Graph Decompositions and Variance Balanced Block Designs of Experiments

by

Meixin Liu
B.Sc., University of Victoria, 2017

A Thesis Submitted in Partial Fulfillment of the
Requirements for the Degree of

MASTER OF SCIENCE

in the Department of Mathematics and Statistics

© Meixin Liu, 2019
University of Victoria

All rights reserved. This thesis may not be reproduced in whole or in part, by photocopying or other means, without the permission of the author.

Graph Decompositions and Variance Balanced Block Designs of Experiments

by

Meixin Liu

B.Sc., University of Victoria, 2017

Supervisory Committee

Dr. Peter Dukes, Co-Supervisor

(Department of Mathematics and Statistics)

Dr. Julie Zhou, Co-Supervisor

(Department of Mathematics and Statistics)

ABSTRACT

We study construction methods for variance balanced design (VBD) with both uncorrelated and correlated errors, where block designs are used to investigate several treatment effects. We begin with a review for the development of VBDs when the errors in the linear effects model are uncorrelated. There are several construction methods of VBDs for equal and unequal block sizes. When the errors are correlated, we introduce graph theory to study construction methods of VBDs. We develop new methods via graph decomposition. In addition, we construct block designs such that the covariance matrix of the least squares estimator of treatment effects is completely symmetric. Various applications are presented for certain specific error covariance matrices.

Contents

List of Tables

List of Figures

List of Abbreviations and Variables

BIBD	Balanced Incomplete Block Design
GDD	Group Divisible Design
PBD	Pairwise Balanced Design
PBIBD	Partially Balanced Incomplete Design
RCBD	Randomized Complete Block Design
VBD	Variance Balanced Block Design

$\boldsymbol{\epsilon}$	error vector
$\hat{\boldsymbol{\theta}}$	least squares estimator of treatment effect
$\boldsymbol{\theta}$	treatment effect vector
$\boldsymbol{C}$	information matrix
$\boldsymbol{I}_v$	$v \times v$ identity matrix
$\boldsymbol{J}_{v,v}$	$v \times v$ matrix with all entries equal to 1

$\boldsymbol{N}$	incidence matrix
$\boldsymbol{X}$	design matrix
λ	total number of times each pair of treatments appears in the same block
$\mathcal{B}$	collection of blocks
$\mathