K_2 are shown below:

$$K_1 = \begin{bmatrix} 2 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 16 & 0 & 0 & 0 & 0 & 0 \\ 2.8358 & 0 & 16 & 0 & 0 & 0 & 0.0896(1_{1,2}) \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 2.9433(1_{2,1}) & 0 & 0 & 0 & 811'_2 & 0 & 0.358211'_2 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 2.1910(1_{2,1}) & 0 & 0 & 0 & 0 & 0 & 6.477611'_2 \end{bmatrix} K_2 = \begin{bmatrix} 2 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 4 & 0 & 0 & 0 & 0 & 0 \\ 0.4060 & 0 & 4 & 0 & 0 & 0 & 0.0149(1_{1,2}) \\ 0 & 0 & 0 & 4 & 0 & 0 & 0 \\ 0.4239(1_{2,1}) & 0 & 0 & 0 & 4 & 0 & 0.059711'_2 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0.2985(1_{2,1}) & 0 & 0 & 0 & 0 & 0 & \begin{bmatrix} 3.4129 & 0.0796 \\ 0.0796 & 3.4129 \end{bmatrix} \end{bmatrix}$$

Based on the numerical evaluation of K_1 and K_2 for balanced split-split-plot designs and unbalanced split-split-plot designs, one can see that using estimation-equivalent conditions to verify whether a design achieves equivalent-estimates is very useful.

CHAPTER 5

ROBUSTNESS OF OLS ESTIMATES TO NONEQUIVALENT ESTIMATION DESIGNS

In the previous chapters, I proposed several classes of equivalent-estimation designs, both balanced and unbalanced. Even with this broad catalog of designs, there are cases where an equivalent design is not known to exist or the available equivalent designs are not suitable. Under such circumstances, one might entertain designs that are logical extensions of classical completely randomized designs. These designs may be balanced or unbalanced, but they do not satisfy the conditions of equivalent-estimation designs. We refer to these designs as nonequivalent designs. With regard to the nonequivalent designs, we may be interested in the measure of departure from equivalence and investigating the robustness of OLS estimates to the designs that are far-from-equivalence and near-to-equivalence designs.

The remainder of this chapter is arranged as follows. First, a measure for departure from equivalence is provided in Section 5.1. Two representative nonequivalent split-split-plot designs for the VKM method are provided in Section 5.2. The performance of the estimation methods is developed in Section 5.3. In Section 5.4, the simulation parameters are presented, and simulation results are discussed in Section 5.5. The description of the simulation algorithm is provided in the last section 5.6.

5.1 Measures of Near Equivalence

Based on the necessary and sufficient condition for equivalence,

$X(X'X)^{-1}X'M_iX = M_tX$ for t $= 1,2$.

As we know that the HAT matrix noted by H = $X(X'X)^{-1}X'$, then the left-hand side can be expressed by

$HM_tX = M_tX$ for t $= 1,2$.

Rearranging the above expression yields

$(I-H)M_tX = 0$ for t $= 1,2$.

We define the difference matrix D as follows:

$D_t = (I-H)M_tX$ for t $= 1,2$.

$D = D_1 + D_2$.

Note that D is $N \times p$ matrix and model dependent. Parker, Kowalski, and Vining (2007a, 2007b) proposed a means to measure the size of D that was based on functions of the Eigen values. I adopted this measure for my research. When the design is an estimation equivalent design, D is a zero matrix. When the design is not an equivalent estimation design, then the farther the design departs from the equivalence, the more nonzeros are in the D matrix.

A common matrix norm is based on the largest singular value, corresponding to the square root of the largest Eigen values of D'D denoted by

$\| (I-H)M_tX \|_2$ for t $= 1,2$.

Let λ_i for i = 1, 2,…,*e* represent the nonzero Eigen values of D'D, then, I defined

$E_{norm} = \max_{i \le e} \lambda_i$ as a measure of departure from equivalence.

5.2 Two Representative Nonequivalent Split-Split-Plot Designs for the VKM Method

In Section 5.1, a measure of departure from equivalence for nonequivalent split-split-plot designs has been derived. In this section, I considered two representative nonequivalent split-split-plot designs for the VKM method:

- VKM construction designs that are unbalanced but not satisfying the conditions derived for unbalanced equivalent-estimation designs. For example, Table 15 shows a central composite split-split-plot design for 1 VHTC, 1 HTC, and 3 ETCs. The sub-subplot axial points have been included in 3 subplots of size 8 within whole-plot 6. Sixteen center points have been included in 2 subplots of size 8 in whole-plot 7. All other whole plots except whole-plot 6 contain 2 subplots. Within each subplot, there are 8 sub-subplots. This construction is not permissible to achieve equivalence as it does not satisfy the criteria for an unbalanced estimation-equivalent split-split-plot design.
- VKM construction designs that are balanced but do not satisfy the conditions derived for balanced designs. For example, Table 16 shows a balanced CCD nonequivalent estimation split-split-plot design with 1 VHTC, 1HTC, and 1ETC. Center points have been combined with sub-subplot axial points. This construction is not permissible to achieve equivalence as it does not satisfy the criteria established for a balanced estimation-equivalent split-split-plot design.

In Table 17, CCD113_NE_CP represents the design in Table 15. Whole-plot replicates are at center level. The first column of Table 17 shows the whole-plot replicates, and the second column shows the Enorms for this design. The whole-plot replicates are executed at center level. The values of the Enorms for this kind of design are high, up to 4300.8, shown in the second column in Table 17. This kind of design is regarded as far-from equivalence. The reason for this is the unbalanced properties in whole-plot 6 shown in Table 15. As there is only one nonzero Eigen value for D’D, the norms do not change with the increase of the whole-plot replicates. It indicates that the departure from equivalence for this kind of design is not influenced by the whole-plot replicates.

CCD111_NE_FP in Table 17 represents the design shown in Table 16. The whole-plot replicates are executed in the factorial points. The Enorms for this design are shown in the third column of Table 17. One can see that the Enorms between 42 and 46 are much smaller than those in Table 15. This kind of design is called near-to-equivalence. With an increase of the whole-plot replicates, the Enorms are changed very slightly.

These two nonequivalent designs represent the far-from-equivalence designs and next-to-equivalence designs, unbalanced designs and balanced designs, whole-plot replicates at center points and factorial points, respectively. Therefore, in this study, the Monte Carlo simulations are based on these two nonequivalent designs.

Table 15

Unbalanced Second-Order Split-Split-Plot Design with 1 VHTC, 1 HTC, and 3 ETCs (Nonequivalent Estimation Design)

WP	SP	A	B	C	D	E
1	1	-1	-1	-1	-1	-1
		-1	-1	1	-1	-1
		-1	-1	-1	1	-1
		-1	-1	1	1	-1
		-1	-1	-1	-1	1
		-1	-1	1	-1	1
		-1	-1	-1	1	1
		-1	-1	1	1	1
	2	-1	1	-1	-1	-1
		-1	1	1	-1	-1
		-1	1	-1	1	-1
		-1	1	1	1	-1
		-1	1	-1	-1	1
		-1	1	1	-1	1
		-1	1	-1	1	1
		-1	1	1	1	1
2	3	1	-1	-1	-1	-1
		1	-1	1	-1	-1
		1	-1	-1	1	-1
		1	-1	1	1	-1
		1	-1	-1	-1	1
		1	-1	1	-1	1
		1	-1	-1	1	1
		1	-1	1	1	1
	4	1	1	-1	-1	-1
		1	1	1	-1	-1
		1	1	-1	1	-1
		1	1	1	1	-1
		1	1	-1	-1	1
		1	1	1	-1	1
		1	1	-1	1	1
		1	1	1	1	1

WP	SP	A	B	C	D	E
3	**5-6**	**-2.24**	**0**	**0**	**0**	**0**
4	**7-8**	**2.24**	**0**	**0**	**0**	**0**
5	**9**	**0**	**-2.24**	**0**	**0**	**0**
	10	**0**	**2.24**	**0**	**0**	**0**
6	11	0	0	-2.24	0	0
		0	0	2.24	0	0
		0	0	-2.24	0	0
		0	0	2.24	0	0
		0	0	-2.24	0	0
		0	0	2.24	0	0
		0	0	-2.24	0	0
		0	0	2.24	0	0
	12	0	0	0	-2.24	0
		0	0	0	2.24	0
		0	0	0	-2.24	0
		0	0	0	2.24	0
		0	0	0	-2.24	0
		0	0	0	2.24	0
		0	0	0	-2.24	0
		0	0	0	2.24	0
	13	0	0	0	0	-2.24
		0	0	0	0	2.24
		0	0	0	0	-2.24
		0	0	0	0	2.24
		0	0	0	0	-2.24
		0	0	0	0	2.24
		0	0	0	0	-2.24
		0	0	0	0	2.24
7	**14-15**	**0**	**0**	**0**	**0**	**0**

Note. Whole-plot 3, whole-plot 4, and whole-plot 7 contain 2 subplots, and each subplot contains 8 sub-subplots. Subplots 9 and 10 in Whole-plot 5 contain 8 sub-subplots each.

Table 16

Balanced Second-Order Split-Split-Plot Design with 1 VHTC, 1 HTC, and 1 ETC (Nonequivalent Estimation Design)

WP	SP	Factor			WP	SP	Factor		
		A	B	C			A	B	C
1	1	-1	-1	-1	6	11	-1.73	0	0
		-1	-1	1			-1.73	0	0
	2	-1	1	-1		12	-1.73	0	0
		-1	1	1			-1.73	0	0
2	3	1	-1	-1	7	13	0	-1.73	0
		1	-1	1			0	-1.73	0
	4	1	1	-1		14	0	1.73	0
		1	1	1			0	1.73	0
3	5	-1	-1	-1	8	15	0	0	-1.73
		-1	-1	1			0	0	1.73
	6	-1	1	-1		16	0	0	0
		-1	1	1			0	0	0
4	7	1	-1	-1	9	17	0	0	-1.73
		1	-1	1			0	0	1.73
	8	1	1	-1		18	0	0	0
		1	1	1			0	0	0
5	9	1.73	0	0					
		1.73	0	0					
	10	1.73	0	0					
		1.73	0	0					

Table 17

Norms of Difference Matrix for Simulation Designs

	CCD113_NE_CP	CCD111_NE_FP
Wprep	Enorm	Enorm
3	4300.8	42.3529
4	4300.8	44.3077
5	4300.8	45.8182

Note. Wprep represents whole-plot replicates.

5.3 Performance of Estimation Methods

How to choose an appropriate method of analysis when executing a nonequivalent design is a must-do job for the practitioner. This section shows an approach that Kowalski, Cornell, and Vining (2002) proposed to investigate the performance of estimation methods for mixed experiments in a split-plot design. This approach was also accepted by Parker, Kowalski, and Vining (2007a, 2007b) to compare the performance of OLS and GLS estimation methods for split-plots. I adopt this approach in our study to compare the performance of OLS and GLS estimation methods for split-split-plot designs.

Regarding the general split-split-plot model defined in chapter 1, it is necessary to review the model parameter estimates and the associated variances. In the simulation context, when the variance components are known, the variance-covariance matrices of the BLUE parameter estimates, OLS estimates $\hat{\beta}_{OLS}$, and GLS estimates $\hat{\beta}_{GLS}$ are shown as follows:

$$Var(\hat{\beta}_{BLUE}) = (X'\Sigma^{-1}X)^{-1},$$

$$Var(\hat{\beta}_{OLS}) = (X'X)^{-1}X'\Sigma^{-1}X(X'X)^{-1},$$

$$Var(\hat{\beta}_{GLS}) = (X'\hat{\Sigma}^{-1}X)^{-1}X'\hat{\Sigma}^{-1}\Sigma^{-1}\hat{\Sigma}^{-1}X(X'\hat{\Sigma}^{-1}X)^{-1},$$

where $\hat{\Sigma}$ is the estimated variance-covariance matrix given by

$$\hat{\Sigma} = \hat{\sigma}^2{}_{\varepsilon}I + \hat{\sigma}^2{}_{\nu}Z_1Z_1' + \hat{\sigma}^2{}_{\delta}Z_2Z_2'$$

In light of the lack of specific information about the model parameters, I chose the determinant of the variance-covariance matrix of the model parameter estimates as a single summary value to measure the efficiency. The relative efficiency is defined as the ratio between two determinants of the variance-covariance matrix:

$$\eta_{OLS/BLUE} = \frac{|Var(\hat{\beta}_{OLS})|}{|Var(\hat{\beta}_{BLUE})|}$$

$$\eta_{GLS/BLUE} = \frac{|Var(\hat{\beta}_{GLS})|}{|Var(\hat{\beta}_{BLUE})|}$$

where the subscript on η denotes the comparison between parameter estimation methods.

In the nonequivalent split-split-plot designs that I considered, pure error estimates of the variance components are available, which enables me to construct an unbiased estimate of the variance-covariance matrix as proposed by Vining, Kowalski, and Montgomery (2005).

5.4 Simulation Parameters

In this section, I provide details of the Monte Carlo simulations for these two nonequivalent second-order split-split-plot designs. By simulation, I compared OLS, GLS, and BLUE estimates and consider if it remains advantageous to use OLS rather than GLS when the design is far from equivalence or near to equivalence.

Recall from chapter 1,

$$\Sigma = \sigma_\varepsilon^{\ 2}(I_{N\times N} + r_1 Z_1 Z_1' + r_2 Z_2 Z_2'),$$

Where r_1 and r_2 are defined as the variance ratios of whole-plot variance to sub-subplot variance, and subplot variance to sub-subplot variance and expressed as:

$$r_1 = \frac{\sigma_\delta^{\ 2}}{\sigma_\varepsilon^{\ 2}},\ r_2 = \frac{\sigma_\nu^{\ 2}}{\sigma_\varepsilon^{\ 2}},$$

As r_1 increases in magnitude, the correlation among observations within a whole plot gets stronger. As r_2 increases in magnitude, the correlation among observations within a subplot gets stronger when holding r_1 constant.

Due to their practical relevance, I chose $r_1 = \{0.5, 1, 2, 5, 10\}$ and $r_2 = \{0.5, 1, 2, 5, 10\}$. Depending on the nonequivalent design of X, model parameters β, and the two ratios of the variance components r_1 and r_2, the vector of response observations y are simulated. Without loss of generality, I set $\sigma_\varepsilon^{\ 2}$ equal to 1.

Because, in the simulation model, the variance component estimates are pure-error estimates, only replicated observations are simulated. I chose whole-plot replicates equal to 3, 4, and 5. For each simulation case, I ran 200,000 trials. For each trial of simulation, I estimated the variance-covariance matrix of the parameter estimates and computed its determinant. The average determinants over all of the simulation trials were computed to achieve relative efficiency.

5.5 Simulation Results

The simulation results for the far-from-equivalence design in Table 15 are provided in Table 18. Figures 3-8 illustrate the relationship between the relative efficiencies and variance ratios based on Table 18. In Table 18, r_1 denotes the variance ratio between whole-plot variance and sub-subplot variance. r_2 denotes the variance ratio between subplot variance and sub-subplot variance. η_OLS/BLUE denotes the relative efficiency between OLS estimates and BLUE estimates. η_GLS/BLUE denotes the relative efficiency between GLS estimates and BLUE estimates. The relative efficiencies for whole-plot replicates = 3 are shown in columns 3 and 4.The relative efficiencies for replicates = 4 are shown in columns 5 and 6. Columns 7 and 8 contain the relative efficiencies for replicates = 5.

One can see that the values of $\eta_{OLS/BLUE}$ were not changed when I changed the whole-plot replicates at center level. This points out that whole-plot center point replicates won't affect the Enorms for this kind of nonequivalent split-split-plot design. Therefore in practical application, one can choose whole-plot center point replicates = 3 for one's research. Because of the high departure from the equivalence, $\eta_{GLS/BLUE}$ is much larger than $\eta_{OLS/BLUE}$.

Table 18

Relative Efficiencies for Far-from-Equivalence CCD with 1 VHTC, 1 HTC, and 3 ETCs

		Wprep = 3		Wprep = 4		5Wprep = 5	
r_1	r_2	eta_OLS/ BLUE	eta_GLS/ BLUE	eta_OLS/ BLUE	eta_GLS/ BLUE	eta_OLS/ BLUE	eta_GLS/ BLUE
0.5	0.5	1	11128	1	1067.8409	1	2707.6
0.5	1	1	11425	1	949.0883	1	24098
0.5	2	1	15587	1	3635.4	1	4380
0.5	5	1	19608	1	3801.1	1	34945
0.5	10	1	20498	1	7949.3	1	88271
1	0.5	1.0221	952.5	1.0221	784.5753	1.0221	176.0012
1	1	1.0163	908.1	1.0163	754.9	1.0163	616.1689
1	2	1	10718	1	1169.9	1	1630.4
1	5	1	15907	1	2621.8	1	8408.5
1	10	1	15840	1	4129.9	1	30123
2	0.5	1.0274	179.1	1.0274	97.0948	1.0274	137.2184
2	1	1.0230	792.4	1.023	711.8752	1.023	117.6669
2	2	1	5796.2	1	1182.1	1	1609.2
2	5	1	9813.1	1	1294.1	1	1376.2
2	10	1	10775	1	2625.3800	1	11411
5	0.5	1.0316	63.1802	1.0316	42.8141	1.0316	1.9777
5	1	1.0293	183.7833	1.0293	102.9651	1.0293	4.0954
5	2	1.0253	433.4387	1.0253	255.3821	1.0253	44.5418
5	5	1.0172	399.0405	1.0172	713.3	1.0172	170.2693
5	10	1	4924.8	1	830.5	1	12266
10	0.5	1.0332	17.9051	1.0332	1.3432	1.0332	1.0692
10	1	1.0319	55.6101	1.0319	16.9877	1.0319	1.2561
10	2	1.0295	345.2812	1.0295	109.8354	1.0295	3.6075
10	5	1.0238	886.9368	1.0248	134.3341	1.0238	49.4811
10	10	1	2292.2	1.0174	110.1812	1.0174	94.0027

Note. r_1 and r_2 denote the variance ratios, eta_OLS/BLUE denotes relative efficiency of OLS and Blue. And eta_GLS/BLUE denotes relative efficiency of GLS and Blue. BLUE is one kind of model parameter estimation method that has been defined in the dissertation.

The top figures in Figures 3, 5, and 7 illustrate the relationship between the relative efficiencies $\eta_{OLS/BLUE}$, $\eta_{GLS/BLUE}$ and the variance ratio r_2 when holding r_1 constant. There are no differences for whole-plot replicates at center level = 3, 4, and 5. With regard to r_1, when r_1 is very small, such as $r_1 = 0.5$, the relative efficiency $\eta_{OLS/BLUE}$ is equal to 1. With r_1 getting bigger, slight differences are shown in $\eta_{OLS/BLUE}$. With the increases of r_2, $\eta_{OLS/BLUE}$ decreases. High values of r_1 give high values of $\eta_{OLS/BLUE}$. The bottom figures in Figures 3, 5, and 7 illustrate the relationship between the relative efficiencies $\eta_{GLS/BLUE}$, $\eta_{GLS/BLUE}$ and the variance ratio r_2 when holding r_1 constant. $\eta_{GLS/BLUE}$ has a positive relationship with r_2. Lower levels of r_1 brings higher values of $\eta_{GLS/BLUE}$. Holding r_2 constant, the top figures in Figure 4, 6, and 8 illustrate the positive relationship between the relative efficiencies $\eta_{OLS/BLUE}$ and the variance ratio r_1. Lower levels of r_2 give higher values of $\eta_{OLS/BLUE}$. The bottom figures in Figure 4, 6, and 8 illustrate the negative relationship between the relative efficiencies $\eta_{GLS/BLUE}$ and the variance ratio r_1. Lower levels of r_1 give higher values of $\eta_{GLS/BLUE}$. The relative efficiency $\eta_{GLS/BLUE}$ has a positive relationship with r_2. Lower levels of r_2 give lower values of $\eta_{GLS/BLUE}$.

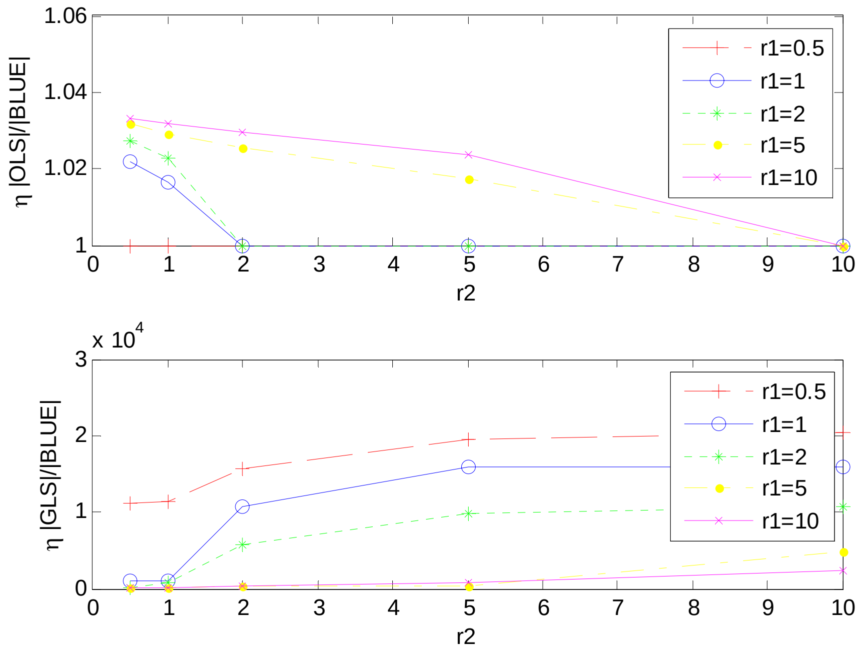

Figure 3. Relationship between relative efficiency and the variance ratios for Far-from-Equivalence CCD with 1 VTHC, 1 HTC, 3 ETCs. Replicates = 3 holding r_1 constant.

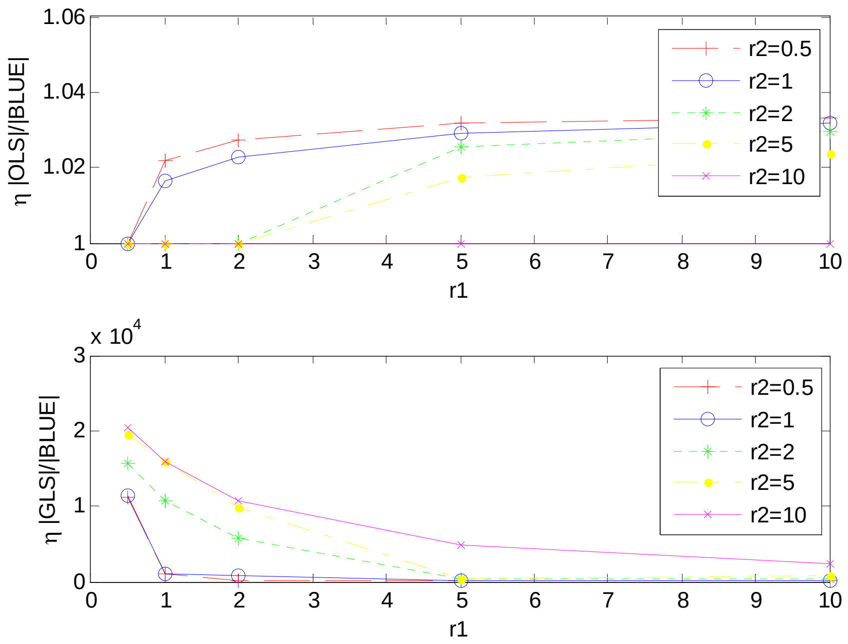

Figure 4. Relationship between relative efficiency and the variance ratios for far-from-equivalence CCD with 1 VTHC, 1 HTC, 3 ETCs. Replicates = 3 holding r_2 constant.

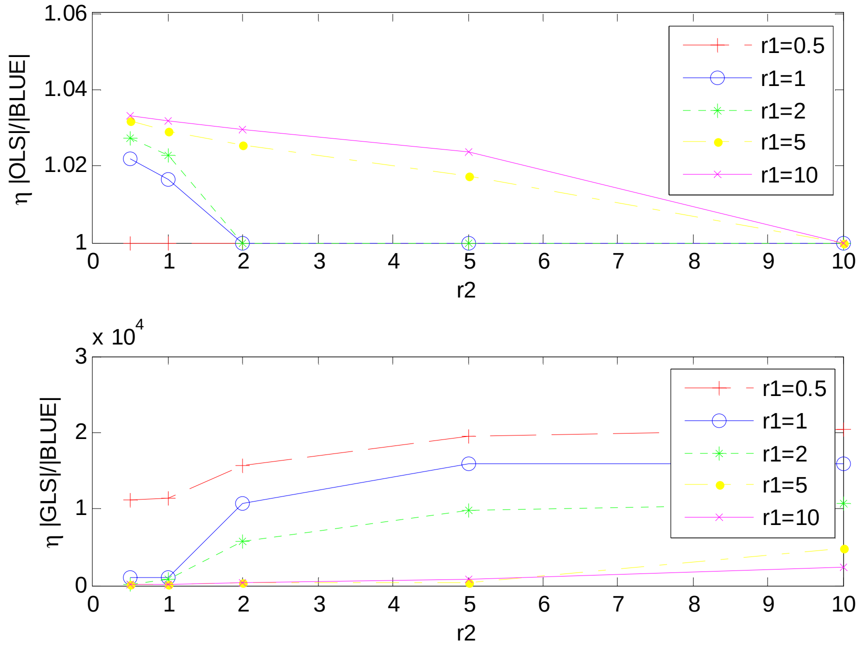

Figure 5. Relationship between relative efficiency and the variance ratios for Far-from-Equivalence CCD with 1 VTHC, 1 HTC, 3 ETCs. Replicates = 4 holding r_1 constant.

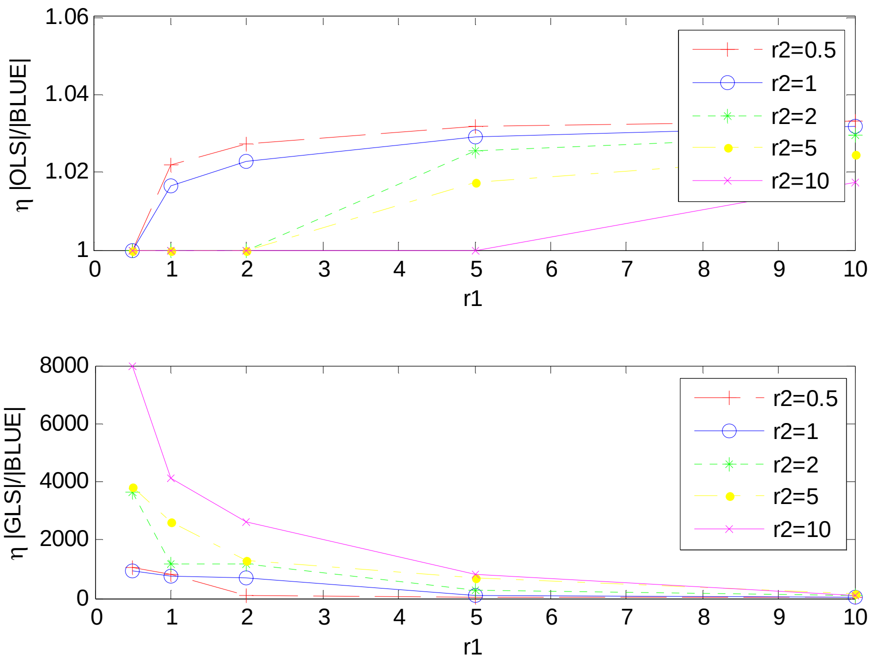

Figure6. Relationship between relative efficiency and the variance ratios for far-from-equivalence CCD with 1 VTHC, 1 HTC, 3 ETCs. Replicates = 4 holding r_2 constant.

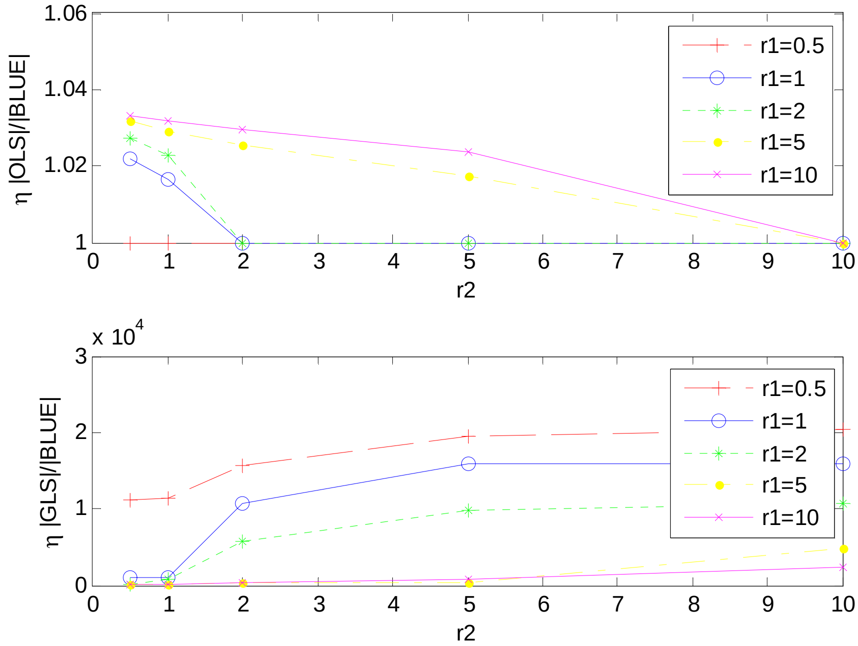

Figure 7. Relationship between relative efficiency and the variance ratios for far-from-equivalence CCD with 1 VTHC, 1 HTC, 3 ETCs. Replicates = 5 holding r_1 constant.

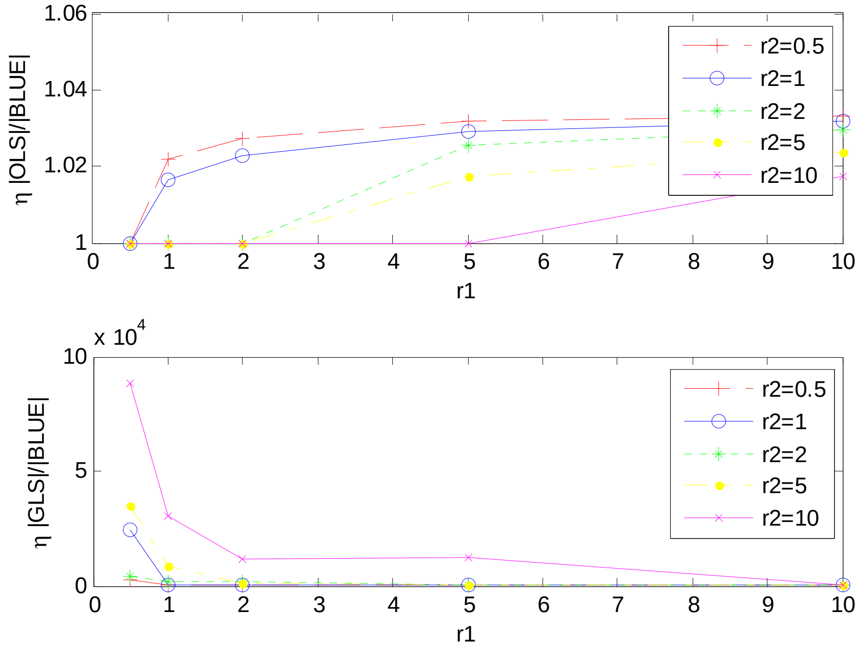

Figure 8. Relationship between relative efficiency and the variance ratios for far-from-equivalence CCD with 1 VTHC, 1 HTC, 3 ETCs. Replicates = 5 holding r_2 constant.

The simulation results for the near-to-equivalence split-split-plot designs in Table 16 are summarized in Table 19. Figures 9-14 illustrate the relationship between the relative efficiencies and variance ratios based on Table 19.

Table 19

Relative Efficiencies for Near-to--Equivalence CCD with 1 VHTC, 1 HTC, and 1 ETC

		Wprep = 3		Wprep = 4		Wprep = 5	
r_1	r_2	eta_OLS/BLUE	eta_GLS/BLUE	eta_OLS/BLUE	eta_GLS/BLUE	eta_OLS/BLUE	eta_GLS/BLUE
0.5	0.5	1	5962.1	1	3389.2	1	4180.7
0.5	1	1	1517.7	1	1085.1	1	1341.6
0.5	2	1	1253.8	1.0049	503.8594	1.0153	126.6821
0.5	5	1.0035	303.5235	1.0036	75.5905	1.0037	2.7899
0.5	10	1.001	91.3367	1.0011	1.991	1.0011	1.3578
1	0.5	1.2	2509.3	1.2	1748.6	1.2	1050.7
1	1	1.1	1144.9	1.0992	989.8079	1.1019	386.8249
1	2	1.0446	392.843	1.0463	359.9161	1.0476	90.9903
1	5	1.0122	81.09	1.0126	17.9283	1.013	7.4163
1	10	1.0038	12.5056	1.004	1.8745	1.0041	5.199
2	0.5	1.4	1961.7	1.4166	568.3827	1.4281	108.2002
2	1	1.2	1402.9	1.2525	514.0637	1.2595	218.3622
2	2	1.1235	904.5428	1.1282	114.9512	1.1317	46.6991
2	5	1.0384	50.4147	1.0399	3.4269	1.041	3.418
2	10	1.0132	3.9513	1.0137	1.539	1.0141	1.197
5	0.5	2.1403	157.7932	2.1834	54.6388	2.2162	21.1757
5	1	1.7271	148.2128	1.7547	79.4963	1.7755	12.8389
5	2	1.4014	106.2934	1.4166	18.2041	1.4281	10.7019
5	5	1.1471	8.1632	1.1527	9.8931	1.1469	4.8756
5	10	1.0583	4.5661	1.0605	1.2485	1.0622	1.1587
10	0.5	3.3892	62.9444	3.4796	66.7437	3.5482	2.2573
10	1	2.5558	58.813	2.6146	5.3411	2.6593	9.389
10	2	1.89	54.1232	1.9257	5.2764	1.9513	1.6726
10	5	1.3577	20.434	1.3713	3.7062	1.3816	1.127
10	10	1.1567	1.6726	1.1626	1.3327	1.1671	1.09

Note. r_1 and r_2 denotes the variance ratios, eta_OLS/BLUE denotes relative efficiency of OLS and Blue. eta_GLS/BLUE denotes relative efficiency of GLS and Blue 0.5, 1, 2 ,5 , 10 are all values set to r_1 and r_2.

Based on Table 19, compared with $\eta_{GLS/BLUE}$, the values of $\eta_{OLS/BLUE}$ changed very slightly when I increased the whole-plot replicates from 3 to 5 at the factorial level.

The relationship between relative efficiency and variance ratios is illustrated in Figures 9-14. The top figures in Figures 9, 11, and 13 illustrate the relationship between the relative efficiencies $\eta_{OLS/BLUE}$ and the variance ratio r_2 when holding r_1 constant. There are tiny differences between whole-plot center point replicates = 3, 4, and 5. r_1 has a positive relationship with $\eta_{OLS/BLUE}$, and r_2 has a negative relationship with $\eta_{OLS/BLUE}$. The bottom figures in Figures 9, 11, and 13 illustrate the relationship between the relative efficiencies $\eta_{GLS/BLUE}$ and the variance ratio r_2 when holding r_1 constant. $\eta_{GLS/BLUE}$ has a negative relationship with r_2. Lower levels of r_2 give higher values of $\eta_{GLS/BLUE}$. Holding r_2 constant, the top figures in Figures 10, 12, and 14 illustrate the positive relationship between the relative efficiencies $\eta_{OLS/BLUE}$ and the variance ratio r_1. Lower levels of r_2 give higher values of $\eta_{OLS/BLUE}$. The bottom figures in Figures 10, 12, and 14 illustrate the negative relationship between the relative efficiencies $\eta_{GLS/BLUE}$ and the variance ratio r_1. Lower levels of r_2 give higher values of $\eta_{GLS/BLUE}$.

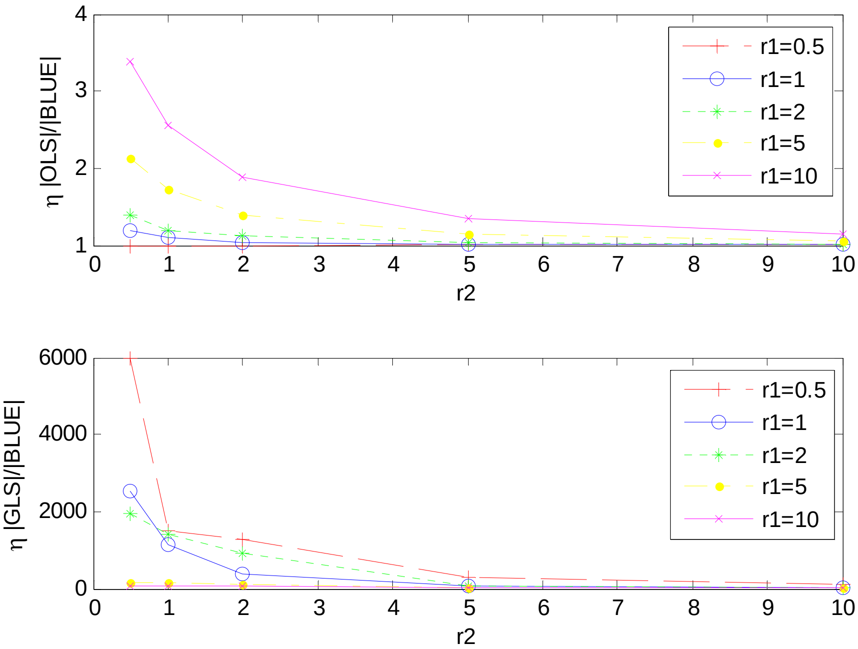

Figure 9. Relationship between relative efficiency and the variance ratios for near-to-equivalence CCD with 1 VTHC, 1 HTC, 1 ETC. Replicates = 3 holding r_1 constant.

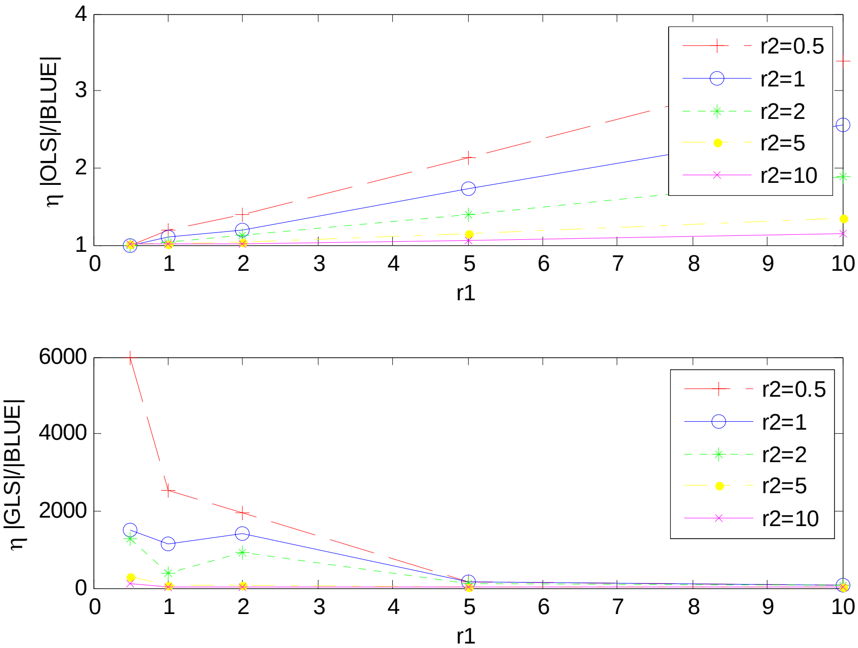

Figure 10. Relationship between relative efficiency and the variance ratios for near-to-equivalence CCD with 1 VTHC, 1 HTC, 1 ETC. Replicates = 3 holding r_2 constant.

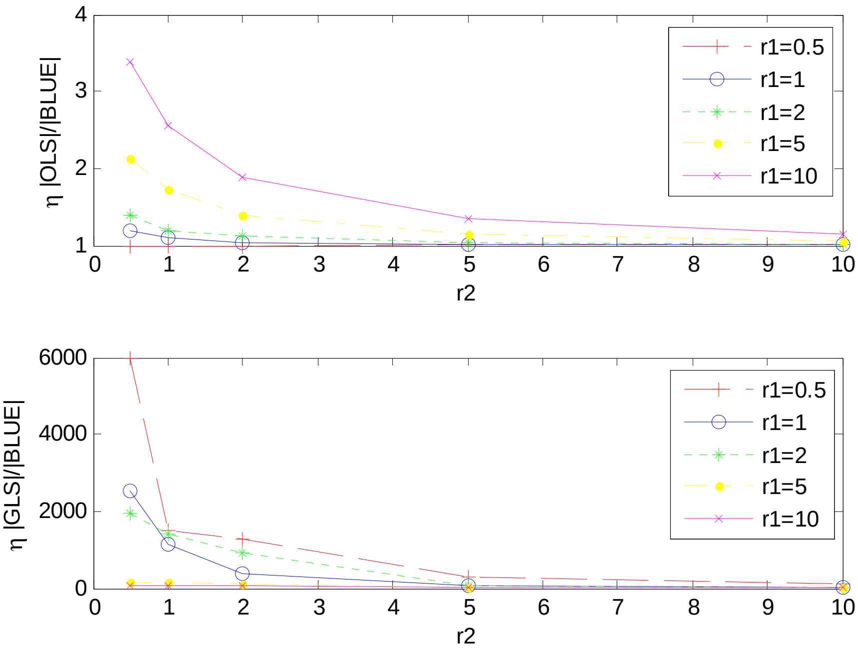

Figure 11. Relationship between relative efficiency and the variance ratios for near-to-equivalence CCD with 1 VTHC, 1 HTC, 1 ETC. Replicates = 4 holding r_1 constant.

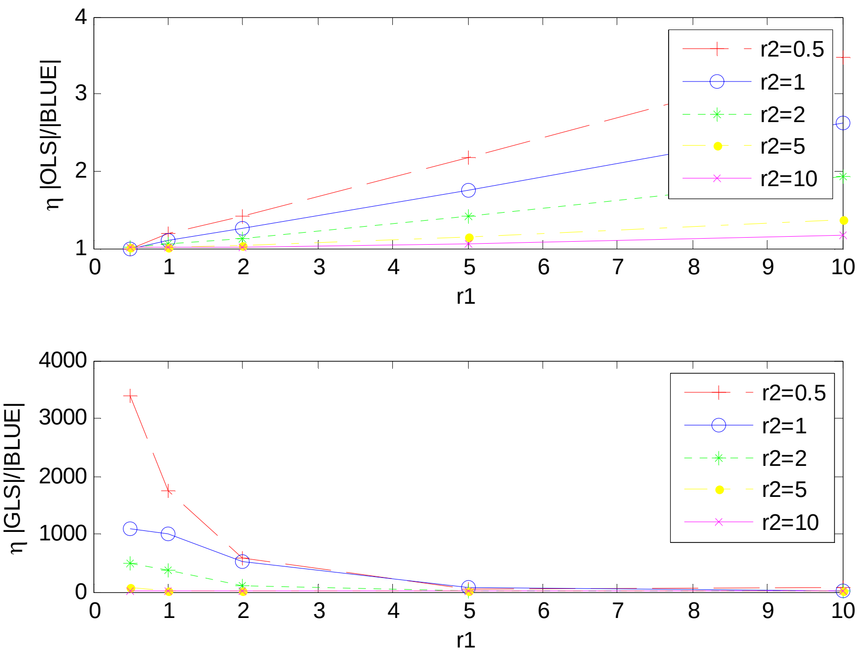

Figure 12. Relationship between relative efficiency and the variance ratios for near-to-equivalence CCD with 1 VTHC, 1 HTC, 1 ETC. Replicates = 4 holding r_2 constant.

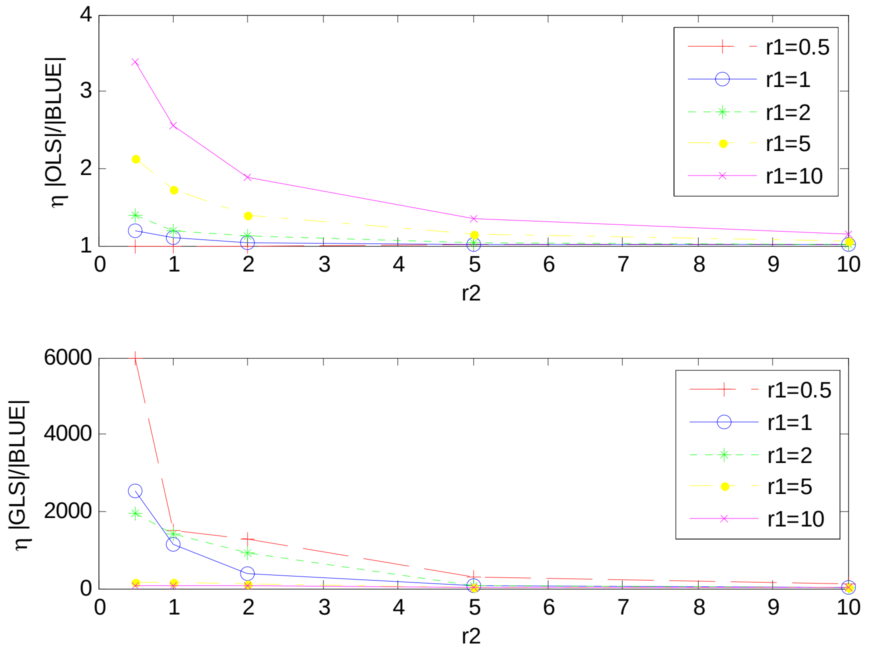

Figure 13. Relationship between relative efficiency and the variance ratios for near-to-equivalence CCD with 1 VTHC, 1 HTC, 1 ETC. Replicates = 5 holding r_1 constant.

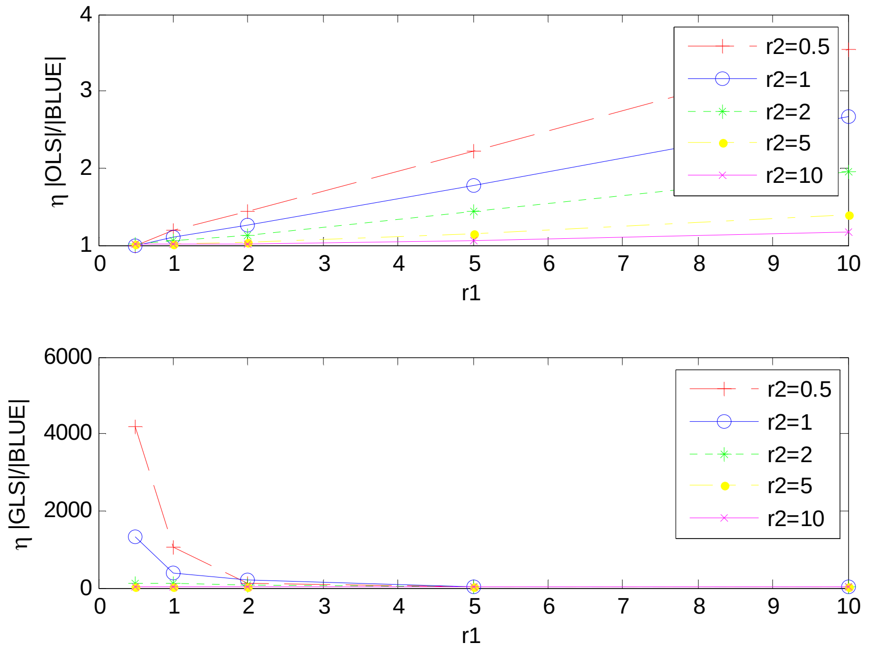

Figure 14. Relationship between relative efficiency and the variance ratios for near-to-equivalence CCD with 1 VTHC, 1 HTC, 1 ETC. Replicates = 5 holding r_2 constant.

5.6 Simulation Algorithm and Diagnostics Procedures

5.6.1 Algorithm Description

In this section, the details of the simulation algorithm are provided. All the computer codes for running the two kinds of nonequivalent designs are shown in Appendix B.

1. Based on the base design without whole-plot replicates, for the far-from-equivalence design in Table 15 with 1 VHTC, 1 HTC, and 3ETCs, the whole-plot replicates at center level are designated at the end of the base design. For the near-to-equivalence design in Table 16 with 1 VHTC, 1 HTC, and 1 ETC, the whole-plot replicates at factorial level are designated between the factorial whole plots and the axial whole plots.

2. From the augmented design, X is generated for a complete second-order CCD design. The difference matrix D is constructed to compute the Enorms.

3. The known variance-covariance matrix of the observations are computed as

$\Sigma = I + r_1 M1 + r_2 M2$,

The covariance matrix of the parameter estimates of BLUE is calculated as

$Var(\hat{\beta}_{BLUE}) = (X'\Sigma^{-1}X)^{-1}$,

and the determinant as

$|Var(\hat{\beta}_{BLUE})| = |(X'\Sigma^{-1}X)^{-1}|$.

The variance-covariance matrix of the OLS estimates is computed by

$Var(\hat{\beta}_{OLS}) = (X'X)^{-1}X'\Sigma^{-1}X(X'X)^{-1}$, and the determinant as

$|Var(\hat{\beta}_{OLS})| = |(X'X)^{-1}X'\Sigma^{-1}X(X'X)^{-1}|$.

4. Based on the augmented design, when computing the pure error estimates of whole plots , subplots, and sub-subplots, I identified the degree of freedom as follows: To compute the estimated sub-subplot error, I identified the whole-plot replicates, the structure of subplots within each whole plot, and the structure of sub-subplots within each subplot. For example, for the design with 1 VHTC, 1 HTC, and 3 ETCs in Table 15, the size of whole plot is 16. Each whole plot contains 2 subplots, within each subplot it contains 8 sub-subplots. If one has three whole-plot replicates, then the degree of freedom for sub-subplot errors is $3 \times 2 \times (8-1) = 42$.

5. Assuming that the replicated whole plot contains subplot replicates and sub-subplot replicates, observations are simulated for each whole plot that contains subplot replicates and sub-subplot replicates. Note that the sample variance calculations are model independent as they are based on the exact replicates. The vector of the response y is randomly generated for the whole-plot replicates from the multivariate normal distribution with mean 0 and the variance-covariance matrix structured as Equation (4).

6. Let *d* represent the whole-plot replicates, *m* represent the subplot replicates within each whole-plot replicate, and *n*0 represent the sub-subplot replicates within each subplot replicate. Let $\overline{Y}_{...}, \overline{Y}_{i..}, \overline{Y}_{ij.}$ represent the overall sample mean of all whole-plot replicates, all subplot replicates within i^{th} whole-plot, and sub-subplot replicates within j^{th} subplot under i^{th} whole plot.

The pure-error estimate of sub-subplot variance can be calculated by:

- Computing the sum-of-squares from the sub-subplot replicates as SS_{total} .

- The estimated sub-subplot variance is calculated as

$$S_{SSP}^2 = \frac{SS_{total}}{df_{total}}$$

where $SS_{total} = \sum_i \sum_j \sum_{k=1}^{SSP_{rep}} (y_{ijk} - \bar{Y}_{ij.})$, $df_{total} = d \times m \times (n0 - 1)$.

- The estimated subplot variance is calculated as

$$S_{SP}^2 = \frac{\sum_i \sum_{j=1}^{m} (\bar{Y}_{ij.} - \bar{Y}_{i..})^2}{d \times (m-1)} - \frac{S_{SSP}^2}{n0} .$$

- The estimated whole-plot variance is calculated as

$$S_{WP}^2 = \frac{\sum_i \sum_{j=1}^{m} (\bar{Y}_{i..} - \bar{Y})^2}{d-1} - \frac{S_{SP}^2}{m} - \frac{S_{SSP}^2}{n0} .$$

7. The estimated variance-covariance matrix of the observations can be expressed as

$$\hat{\Sigma} = \hat{\sigma}_{\varepsilon}^2 I + \hat{\sigma}_{\nu}^2 M_1 + \hat{\sigma}_{\delta}^2 M_2 .$$

The variance-covariance matrix of the GLS parameter estimates can be calculated as

$$Var(\hat{\beta}_{GLS}) = (X'\hat{\Sigma}^{-1}X)^{-1} X'\hat{\Sigma}^{-1}\Sigma^{-1}\hat{\Sigma}^{-1}X(X'\hat{\Sigma}^{-1}X)^{-1}$$

and the determinant as

$$|Var(\hat{\beta}_{GLS})| = |(X'\hat{\Sigma}^{-1}X)^{-1} X'\hat{\Sigma}^{-1}\Sigma^{-1}\hat{\Sigma}^{-1}X(X'\hat{\Sigma}^{-1}X)^{-1}| .$$

8. Based on 200,000 simulations, steps 5 to 7 are replicated for each whole-plot replicate. The sum of the determinants over all of the simulations are calculated, and the average determinant is computed and expressed by

$$\overline{|Var(\hat{\beta}_{GLS})|} .$$

Based on the squared values of the determinant, the sample variance of the simulations can be computed.

9. The relative efficiency denoted by η are calculated by

$$\eta_{OLS\,/\,BLUE} = \frac{|\operatorname{var}(\hat{\beta}_{OLS})|}{|\operatorname{var}(\hat{\beta}_{BLUE})|},$$

$$\eta_{GLS\,/\,BLUE} = \frac{\overline{|\operatorname{var}(\hat{\beta}_{GLS})|}}{|\operatorname{var}(\hat{\beta}_{BLUE})|}.$$

5.6.2 Diagnostics

To check the simulation code for errors and verify the validation of the algorithm, some diagnostics were performed.

- I ran an estimation-equivalent design through the simulation to verify that

$$|\operatorname{var}(\hat{\beta}_{OLS})| = \overline{|Var(\hat{\beta}_{GLS})|}.$$

Therefore

$$\eta_{OLS\,/\,BLUE} = \eta_{GLS\,/\,BLUE}.$$

- To check the distribution of the simulated values, based on the individual samples of the determinant of the variance-covariance matrix of the GLS estimates, and the estimated $\hat{\sigma}_{\varepsilon}^2, \hat{\sigma}_{\nu}^2$, the nonequivalent designs in Table 15 and Table 16 are performed with whole-plot replicates = 3. I chose $r_1 = 1, \mathrm{r}_2 = 1$, which implied that $\sigma_{\varepsilon}^2 = \sigma_{\nu}^2 = \sigma_{\delta}^2 = 1$.
- Based on 200,000 simulation trials, the values of the determinants and the standard deviation are shown below:

CCD_113 in Table 15		CCD_111 in Table 16	
detBLUE=	3.2574E-29	detBLUE=	4.5319E-12
detOLS=	3.3105E-29	detOLS=	4.965E-12
ave_detGLS=	6.9763E-26	avedetGLS=	2.0248E-08
std_detGLS=	1.5235E-25	std_detGLS=	5.1924E-08
avestd_detGLS=	3.40665E-28	avestd_detGLS=	1.16106E-10

The investigations into the samples show that as $\hat{\sigma}_\delta^2$ and $\hat{\sigma}_\nu^2$ approach zero, $\hat{\Sigma} = \hat{\sigma}_\varepsilon^2 I$, which results in a completely randomized design. The values of detBLUE and detOLS are very close to each other. For CCD_111 in Table 16, the extreme value of the GLS determinant is 4.5319E-12, which is identical to detOLS. A histogram of the individual observations for the estimated variances is shown in Figure 5.13 which shows that a large number of extreme values are on the left tail of the distribution of the determinant of GLS estimates. The estimated whole-plot errors $\hat{\sigma}_\delta^2$, subplot errors $\hat{\sigma}_\nu^2$ and sub-subplot errors $\hat{\sigma}_\varepsilon^2$ follow chi-square distribution. For the design CCD_113 in Table 15, the sample means are 0.9998, 0.9437, and 1.0003, respectively. For the design CCD111 in Table 16, the sample means are 1.0894, 1.0009, and 1.0001, respectively. Both of the distributions and the sample means are consistent with my expectations.

- Coefficient of Variation (CV) is a statistical measure to determine the dispersion of data points around the mean. To check whether the 200,000 simulation trials would be sufficient, I computed the CV of the GLS determinant based on the sample standard deviation.
- The standard deviation of detGLS estimates for the design of CCD_111 in Table 15:

$$stde\_\det GLS = 5.1924 \times 10^{-8}.$$

The mean of standard deviations over the 200,000 simulation trials is

$$\frac{5.1924 \times 10^{-8}}{\sqrt{200,000}} = 1.1611 \times 10^{-10}.$$

The ratio of variation is equal to

$$\frac{1.1611 \times 10^{-10}}{2.0248 \times 10^{-8}} \times 100 = 0.5734\%.$$

- The standard deviation of detGLS estimates for the design of CCD_113 in Table 16:

$$stde\_\det GLS = 1.5235 \times 10^{-25},$$

The mean of standard deviation over the 200,000 simulation trials is

$$\frac{1.5235 \times 10^{-25}}{\sqrt{200,000}} = 3.4067 \times 10^{-28}.$$

The ratio of variation is equal to

$$\frac{3.4067 \times 10^{-28}}{6.9763 \times 10^{-26}} \times 100 = 0.4883\%.$$

As the variation of the results is very small, there is high precision of the results. In future study, a smaller simulation may be required.

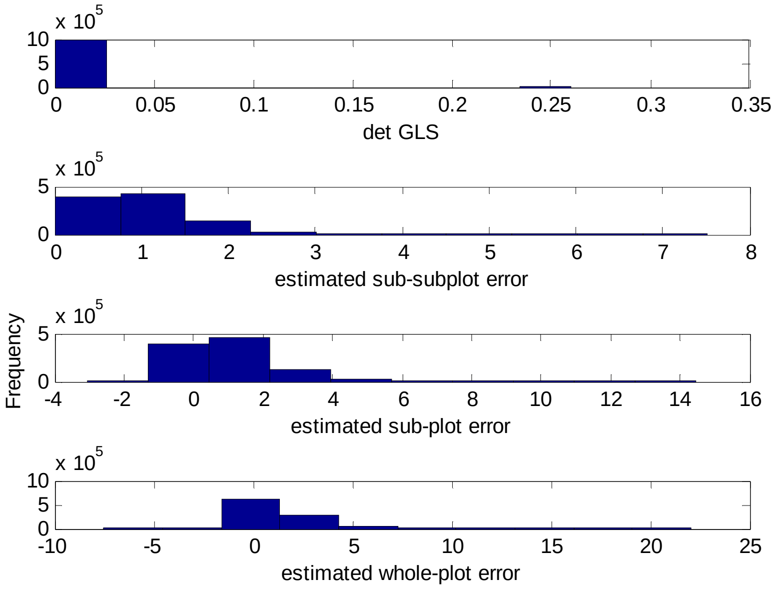

Figure 15. Distribution of simulation observations. (Near-to-equivalence CCD with 1 VHTC, 1 HTC, and 1 ETC).

CHAPTER 6

CONCLUSIONS

Parker, Kowalski, and Vining (2007a, 2007b) discovered the equivalent-estimation second-order split-plot designs in the area of central composite designs and Box-Behnken designs, where the ordinary least square estimates are equal to the generalized least square estimates. Equivalent-estimation designs enjoy a series of equivalence properties: Model parameter estimates are independent of the variance components and robust to the assumption of normality. Model parameter estimates are best linear unbiased estimates (BLUE). The model parameter estimation is simplified by using OLS instead of GLS. Estimation equivalent designs can be constructed independent of any model assumption. Design selection is independent of variance components. Moreover, these designs are very easy to augment to obtain pure-error variance components estimates.

In this study, I extended the work of Parker, Vining, and Montgomery (2007a, 2007b) on split-plot designs to split-split-plot designs. Several categories of designs were studied: balanced second-order split-split-plot designs, unbalanced second-order split-split-plot designs, far-from-equivalence designs, and near-to-equivalence designs.

In general, with regard to the balanced second-order split-split-plot designs for the VKM and MWP methods, I needed to consider three aspects for the design structure: center points, factorial points, and axial points. As to axial points, two cases were considered, depending on whether the number of subplot factors and the number of sub-subplot factors were powers of two. The center points are run in a separate whole plot. For the MWP method, I studied the balanced equivalent-estimation split-split-plot designs for MWP with only one VHTC whole-plot factor and $\alpha = 1$. These designs contained three whole plots at high level, low level, and center level.

Regarding the unbalanced estimation-equivalent second-order split-split-plot designs for the VKM method, similar to a balanced case, three aspects needed to be considered in the design construction: factorial points, axial points, and center points. Among the variety of unbalanced split-split-plot designs, I considered the unbalanced designs in which the unbalance at the whole-plot center level.

Regarding the nonequivalent split-split-plot designs, I provided the measure of departure from equivalence. I considered an unbalanced CCD113 in Table 15 that was far-from equivalence, and a balanced CCD111 in Table 16 that was near-to equivalence. The Monte Carlo simulation method was used to compare the three model parameter estimation methods: OLS, GLS, and BLUE. The simulation results showed that using OLS estimates took the advantage over using GLS estimates for the nonequivalence split-split-plot designs.

In general, throughout this research, I focused on experimental strategies that properly considered the three stratum designs with three kinds of experimental factors: whole-plot factors, subplot factors, and sub-subplot factors. This kind of design with two restricted randomizations represented a new facet of response surface methodology (RSM).

The following list is for future research corresponding to second-order split-split-plot designs:

1. One may be interested in investigating the equivalent-estimation split-split-plot BBD designs that are not easily extended from the split-plot case to split-split-plot case.

2. For unbalanced equivalent-estimation split-split-plot designs, I studied the VKM method. More research needs to be done for the MWP method.

3. If a significant proportion of total experimental cost is also associated with the number of experiments, then the experimenter will often fractionate the factorial portion of the central composite design so as to achieve resolution V or even resolution III^*. Assuming three-factor and higher interaction effects are negligible, the resolution V or resolution III^* fractional factorial designs permit the estimation of main effects and two-factor interaction terms freely (e.g., see Montgomery, 2005). In some cases, fractionating the factorial portion of the CCD violates the proposed equivalent conditions. In the future, more work can be done to check the robustness of OLS estimates to this kind of designs.

REFERENCES

Bingham, D. R., Schoen, E. D., & Sitter, R. R. (2004). Designing fractional factorial split-plot experiments with few whole-plot factors. *Applied Statistics, vol. 53,* Part 2, pp. 325-339.

Bingham, D. R., & Sitter, R. R. (1999a). Minimum-aberration two-level fractional factorial split-plot designs. *Technometrics, 41*(1), 62-70.

Bingham, D. R., & Sitter, R. R. (1999b). Some theoretical results for fractional factorial split-plot designs. *The Annals of Statistics, 27*(4), 1240-1255.

Bingham, D., & Sitter, R. R. (2001). Design issues in fractional factorial split-plot designs. *Journal of Quality Technology, 33,* 2-15.

Bisgaard, S. (2000). The design and analysis of 2^{k-p} x 2^{q-r} split plot experiments. *Journal of Quality Technology, 32*(1), 39-56.

Box, G. E. P. (1996). Split-Plot Experiments. *Quality Engineering 8,* pp. 515-520.

Box, G., Hunter, W., & Hunter, S. (2005). *Statistics for experiments: Design, innovation, and discovery* (2^{nd} ed.). New York: Wiley-Interscience.

Castillo, F. (2010). Split-split-plot experimental design in a high-throughput reactor. *Quality Engineering,* 22, 328-335.

Draper, N. R., & John, J. A. (1998). Response surface designs where levels of some factors are difficult to change. *Australian and New-Zealand Journal of Statistics, 40,* 487-495.

Ferryanto, L., Tollefson, N. (2010). A split-split-plot design of experiments for foil lidding of contact lens packages. *Quality Engineering, 22,* 317-327.

Fisher, R. A. (1925). *Statistical methods for research workers.* Edinburgh: Oliver and Boyd.

Ganju, J., & Lucas, J. M. (1997). Bias in test statistics when restrictions in randomization are caused by factors. *Communications in Statistics: Theory and Methods, 26*(*1*), 47-63.

Ganju, J., & Lucas, J. M. (1999). Detecting randomization restrictions caused by factors. *Journal of Statistical Planning and Inference, 81*(1), 129-140.

Goos, P. (2002). *The optimal design of blocked and split-plot experiments: Lecture notes in statistics.* New York: Springer.

Goos, P. (2006). Optimal versus orthogonal and equivalent-estimation design of blocked and split-plot experiments. *Statistica Neerlandica, 60*(3), 361–378.

Goos, P., & Vandebroek, M. (2003). D-optimal split-plot designs with given numbers and sizes of whole-plots. *Technometrics, 45*, 235 – 245.

Gotu, B. (2001). The equality of OLS and GLS estimators in the linear regression model when the disturbances are spatially correlated. ***Statistical Papers***, *42*(2), 253-263.

Hahn,G. J. (1978). More on randomization. *Chemical Technology*, *8*, 164-168.

Huang, P., Chen, D., & Voelkel, J. O. (1998). Minimum-aberration two-level split-plot designs. *Technometrics, 40*(4), 314-326.

Jones, B., & Goos, P. (2009). D-optimal design of split-split-plot experiments. *Biometrika (2009)* 96 (1): 67-82.

Jones, B., & Nachtsheim, C. J. (2009). Split plot designs: What, why, and how. *Journal of Quality Technology, 41*(4), 340-361.

Kowalski, S. M., Cornell, J. A., & Vining, G. G. (2002). Split-plot designs and estimation methods for mixture experiments with process variables. *Technometrics, 44,* 72-79.

Kowalski, S. M., & Potcner, K. J. (2003). How to recognize a split-plot experiment. *Experimental Design* (November), 60-66

Langhans, I., Goos, P., & Vandebroek, M. (2005). Identifying effects under a split-plot design structure. *Journal of Chemometrics*, *19*, 5-15.

Letsinger, J. D., Myers, R. H., & Lentner, M. (1996). Response surface methods for bi-randomization structures. *Journal of Quality Technology, 28*, 381-397.

Mather, K. (1951). R. A. Fisher's statistical methods for research workers: An appreciation. *Journal of American Statistical Association, 4*6(253), 51-54.

McElroy, F. W. (1967). A necessary and sufficient condition that ordinary least square estimators be best linear unbiased. *Journal of American Statistical Association, 62,* 1302-1304.

Montgomery, D. C. (2005). *Design and analysis of experiments* (7th ed.). New York: Wiley.

Myers, R. H. (1999). Response Surface Methodology-Current Status and Future Directions. *Journal of Quality Technology.* 31, pp. 30-44.

Myers, R. H.; Montgomory, D. C.; Vining, G. G.; Borror, C. M.; and Kowalski, S. M. (2004). Response Surface Methodology: A retrospective and Literature Survey. *Journal of Quality Technology.* 36, pp. 409-419.

Myers, R. H., Montgomery, D. C., & Anderson-Cook , C. M. (2009). *Response surface methodology: Process and product optimization using designed experiments.* New York: Wiley.

Parker, P. A., Kowalski, S. M., & Vining, G. G. (2005). Classes of split-plot response surface designs for equivalent estimation. *Quality and Reliability Engineering International, 22*, 291-305.

Parker, P. A., Kowalski, S. M., & Vining, G. G. (2007a). Construction of balanced equivalent estimation second-order split-plot designs. *Technometrics,4*9(1),56-65.

Parker, P. A., Kowalski, S. M., & Vining, G. G. (2007b). Unbalanced and minimal point equivalent estimation second-order split-plot designs. *Journal of Quality Technology, 39*, 376-388.

Schoen, E. D. (1999). Designing fractional two-level experiments with nested error structures. *Journal of Applied Statistics, 26,* 495-508.

Simpson, J. R., Kowalski, S. M., & Landman, D. (2004). Experimentation with randomization restrictions: Targeting practical implementation. *Quality and Reliability Engineering International, 20,* 481-495.

Taguchi, G. (1987). *System of experimental design, Vol. 1.* White Plains, NY: Kraus International.

Trinca, L. A., & Gilmour, S. G. (2001). Multi-stratum response surface designs. *Technometrics 43*, 25-33.

Vining, G. G.; Kowalski, S. M.; and Montgomery, D. C. (2005), Reponse Surface Designs Within a Split-Plot Structure. *Journal of Quality Technology,* 37, pp. 115-129

Wooding,W. M. (1973). The split-plot design. *Journal of Quality Technology, 5,* 16-33.

APPENDIX A

DEVELOPMENT OF BALANCED FORMS OF K_1 AND K_2 FOR THE VKM METHOD AND THE MWP METHOD

The general estimation equivalent conditions for a split-split-plot design are given by

(AI. 1) $XK_1 = \mathrm{M}_1\mathrm{X} = Z_1Z_1'X$

and

(AI. 2) $XK_2 = \mathrm{M}_2\mathrm{X} = Z_2Z_2'X$

where

$$X = \begin{bmatrix} 1 & W_{D1} & W_{Q1} & S_{D1} & S_{Q1} & SS_{D1} & SS_{Q1} \\ 1 & W_{D2} & W_{Q2} & S_{D2} & S_{Q2} & SS_{D2} & SS_{Q2} \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ 1 & W_{Dw} & W_{Qw} & S_{Dw} & S_{Qw} & SS_{Dw} & SS_{Qw} \end{bmatrix} X = \begin{bmatrix} 1 & W_{D11} & W_{Q11} & S_{D11} & S_{Q11} & SS_{D11} & SS_{Q11} \\ 1 & . & . & . & . & . & . \\ 1 & . & . & . & . & . & . \\ 1 & . & . & . & . & . & . \\ 1 & W_{D1m1} & W_{Q1m1} & S_{D1m1} & S_{Q1m1} & SS_{D1m1.} & SS_{Q1m1} \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ 1 & W_{Dwmw} & W_{Qwmw} & S_{Dwmw} & S_{Qwmw} & SS_{Dwmw} & SS_{Qwmw} \end{bmatrix}.$$

where

$$W_{Di} = \begin{bmatrix} W_{Di1} \\ W_{Di2} \\ . \\ . \\ . \\ W_{Dim_i} \end{bmatrix}, W_{Qi} = \begin{bmatrix} W_{Qi1} \\ W_{Qi2} \\ . \\ . \\ . \\ W_{Qim_i} \end{bmatrix}, S_{Di} = \begin{bmatrix} S_{Di1} \\ S_{Di2} \\ . \\ . \\ . \\ S_{Dim_i} \end{bmatrix},$$

$$S_{Qi} = \begin{bmatrix} S_{Qi1} \\ S_{Qi2} \\ . \\ . \\ . \\ S_{Qim_i} \end{bmatrix}, SS_{Di} = \begin{bmatrix} SS_{Di1} \\ SS_{Di2} \\ . \\ . \\ . \\ SS_{Dim_i} \end{bmatrix}, SS_{Qi} = \begin{bmatrix} SS_{Qi1} \\ SS_{Qi2} \\ . \\ . \\ . \\ SS_{Qim_i} \end{bmatrix} \text{ for i =1, 2, …, w.}$$

The first column of ones in X denotes the intercept. W_{Dij} denotes the model sub matrix for the whole-plot main effect and two factor interaction terms contained in the j^{th} subplot of i^{th} whole plot. W_{Qij} denotes the model sub matrix for the whole-plot pure quadratic terms contained in the j^{th} subplot of i^{th} whole plot. S_{Dij} denotes the model sub matrix for the subplot main effect and two factor interaction terms between whole plot and subplot, subplot and subplot interaction terms contained in the j^{th} subplot of i^{th} whole plot. S_{Qij} denotes the model sub matrix for the subplot pure quadratic terms contained in the j^{th} subplot of i^{th} whole plot. SS_{Dij} denotes the model sub matrix for the sub-subplot main effect and two factor interaction terms between whole plot and sub-subplot, subplot and sub-subplot, sub-subplot and sub-subplot interaction terms contained in the j^{th} subplot of i^{th} whole plot. SS_{Qij} denotes the model sub matrix for the sub-subplot pure quadratic terms contained in the j^{th} subplot of i^{th} whole plot.

$\mathrm{Z}_1 = blkdiag(1_{n_1}, 1_{n_2}, ..., 1_{n_w}) : N \times w$ known indicator matrix for the whole-plot factors

$\mathrm{Z}_2 = blkdiag(1_{n_{11}}, 1_{n_{12}}, ..., 1_{n_{1m1}}, ..., 1_{n_{21}}, 1_{n_{22}}, ..., 1_{n_{2m2}}, ..., 1_{n_{w1}}, 1_{n_{w2}}, ..., 1_{n_{wmw}}) : N \times k$ known indicator matrix for subplot factors

w : number of whole plots

m_i : number of subplots in i^{th} whole plot

n_{ij} : number of sub-subplots in j^{th} subplot of i^{th} whole plot

$n_i = \sum_{j=1}^{m_i} n_{ij}$: number of sub-subplots in i^{th} whole plot

n_w : number of sub-subplots within each whole plot for balanced case.

n_k : number of sub-subplots within each subplot for balanced case.

The forms of K_1 and K_2 in balanced case are chosen as following for the VKM method:

$$K_1 = \begin{bmatrix} n_w & 0 & 0 & q' & 0 & v1' & 0 \\ 0 & n_w I_D & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & n_w I_Q & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & V_{SQ} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & V_{SSQ} \end{bmatrix} \quad K_2 = \begin{bmatrix} n_k & 0 & 0 & 0 & 0 & v2' & 0 \\ 0 & n_k\ I_D & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & n_k\ I_Q & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & n_k\ I_{SD} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & n_k I_{SQ} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & G_{SSQ} \end{bmatrix}$$

$$\mathrm{XK_1}= \begin{bmatrix} n_w 1_{n_w} & n_w W_{D1} & n_w W_{Q1} & q' & S_{Q1} V_{SQ} & v1' & SSQ_1 V_{SSQ} \\ n_w 1_{n_w} & n_w W_{D2} & n_w W_{Q2} & q' & S_{Q2} V_{SQ} & v1' & SSQ_2 V_{SSQ} \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ n_w 1_{n_w} & n_w W_{Dwm_w} & n_w W_{Qwm_w} & q' & S_{Qm_w} V_{SQ} & v1' & SSQ_{m_w} V_{SSQ} \end{bmatrix}$$

$$\mathrm{M_1X}= \begin{bmatrix} 1_{n_w} 1_{n_w}' 1_{n_w} & 1_{n_w} 1_{n_w}' W_{D1} & 1_{n_w} 1_{n_w}' W_{Q1} & 1_{n_w} 1_{n_w}' S_{D1} & 1_{n_w} 1_{n_w}' S_{Q1} & 1_{n_w} 1_{n_w}' SS_{D1} & 1_{n_w} 1_{n_w}' SS_{Q1} \\ 1_{n_w} 1_{n_w}' 1_{n_w} & 1_{n_w} 1_{n_w}' W_{D2} & 1_{n_w} 1_{n_w}' W_{Q2} & 1_{n_w} 1_{n_w}' S_{D1} & 1_{n_w} 1_{n_w}' S_{Q1} & 1_{n_w} 1_{n_w}' SS_{D1} & 1_{n_w} 1_{n_w}' SS_{Q1} \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ 1_{n_w} 1_{n_w}' 1_{n_w} & 1_{n_w} 1_{n_w}' W_{Dw} & 1_{n_w} 1_{n_w}' W_{Qw} & 1_{n_w} 1_{n_w}' S_{Dw} & 1_{n_w} 1_{n_w}' S_{Qw} & 1_{n_w} 1_{n_w}' SS_{Dw} & 1_{n_w} 1_{n_w}' SS_{Qw} \end{bmatrix}$$

I state a few facts of an equivalent design for balanced designs for the VKM method as follows:

$$1_{n_w} 1_{n_w}' = n_w$$

$$1_{n_w}' W_{Di} = n_w\, W_{Di} \qquad \text{for } i = 1,2,...,w$$

$$1_{n_w}' W_{Qi} = n_w\, W_{Qi} \qquad \text{for } i = 1,2,...,w$$

$$S_{Di}' 1_{n_w} = q \qquad \text{for i} = 1,2,..., \text{w}$$

$$SS_{Di}' 1_{n_w} = v1 \qquad \text{for i} = 1,2,..., \text{w}$$

q and $v1$ are two constant vectors. $q = 0$ and $v1 = 0$ if the design is an orthogonal design.

$\mathrm{XK_1} = \mathrm{M_1X}$ if

$$S_{Qi}V_{SQ} = 1_{n_w}1_{n_w}{}'S_{Qi} \quad \text{for i} = 1,2,...,\text{w}$$

$$SS_{Q_i}V_{SSQ} = 1_{n_w}1_{n_w}{}'SS_{Q_i} \quad \text{for i} = 1,2,...,\text{w}$$

If the number of subplot factors is a power of two, the number of sub-subplot factors is a power of two, then

$$V_{SQ} = \frac{n_w}{b}(11')_b \,, V_{SSQ} = \frac{n_w}{l}(11')_l$$

If the number of subplot factors is not power of two, the number of sub-subplot factors is not a power of two, then

$$V_{SQ} = n_w I_b \,, V_{SSQ} = n_w I_l$$

Similarly,

$$XK_2 = \begin{bmatrix} n_k & n_k W_{D11} & n_k W_{Q11} & n_k S_{D11} & n_k S_{Q11} & v2' & SS_{D11}G_{SSQ} \\ n_k & n_k W_{D12} & n_k W_{Q12} & n_k S_{D12} & n_k S_{Q12} & v2 & SS_{Q12}G_{SSQ} \\ .. & . & . & . & . & . & 0 \\ .. & . & . & . & . & . & 0 \\ .. & . & . & . & . & . & 0 \\ .. & . & . & . & . & . & 0 \\ n_k & n_k W_{Dwm_w} & n_k W_{Qwm_w} & n_k S_{Dwm_w} & n_k S_{Qwm_w} & v2 & SS_{Qwm_w}G_{SSQ} \end{bmatrix}$$

$M_2X=$

$$\begin{bmatrix} 1_{11}1_{11}{}'1_{11} & 1_{11}1_{11}{}'W_{D11} & 1_{11}1_{11}{}'W_{Q11} & 1_{11}1_{11}{}'S_{D11} & 1_{11}1_{11}{}'S_{Q11} & 1_{11}1_{11}{}'SS_{D11} & 1_{11}1_{11}{}'SS_{Q11} \\ 1_{12}1_{12}{}'1_{12} & 1_{12}1_{12}{}'W_{D12} & 1_{12}1_{12}{}'W_{Q12} & 1_{12}1_{12}{}'S_{D12} & 1_{12}1_{12}{}'S_{Q12} & 1_{12}1_{12}{}'SS_{D12} & 1_{12}1_{12}{}'SS_{Q12} \\ . & . & . & . & . & . & . \\ 1_{1m1}1_{1m1}{}'1_{1m1} & 1_{1m1}1_{1m1}{}'W_{D1m1} & 1_{1m1}1_{1m1}{}'W_{Q1m1} & 1_{1m1}1_{1m1}{}'S_{D1m1} & 1_{1m1}1_{1m1}{}'S_{Q1m1} & 1_{1m1}1_{1m1}{}'SS_{D1m1} & 1_{1m1}1_{1m1}{}'SS_{Q1m1} \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ 1_{wmw}1_{wmw}{}'1_{wmw} & 1_{wmw}1_{wmw}{}'W_{Dwmw} & 1_{wmw}1_{wmw}{}'W_{Qwmw} & 1_{wmw}1_{wmw}{}'S_{Dwmw} & 1_{wmw}1_{wmw}{}'S_{Qwmw} & 1_{wmw}1_{wmw}{}'SS_{Dwmw} & 1_{wmw}1_{wmw}{}'SS_{Qwmw} \end{bmatrix}$$

I state a few facts of an equivalent design for balanced designs for the VKM method as follows:

$1_{ij}1_{ij}' = n_k \quad \text{for i} = 1,2,...,\text{w}; \quad \text{j} = 1,2,...,\text{m}_\text{w}$

$1_{ij}'W_{Dij} = n_k\, W_{Dij} \quad \text{for } i = 1,2,...,w; \quad \text{j} = 1,2,...,\text{m}_\text{w}$

$1_{ij}'W_{Qij} = n_k\, W_{Qij} \quad \text{for } i = 1,2,...,w; \quad \text{j} = 1,2,...,\text{m}_\text{w}$

$SS_{Dij}'1_k = v2 \quad \text{for i} = 1,2,...,\text{w}; \quad \text{j} = 1,2,...,\text{m}_\text{w}$

$XK_2 = M_2X$ if

$SS_{Q_{ij}}G_{SSQ} = 1_{n_k}1_{n_k}'SS_{Q_{ij}} \quad \text{for i} = 1,2,...,\text{w, j} = 1,2,...,\text{m}_\text{w}$

If number of sub-subplot factors is power of two, then

$$G_{SSQ} = \frac{n_k}{l}(11')_l$$

If number of sub-subplot factors is not power of two, then

$G_{SSQ} = n_k I_l$

$v2$ are two constant vectors. $v2 = 0$ if the design is an orthogonal design.

Regarding balanced case for the MWP method, I defined n_{nzf} as the number of nonzero factorial points within the whole plot at high level. n_{nzsa} is the number of nonzero subplot axial points within the whole plot at center points, n_{nzssa} is the number of nonzero sub-subplot axial points within the whole plot at center points.

I chose K_1 and K_2 as follows:

$$K_1 = \begin{bmatrix} n_w & 0 & 0 & q' & t_1' & v1 & t_0' \\ 0 & n_w I_D & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & n_w I_Q & 0 & M_{W1} & 0 & M_{W0} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \quad K_2 = \begin{bmatrix} n_k & 0 & 0 & 0 & 0 & v2 & 0 \\ 0 & n_k I_D & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & n_k I_Q & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & n_k\, I_{SD} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & n_k\, I_{SQ} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & M_{SSQ} \end{bmatrix}$$

In this case, they share the same facts as the balanced case for the VKM method except the following:

$$1_{n_w} t_1' + W_{Qi} M_{w1} = 1_{n_w} 1_{n_w}' S_{Qi} \quad \text{for } i = 1,2,\ldots, w$$

$$1_{n_w} t_0' + W_{Qi} M_{w0} = 1_{n_w} 1_{n_w}' SS_{Qi} \quad \text{for } i = 1,2,\ldots, w$$

$$SS_{Qij} M_{SSQ} = 1_{n_k} 1_{n_k}' SS_{Qij} \quad \text{for } j = 1,2,\ldots, m_w, \ i = 1,2,\ldots, w$$

In the whole plot with the VHTC factors at center points, we have:

If the number of subplot factor is power of two, then

$$1_{n_k}' S_{Qij} = \frac{n_{nzf}}{b} \phi^2 1_b' ,$$

If the number of subplot factor is not power of two, then

$$1_{n_k}' S_{Qij} = n_{nzf} \phi^2 1_b' ,$$

For the whole plots in a balanced CCD split-split-plot design, $W_{Qij} M_{w1}$, $W_{Qij} M_{w0}$ are vectors of 0. Therefore, if the number of subplot factors (sub-subplot factors) is power of two, then

$$t_1' = \frac{n_{nzf}}{b} \phi^2 1_b'$$

$$t_0' = \frac{n_k}{l} \gamma^2 1_l'$$

If the number of subplot factors is not power of two, the number of sub-subplot factors is not power of two, then

$$t_1' = n_{nzf} \phi^2 1_b'$$

$$t_0' = n_k \gamma^2 1_l'$$

Therefore,

If the number of subplot factor is power of two, the number of sub-subplot factor is power of two, then

$$M_{W1} = (n_{nzf} - \frac{\mathrm{n}_{\mathrm{nzf}}}{b}\phi^2)1_{\mathrm{b}}'$$

$$M_{W0} = (\mathrm{n}_{\mathrm{nzf}} - \frac{\mathrm{n}_{\mathrm{k}}}{l}\gamma^2)1_{\mathrm{l}}'$$

If the number of subplot factor is not power of two, the number of subplot factor is not power of two, then

$$\mathrm{M}_{\mathrm{W1}} = (\mathrm{n}_{\mathrm{nzf}} - \mathrm{n}_{\mathrm{nzf}}\phi^2)1_{\mathrm{b}}'$$

$$\mathrm{M}_{0} = (\mathrm{n}_{\mathrm{nzf}} - \mathrm{n}_{\mathrm{k}}\gamma^2)1_{\mathrm{l}}'$$

If the number of sub-subplot factor is not power of two, then

$$M_{SSQ} = \frac{n_k}{l} I_l$$

If the number of sub-subplot factor is not power of two, then

$$M_{SSQ} = n_k 1_l 1_l'$$

APPENDIX B

SIMULATION CODES

```
1. function
[AVE_BLUE,AVE_OLS,AVE_GLS,max_GLS,min_GLS,Ave_sigmaEPS,Ave_sigmaMU,Ave_
sigmaDELTA,Stdev_OLS,Stdev_GLS]=reff_unbalance(d,r1,r2,sim)
% X is complete model matrix
% d is number of whole-plot replicates
% m is number of subplots per whole plot
% n0 is number of sub-subplots per subplot
% Z1 is Nxw matrix (w=total number of whole plots)
% Z2 is Nxs matrix (s=total number of subplots)
% r1 is true ratio of wp to ssp variance
% r2 is true ratio of sp to ssp variance

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%center
points
nn=16;
mm=8;
m=2;
n0=8;
%rep=3
X = xlsread('C:\reeff.xls','CCD113NE','c2:w169');
MT=size(X);
N=MT(1);
Z1=blkdiag(ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(24,1),ones(nn,1),ones(
nn,1),ones(nn,1),ones(nn,1));
Z2=blkdiag(ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(m
m,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),one
s(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1));

%rep=4
%X = xlsread('C:\reeff.xls','CCD113NE','c2:w185');
%MT=size(X);
%N=MT(1);
%Z1=blkdiag(ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(24,1),ones(nn,1),one
s(nn,1),ones(nn,1),ones(nn,1),ones(nn,1));
%Z2=blkdiag(ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(
mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),o
nes(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,
1),ones(mm,1));

%rep=5
%X = xlsread('C:\reeff.xls','CCD113NE','c2:w201');
```

```
%MT=size(X);
%N=MT(1);
%Z1=blkdiag(ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(24,1),ones(nn,1),one
s(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1));
%Z2=blkdiag(ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(
mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),o
nes(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,
1),ones(mm,1));

%rep=6
%X = xlsread('C:\reeff.xls','CCD113NE','c2:w217');
%
%Z1=blkdiag(ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(24,1),ones(nn,1),one
s(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1));
%Z2=blkdiag(ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(
mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),o
nes(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,
1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1));
%varrat=pure_error_ssp(y,d,m,n0,M1,M2)

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%% factorial points
%rep=3
%X = xlsread('C:\reeff.xls','CCD111NE_FP','c2:l61');
%MT=size(X);
%N=MT(1);
%nn=4;
%mm=2;
%m=2;
%n0=2;
%Z1=blkdiag(ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),one
s(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1));
%Z2=blkdiag(ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(
mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),o
nes(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,
1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(
mm,1));
%varrat=pure_error_ssp(y,d,m,n0,M1,M2)

%rep=4
%X = xlsread('C:\reeff.xls','CCD111NE_FP','c2:l69');
```

```
%MT=size(X);
%N=MT(1);
%nn=4;
%mm=2;
%m=2;
%n0=2;
%%%% CCD111NE rep=4
%Z1=blkdiag(ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),one
s(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1)
,ones(nn,1));
%Z2=blkdiag(ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(
mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),o
nes(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,
1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(
mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1));

%rep=5
%X = xlsread('C:\reeff.xls','CCD111NE_FP','c2:l77');
%MT=size(X);
%N=MT(1);
%nn=4;
%mm=2;
%m=2;
%n0=2;
%%%% CCD111NE rep=5
%Z1=blkdiag(ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),one
s(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1)
,ones(nn,1),ones(nn,1),ones(nn,1));
%Z2=blkdiag(ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(
mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),o
nes(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,
1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(
mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),o
nes(mm,1));


for iii=1:sim
    DETERM(iii,:)=releff(X,d,m,n0,Z1,Z2,r1,r2);

end
```

```
AVE_DETERM=mean(DETERM);
AVE_OLS=AVE_DETERM(1);
AVE_GLS=AVE_DETERM(2);
AVE_BLUE=AVE_DETERM(3);
Ave_sigmaEPS=AVE_DETERM(4);
Ave_sigmaMU=AVE_DETERM(5);
Ave_sigmaDELTA=AVE_DETERM(6);
Stdev_OLS=std(DETERM(:,1));
Stdev_GLS=std(DETERM(:,2));
max_GLS=max(DETERM(:,2));
min_GLS=min(DETERM(:,2));
%
subplot(4,1,1);
hist(DETERM(:,2));xlabel('det GLS');title({'Figure 15: Distribution of simulation
observations';'(the CCD Near Equivalent design with 1VHTC, 1HTC and 3ETCs)'});
subplot(4,1,2);
hist(DETERM(:,4));xlabel('estimated sub-subplot error');
subplot(4,1,3);
hist(DETERM(:,5));xlabel('estimated subplot error');ylabel('Frequency');
subplot(4,1,4);
hist(DETERM(:,6));xlabel('estimated whole-plot error');
yita_OB=AVE_OLS/AVE_BLUE;
yita_GB=AVE_GLS/AVE_BLUE;
yita_OG=AVE_OLS/AVE_GLS;
yita=[yita_OB yita_GB yita_OG]'
```

2. function [Enorm,EV]=Departure(replicates)

```
% X is complete model matrix
% d is number of whole-plot replicates
% m is number of subplots per whole plot
% n0 is number of sub-subplots per subplot
% M1 is Nxw matrix (w=total number of whole plots)
% M2 is Nxs matrix (s=total number of subplots)
% r1 is true ratio of wp to ssp variance
% r2 is true ratio of sp to ssp variance

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%center points
nn=16;
mm=8;
m=2;
```

```
n0=8;
%rep=3
X = xlsread('C:\reeff.xls','CCD113NE','c2:w169');
MT=size(X);
N=MT(1);
M1=blkdiag(ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(24,1),ones(nn,1),ones(
nn,1),ones(nn,1),ones(nn,1));
M2=blkdiag(ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(m
m,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),one
s(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1));

%rep=4
%X = xlsread('C:\reeff.xls','CCD113NE','c2:w185');
%MT=size(X);
%N=MT(1);
%M1=blkdiag(ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(24,1),ones(nn,1),on
es(nn,1),ones(nn,1),ones(nn,1),ones(nn,1));
%M2=blkdiag(ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(
mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),o
nes(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,
1),ones(mm,1));

%rep=5
%X = xlsread('C:\reeff.xls','CCD113NE','c2:w201');
%MT=size(X);
%N=MT(1);
%
%M1=blkdiag(ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(24,1),ones(nn,1),on
es(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1));
%M2=blkdiag(ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(
mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),o
nes(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,
1),ones(mm,1),ones(mm,1),ones(mm,1));

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%% factorial points
%nn=4;
%mm=2;
%m=2;
%n0=2;
%rep=3
```

```
%X = xlsread('C:\reeff.xls','CCD111NE_FP','c2:l61');
%MT=size(X);
%N=MT(1);
%M1=blkdiag(ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),on
es(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1));
%M2=blkdiag(ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(
mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),o
nes(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,
1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(
mm,1));
%varrat=pure_error_ssp(y,d,m,n0,M1,M2)

%rep=4
%X = xlsread('C:\reeff.xls','CCD111NE_FP','c2:l69');
%MT=size(X);
%N=MT(1);
%M1=blkdiag(ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),on
es(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1
),ones(nn,1));
%M2=blkdiag(ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(
mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),o
nes(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,
1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(
mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1));


%rep=5
%X = xlsread('C:\reeff.xls','CCD111NE_FP','c2:l77');
%MT=size(X);
%N=MT(1);
%M1=blkdiag(ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),on
es(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1
),ones(nn,1),ones(nn,1),ones(nn,1));
%M2=blkdiag(ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(
mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),o
nes(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,
1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(
mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),o
nes(mm,1));

H=X*inv(X'*X)*X';
```

```
D1=(eye(N)-H)*M1*M1'*X;
D2=(eye(N)-H)*M2*M2'*X;

D=D1+D2;
EV=eig(D'*D);
Enorm=max(eig(D'*D));
```

3. function [Enorm,EV]=Departure_resolutionV(replicates)

```
% X is complete model matrix
% d is number of whole-plot replicates
% m is number of subplots per whole plot
% n0 is number of sub-subplots per subplot
% M1 is Nxw matrix (w=total number of whole plots)
% M2 is Nxs matrix (s=total number of subplots)
% r1 is true ratio of wp to ssp variance
% r2 is true ratio of sp to ssp variance

%X = xlsread('C:\Resolution V.xls','113','c2:w177');
%X = xlsread('C:\Resolution V.xls','113','c2:w209');
%X = xlsread('C:\Resolution V.xls','113','c2:w225');
%nn=16;
%mm=8;
%MT=size(X);
%N=MT(1);
%M1=blkdiag(ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1));
%M2=blkdiag(ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1));



%X = xlsread('C:\Resolution V.xls','122','c2:w177');
%X = xlsread('C:\Resolution V.xls','122','c2:w193');
%X = xlsread('C:\Resolution V.xls','122','c2:w209');
%nn=16;
%mm=4;
%MT=size(X);
%N=MT(1);
```

```
%M1=blkdiag(ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),on
es(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1));
%M2=blkdiag(ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(
mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),o
nes(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,
1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(
mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),o
nes(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,
1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(
mm,1),ones(mm,1),ones(mm,1));

%X = xlsread('C:\Resolution V.xls','131','c2:w177');
%X = xlsread('C:\Resolution V.xls','131','c2:w193');
%X = xlsread('C:\Resolution V.xls','131','c2:w209');
%nn=16;
%mm=2;
%MT=size(X);
%N=MT(1);
%M1=blkdiag(ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),on
es(nn,1),ones(nn,1),ones(nn,1),ones(nn,1));
%M2=blkdiag(ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(
mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),o
nes(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,
1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(
mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),o
nes(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,
1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(
mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),o
nes(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,
1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(
mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),o
nes(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1));

%X = xlsread('C:\Resolution V.xls','212','c2:w113');
%X = xlsread('C:\Resolution V.xls','212','c2:w121');rep=4
%X = xlsread('C:\Resolution V.xls','212','c2:w129');rep=5
%nn=8;
%mm=4;
%MT=size(X);
%N=MT(1);
%M1=blkdiag(ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),on
```

```
es(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1));
%M2=blkdiag(ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(
mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),o
nes(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,
1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1));

%X = xlsread('C:\Resolution V.xls','221','c2:w113');rep=3
%X = xlsread('C:\Resolution V.xls','221','c2:w121');rep=4
X = xlsread('C:\Resolution V.xls','221','c2:w129');
nn=8;
mm=2;
MT=size(X);
N=MT(1);
M1=blkdiag(ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(
nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1));
M2=blkdiag(ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(m
m,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),one
s(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),
ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(m
m,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),one
s(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),
ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(m
m,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),one
s(mm,1),ones(mm,1),ones(mm,1),ones(mm,1));

%X = xlsread('C:\Resolution V.xls','311','c2:w77');
%X = xlsread('C:\Resolution V.xls','311','c2:w81');
%nn=4;
%mm=2;
%MT=size(X);
%N=MT(1);
%M1=blkdiag(ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),on
es(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1
),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1));
%M2=blkdiag(ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(
mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),o
nes(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,
1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(
mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),o
nes(mm,1),ones(mm,1),ones(mm,1));
```

```
H=X*inv(X'*X)*X';

D1=(eye(N)-H)*M1*M1'*X;
D2=(eye(N)-H)*M2*M2'*X;

D=D1+D2;
EV=eig(D'*D);
Enorm=max(eig(D'*D));
```

4. function [Enorm,EV]=Departure_resolutionV(replicates)

```
% X is complete model matrix
% d is number of whole-plot replicates
% m is number of subplots per whole plot
% n0 is number of sub-subplots per subplot
% M1 is Nxw matrix (w=total number of whole plots)
% M2 is Nxs matrix (s=total number of subplots)
% r1 is true ratio of wp to ssp variance
% r2 is true ratio of sp to ssp variance

%X = xlsread('C:\Resolution V.xls','113','c2:w177');
%X = xlsread('C:\Resolution V.xls','113','c2:w209');
%X = xlsread('C:\Resolution V.xls','113','c2:w225');
%nn=16;
%mm=8;
%MT=size(X);
%N=MT(1);
%M1=blkdiag(ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1));
%M2=blkdiag(ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1));



%X = xlsread('C:\Resolution V.xls','122','c2:w177');
%X = xlsread('C:\Resolution V.xls','122','c2:w193');
%X = xlsread('C:\Resolution V.xls','122','c2:w209');
%nn=16;
%mm=4;
%MT=size(X);
```

```
%N=MT(1);
%M1=blkdiag(ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),on
es(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1));
%M2=blkdiag(ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(
mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),o
nes(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,
1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(
mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),o
nes(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,
1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(
mm,1),ones(mm,1),ones(mm,1));

%X = xlsread('C:\Resolution V.xls','131','c2:w177');
%X = xlsread('C:\Resolution V.xls','131','c2:w193');
%X = xlsread('C:\Resolution V.xls','131','c2:w209');
%nn=16;
%mm=2;
%MT=size(X);
%N=MT(1);
%M1=blkdiag(ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),on
es(nn,1),ones(nn,1),ones(nn,1),ones(nn,1));
%M2=blkdiag(ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(
mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),o
nes(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,
1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(
mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),o
nes(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,
1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(
mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),o
nes(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,
1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(
mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),o
nes(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1));

%X = xlsread('C:\Resolution V.xls','212','c2:w113');
%X = xlsread('C:\Resolution V.xls','212','c2:w121');rep=4
%X = xlsread('C:\Resolution V.xls','212','c2:w129');rep=5
%nn=8;
%mm=4;
%MT=size(X);
%N=MT(1);
```

```
%M1=blkdiag(ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),on
es(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1));
%M2=blkdiag(ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(
mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),o
nes(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,
1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1));

%X = xlsread('C:\Resolution V.xls','221','c2:w113');rep=3
%X = xlsread('C:\Resolution V.xls','221','c2:w121');rep=4
X = xlsread('C:\Resolution V.xls','221','c2:w129');
nn=8;
mm=2;
MT=size(X);
N=MT(1);
M1=blkdiag(ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(
nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1));
M2=blkdiag(ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(m
m,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),one
s(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),
ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(m
m,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),one
s(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),
ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(m
m,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),one
s(mm,1),ones(mm,1),ones(mm,1),ones(mm,1));

%X = xlsread('C:\Resolution V.xls','311','c2:w77');
%X = xlsread('C:\Resolution V.xls','311','c2:w81');
%nn=4;
%mm=2;
%MT=size(X);
%N=MT(1);
%M1=blkdiag(ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),on
es(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1
),ones(nn,1),ones(nn,1),ones(nn,1),ones(nn,1));
%M2=blkdiag(ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(
mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),o
nes(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,
1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(
mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),ones(mm,1),o
nes(mm,1),ones(mm,1),ones(mm,1));
```

```
H=X*inv(X'*X)*X';

D1=(eye(N)-H)*M1*M1'*X;
D2=(eye(N)-H)*M2*M2'*X;

D=D1+D2;
EV=eig(D'*D);
Enorm=max(eig(D'*D));
```

5. function figure5_1

```
X = xlsread('C:\Dissertation tables.xls','Table 18','a4:h28');
r1=X(:,1);
r2=X(:,2);
OB3=X(:,3);
GB3=X(:,4);
OB4=X(:,5);
GB4=X(:,6);
OB5=X(:,7);
GB5=X(:,8);

hold on;
subplot(2,1,1);
plot(r2(1:5),OB3(1:5),'--r+',r2(6:10),OB3(6:10),'-bo',r2(11:15),OB3(11:15),':g*',r2(16:20),OB3(1
6:20),'-.y.',r2(21:25),OB3(21:25),'-mx');
legend('r1=0.5','r1=1','r1=2','r1=5','r1=10');title({'Figure 3: Relative efficiency for
Near-Equivalent CCD with 1VTHC,1HTC,3ETCs';'Replicates=3 holding r1
constant'});xlabel('r2');ylabel('\eta |OLS|/|BLUE|');
subplot(2,1,2);
plot(r2(1:5),GB3(1:5),'--r+',r2(6:10),GB3(6:10),'-bo',r2(11:15),GB3(11:15),':g*',r2(16:20),GB3(1
6:20),'-.y.',r2(21:25),GB3(21:25),'-mx');
legend('r1=0.5','r1=1','r1=2','r1=5','r1=10');xlabel('r2');ylabel('\eta |GLS|/|BLUE|');
hold off;
```

6. function figure5_2

```
X = xlsread('C:\Dissertation tables.xls','Table 18','a4:h28');
r1=X(:,1);
r2=X(:,2);
OB3=X(:,3);
GB3=X(:,4);
OB4=X(:,5);
```

```
GB4=X(:,6);
OB5=X(:,7);
GB5=X(:,8);
xx=[0.5,1,2,5,10];
yy1=[OB3(1),OB3(6),OB3(11),OB3(16),OB3(21)];
yy2=[OB3(2),OB3(7),OB3(12),OB3(17),OB3(22)];
yy3=[OB3(3),OB3(8),OB3(13),OB3(18),OB3(23)];
yy4=[OB3(4),OB3(9),OB3(14),OB3(19),OB3(24)];
yy5=[OB3(5),OB3(10),OB3(15),OB3(20),OB3(25)];
yyy1=[GB3(1),GB3(6),GB3(11),GB3(16),GB3(21)];
yyy2=[GB3(2),GB3(7),GB3(12),GB3(17),GB3(22)];
yyy3=[GB3(3),GB3(8),GB3(13),GB3(18),GB3(23)];
yyy4=[GB3(4),GB3(9),GB3(14),GB3(19),GB3(24)];
yyy5=[GB3(5),GB3(10),GB3(15),GB3(20),GB3(25)];
hold on;
subplot(2,1,1);
plot(xx,yy1,'--r+',xx,yy2,'-bo',xx,yy3,':g*',xx,yy4,'-.y.',xx,yy5,'-mx');
legend('r2=0.5','r2=1','r2=2','r2=5','r2=10');title({'Figure 4: Relative efficiency for
Near-Equivalent CCD with 1VTHC,1HTC,3ETCs';' Replicates=3 holding r2
constant'});xlabel('r1');ylabel('\eta |OLS|/|BLUE|');
subplot(2,1,2);
plot(xx,yyy1,'--r+',xx,yyy2,'-bo',xx,yyy3',':g*',xx,yyy4,'-.y.',xx,yyy5,'-mx');
legend('r2=0.5','r2=1','r2=2','r2=5','r2=10');xlabel('r1');ylabel('\eta |GLS|/|BLUE|');
hold off;
```

7．function figure5_3

```
X = xlsread('C:\Dissertation tables.xls','Table 18','a4:h28');
r1=X(:,1);
r2=X(:,2);
OB3=X(:,3);
GB3=X(:,4);
OB4=X(:,5);
GB4=X(:,6);
OB5=X(:,7);
GB5=X(:,8);

hold on;
subplot(2,1,1);
plot(r2(1:5),OB3(1:5),'--r+',r2(6:10),OB3(6:10),'-bo',r2(11:15),OB3(11:15),':g*',r2(16:20),OB3(1
6:20),'-.y.',r2(21:25),OB3(21:25),'-mx');
legend('r1=0.5','r1=1','r1=2','r1=5','r1=10');title({'Figure 5: Relative efficiency for
Near-Equivalent CCD with 1VTHC,1HTC,3ETCs';'Replicates=4 holding r1
```

```
constant'});xlabel('r2');ylabel('\eta |OLS|/|BLUE|');
subplot(2,1,2);
plot(r2(1:5),GB3(1:5),'--r+',r2(6:10),GB3(6:10),'-bo',r2(11:15),GB3(11:15),':g*',r2(16:20),GB3(1
6:20),'-.y.',r2(21:25),GB3(21:25),'-mx');
legend('r1=0.5','r1=1','r1=2','r1=5','r1=10');xlabel('r2');ylabel('\eta |GLS|/|BLUE|');
hold off;
```

8． function figure5_4

```
X = xlsread('C:\Dissertation tables.xls','Table 18','a4:h28');
r1=X(:,1);
r2=X(:,2);
OB3=X(:,3);
GB3=X(:,4);
OB4=X(:,5);
GB4=X(:,6);
OB5=X(:,7);
GB5=X(:,8);
xx=[0.5,1,2,5,10];
yy1=[OB4(1),OB4(6),OB4(11),OB4(16),OB4(21)];
yy2=[OB4(2),OB4(7),OB4(12),OB4(17),OB4(22)];
yy3=[OB4(3),OB4(8),OB4(13),OB4(18),OB4(23)];
yy4=[OB4(4),OB4(9),OB4(14),OB4(19),OB4(24)];
yy5=[OB4(5),OB4(10),OB4(15),OB4(20),OB4(25)];
yyy1=[GB4(1),GB4(6),GB4(11),GB4(16),GB4(21)];
yyy2=[GB4(2),GB4(7),GB4(12),GB4(17),GB4(22)];
yyy3=[GB4(3),GB4(8),GB4(13),GB4(18),GB4(23)];
yyy4=[GB4(4),GB4(9),GB4(14),GB4(19),GB4(24)];
yyy5=[GB4(5),GB4(10),GB4(15),GB4(20),GB4(25)];
hold on;
subplot(2,1,1);
plot(xx,yy1,'--r+',xx,yy2,'-bo',xx,yy3,':g*',xx,yy4,'-.y.',xx,yy5,'-mx');
legend('r2=0.5','r2=1','r2=2','r2=5','r2=10');title({'Figure 6: Relative efficiency for
Near-Equivalent CCD with 1VTHC,1HTC,3ETCs';' Replicates=4 holding r2
constant'});xlabel('r1');ylabel('\eta |OLS|/|BLUE|');
subplot(2,1,2);
plot(xx,yyy1,'--r+',xx,yyy2,'-bo',xx,yyy3',':g*',xx,yyy4,'-.y.',xx,yyy5,'-mx');
legend('r2=0.5','r2=1','r2=2','r2=5','r2=10');xlabel('r1');ylabel('\eta |GLS|/|BLUE|');
hold off;
```

9． function figure5_5

```
X = xlsread('C:\Dissertation tables.xls','Table 18','a4:h28');
```

```
r1=X(:,1);
r2=X(:,2);
OB3=X(:,3);
GB3=X(:,4);
OB4=X(:,5);
GB4=X(:,6);
OB5=X(:,7);
GB5=X(:,8);

hold on;
subplot(2,1,1);
plot(r2(1:5),OB3(1:5),'--r+',r2(6:10),OB3(6:10),'-bo',r2(11:15),OB3(11:15),':g*',r2(16:20),OB3(1
6:20),'-.y.',r2(21:25),OB3(21:25),'-mx');
legend('r1=0.5','r1=1','r1=2','r1=5','r1=10');title({'Figure 7: Relative efficiency for
Near-Equivalent CCD with 1VTHC,1HTC,3ETCs';'Replicates=5 holding r1
constant'});xlabel('r2');ylabel('\eta |OLS|/|BLUE|');
subplot(2,1,2);
plot(r2(1:5),GB3(1:5),'--r+',r2(6:10),GB3(6:10),'-bo',r2(11:15),GB3(11:15),':g*',r2(16:20),GB3(1
6:20),'-.y.',r2(21:25),GB3(21:25),'-mx');
legend('r1=0.5','r1=1','r1=2','r1=5','r1=10');xlabel('r2');ylabel('\eta |GLS|/|BLUE|');
hold off;
```

10． function figure5_6

```
X = xlsread('C:\Dissertation tables.xls','Table 18','a4:h28');
r1=X(:,1);
r2=X(:,2);
OB3=X(:,3);
GB3=X(:,4);
OB4=X(:,5);
GB4=X(:,6);
OB5=X(:,7);
GB5=X(:,8);
xx=[0.5,1,2,5,10];
yy1=[OB5(1),OB5(6),OB5(11),OB5(16),OB5(21)];
yy2=[OB5(2),OB5(7),OB5(12),OB5(17),OB5(22)];
yy3=[OB5(3),OB5(8),OB5(13),OB5(18),OB5(23)];
yy4=[OB5(4),OB5(9),OB5(14),OB5(19),OB5(24)];
yy5=[OB5(5),OB5(10),OB5(15),OB5(20),OB5(25)];
yyy1=[GB5(1),GB5(6),GB5(11),GB5(16),GB5(21)];
yyy2=[GB5(2),GB5(7),GB5(12),GB5(17),GB5(22)];
yyy3=[GB5(3),GB5(8),GB5(13),GB5(18),GB5(23)];
```

```
yyy4=[GB5(4),GB5(9),GB5(14),GB5(19),GB5(24)];
yyy5=[GB5(5),GB5(10),GB5(15),GB5(20),GB5(25)];
hold on;
subplot(2,1,1);
plot(xx,yy1,'--r+',xx,yy2,'-bo',xx,yy3,':g*',xx,yy4,'-.y.',xx,yy5,'-mx');
legend('r2=0.5','r2=1','r2=2','r2=5','r2=10');title({'Figure 8: Relative efficiency for
Near-Equivalent CCD with 1VTHC,1HTC,3ETCs';' Replicates=5 holding r2
constant'});xlabel('r1');ylabel('\eta |OLS|/|BLUE|');
subplot(2,1,2);
plot(xx,yyy1,'--r+',xx,yyy2,'-bo',xx,yyy3',':g*',xx,yyy4,'-.y.',xx,yyy5,'-mx');
legend('r2=0.5','r2=1','r2=2','r2=5','r2=10');xlabel('r1');ylabel('\eta |GLS|/|BLUE|');
hold off;
```

11． function figure5_7

```
X = xlsread('C:\Dissertation tables.xls','Table 19','a4:h28');
r1=X(:,1);
r2=X(:,2);
OB3=X(:,3);
GB3=X(:,4);
OB4=X(:,5);
GB4=X(:,6);
OB5=X(:,7);
GB5=X(:,8);

hold on;
subplot(2,1,1);
plot(r2(1:5),OB3(1:5),'--r+',r2(6:10),OB3(6:10),'-bo',r2(11:15),OB3(11:15),':g*',r2(16:20),OB3(1
6:20),'-.y.',r2(21:25),OB3(21:25),'-mx');
legend('r1=0.5','r1=1','r1=2','r1=5','r1=10');title({'Figure 9: Relative efficiency for
Near-Equivalent CCD with 1VTHC,1HTC,1ETC';'Replicates=3 holding r1
constant'});xlabel('r2');ylabel('\eta |OLS|/|BLUE|');
subplot(2,1,2);
plot(r2(1:5),GB3(1:5),'--r+',r2(6:10),GB3(6:10),'-bo',r2(11:15),GB3(11:15),':g*',r2(16:20),GB3(1
6:20),'-.y.',r2(21:25),GB3(21:25),'-mx');
legend('r1=0.5','r1=1','r1=2','r1=5','r1=10');xlabel('r2');ylabel('\eta |GLS|/|BLUE|');
hold off;
```

12． function figure5_8

```
X = xlsread('C:\Dissertation tables.xls','Table 19','a4:h28');
r1=X(:,1);
r2=X(:,2);
```

```
OB3=X(:,3);
GB3=X(:,4);
OB4=X(:,5);
GB4=X(:,6);
OB5=X(:,7);
GB5=X(:,7);
xx=[0.5,1,2,5,10];
yy1=[OB3(1),OB3(6),OB3(11),OB3(16),OB3(21)];
yy2=[OB3(2),OB3(7),OB3(12),OB3(17),OB3(22)];
yy3=[OB3(3),OB3(8),OB3(13),OB3(18),OB3(23)];
yy4=[OB3(4),OB3(9),OB3(14),OB3(19),OB3(24)];
yy5=[OB3(5),OB3(10),OB3(15),OB3(20),OB3(25)];
yyy1=[GB3(1),GB3(6),GB3(11),GB3(16),GB3(21)];
yyy2=[GB3(2),GB3(7),GB3(12),GB3(17),GB3(22)];
yyy3=[GB3(3),GB3(8),GB3(13),GB3(18),GB3(23)];
yyy4=[GB3(4),GB3(9),GB3(14),GB3(19),GB3(24)];
yyy5=[GB3(5),GB3(10),GB3(15),GB3(20),GB3(25)];
hold on;
subplot(2,1,1);
plot(xx,yy1,'--r+',xx,yy2,'-bo',xx,yy3,':g*',xx,yy4,'-.y.',xx,yy5,'-mx');
legend('r2=0.5','r2=1','r2=2','r2=5','r2=10');title({'Figure 10: Relative efficiency for
Near-Equivalent CCD with 1VTHC,1HTC,1ETC';' Replicates=3 holding r2
constant'});xlabel('r1');ylabel('\eta |OLS|/|BLUE|');
subplot(2,1,2);
plot(xx,yyy1,'--r+',xx,yyy2,'-bo',xx,yyy3',':g*',xx,yyy4,'-.y.',xx,yyy5,'-mx');
legend('r2=0.5','r2=1','r2=2','r2=5','r2=10');xlabel('r1');ylabel('\eta |GLS|/|BLUE|');
hold off;
```

13． function figure5_9

```
X = xlsread('C:\Dissertation tables.xls','Table 19','a4:h28');
r1=X(:,1);
r2=X(:,2);
OB3=X(:,3);
GB3=X(:,4);
OB4=X(:,5);
GB4=X(:,6);
OB5=X(:,7);
GB5=X(:,7);

hold on;
subplot(2,1,1);
```

```
plot(r2(1:5),OB3(1:5),'--r+',r2(6:10),OB3(6:10),'-bo',r2(11:15),OB3(11:15),':g*',r2(16:20),OB3(1
6:20),'-.y.',r2(21:25),OB3(21:25),'-mx');
legend('r1=0.5','r1=1','r1=2','r1=5','r1=10');title({'Figure 11: Relative efficiency for
Near-Equivalent CCD with 1VTHC,1HTC,1ETC';'Replicates=4 holding r1
constant'});xlabel('r2');ylabel('\eta |OLS|/|BLUE|');
subplot(2,1,2);
plot(r2(1:5),GB3(1:5),'--r+',r2(6:10),GB3(6:10),'-bo',r2(11:15),GB3(11:15),':g*',r2(16:20),GB3(1
6:20),'-.y.',r2(21:25),GB3(21:25),'-mx');
legend('r1=0.5','r1=1','r1=2','r1=5','r1=10');xlabel('r2');ylabel('\eta |GLS|/|BLUE|');
hold off;
```

14． function figure5_10

```
X = xlsread('C:\Dissertation tables.xls','Table 19','a4:h28');
r1=X(:,1);
r2=X(:,2);
OB3=X(:,3);
GB3=X(:,4);
OB4=X(:,5);
GB4=X(:,6);
OB5=X(:,7);
GB5=X(:,7);
xx=[0.5,1,2,5,10];
yy1=[OB4(1),OB4(6),OB4(11),OB4(16),OB4(21)];
yy2=[OB4(2),OB4(7),OB4(12),OB4(17),OB4(22)];
yy3=[OB4(3),OB4(8),OB4(13),OB4(18),OB4(23)];
yy4=[OB4(4),OB4(9),OB4(14),OB4(19),OB4(24)];
yy5=[OB4(5),OB4(10),OB4(15),OB4(20),OB4(25)];
yyy1=[GB4(1),GB4(6),GB4(11),GB4(16),GB4(21)];
yyy2=[GB4(2),GB4(7),GB4(12),GB4(17),GB4(22)];
yyy3=[GB4(3),GB4(8),GB4(13),GB4(18),GB4(23)];
yyy4=[GB4(4),GB4(9),GB4(14),GB4(19),GB4(24)];
yyy5=[GB4(5),GB4(10),GB4(15),GB4(20),GB4(25)];
hold on;
subplot(2,1,1);
plot(xx,yy1,'--r+',xx,yy2,'-bo',xx,yy3,':g*',xx,yy4,'-.y.',xx,yy5,'-mx');
legend('r2=0.5','r2=1','r2=2','r2=5','r2=10');title({'Figure 12: Relative efficiency for
Near-Equivalent CCD with 1VTHC,1HTC,1ETC';' Replicates=4 holding r2
constant'});xlabel('r1');ylabel('\eta |OLS|/|BLUE|');
subplot(2,1,2);
plot(xx,yyy1,'--r+',xx,yyy2,'-bo',xx,yyy3',':g*',xx,yyy4,'-.y.',xx,yyy5,'-mx');
legend('r2=0.5','r2=1','r2=2','r2=5','r2=10');xlabel('r1');ylabel('\eta |GLS|/|BLUE|');
```

```
hold off;

15. function figure5_11
X = xlsread('C:\Dissertation tables.xls','Table 19','a4:h28');
r1=X(:,1);
r2=X(:,2);
OB3=X(:,3);
GB3=X(:,4);
OB4=X(:,5);
GB4=X(:,6);
OB5=X(:,7);
GB5=X(:,8);

hold on;
subplot(2,1,1);
plot(r2(1:5),OB3(1:5),'--r+',r2(6:10),OB3(6:10),'-bo',r2(11:15),OB3(11:15),':g*',r2(16:20),OB3(1
6:20),'-.y.',r2(21:25),OB3(21:25),'-mx');
legend('r1=0.5','r1=1','r1=2','r1=5','r1=10');title({'Figure 13: Relative efficiency for
Near-Equivalent CCD with 1VTHC,1HTC,1ETC';'Replicates=5 holding r1
constant'});xlabel('r2');ylabel('\eta |OLS|/|BLUE|');
subplot(2,1,2);
plot(r2(1:5),GB3(1:5),'--r+',r2(6:10),GB3(6:10),'-bo',r2(11:15),GB3(11:15),':g*',r2(16:20),GB3(1
6:20),'-.y.',r2(21:25),GB3(21:25),'-mx');
legend('r1=0.5','r1=1','r1=2','r1=5','r1=10');xlabel('r2');ylabel('\eta |GLS|/|BLUE|');
hold off;

16. function figure5_12
X = xlsread('C:\Dissertation tables.xls','Table 19','a4:h28');
r1=X(:,1);
r2=X(:,2);
OB3=X(:,3);
GB3=X(:,4);
OB4=X(:,5);
GB4=X(:,6);
OB5=X(:,7);
GB5=X(:,8);
xx=[0.5,1,2,5,10];
yy1=[OB5(1),OB5(6),OB5(11),OB5(16),OB5(21)];
yy2=[OB5(2),OB5(7),OB5(12),OB5(17),OB5(22)];
yy3=[OB5(3),OB5(8),OB5(13),OB5(18),OB5(23)];
yy4=[OB5(4),OB5(9),OB5(14),OB5(19),OB5(24)];
```

```
yy5=[OB5(5),OB5(10),OB5(15),OB5(20),OB5(25)];
yyy1=[GB5(1),GB5(6),GB5(11),GB5(16),GB5(21)];
yyy2=[GB5(2),GB5(7),GB5(12),GB5(17),GB5(22)];
yyy3=[GB5(3),GB5(8),GB5(13),GB5(18),GB5(23)];
yyy4=[GB5(4),GB5(9),GB5(14),GB5(19),GB5(24)];
yyy5=[GB5(5),GB5(10),GB5(15),GB5(20),GB5(25)];
hold on;
subplot(2,1,1);
plot(xx,yy1,'--r+',xx,yy2,'-bo',xx,yy3,':g*',xx,yy4,'-.y.',xx,yy5,'-mx');
legend('r2=0.5','r2=1','r2=2','r2=5','r2=10');title({'Figure 14: Relative efficiency for
Near-Equivalent CCD with 1VTHC,1HTC,1ETC';'Replicates=5 holding r2
constant'});xlabel('r1');ylabel('\eta |OLS|/|BLUE|');
subplot(2,1,2);
plot(xx,yyy1,'--r+',xx,yyy2,'-bo',xx,yyy3',':g*',xx,yyy4,'-.y.',xx,yyy5,'-mx');
legend('r2=0.5','r2=1','r2=2','r2=5','r2=10');xlabel('r1');ylabel('\eta |GLS|/|BLUE|');
hold off;
```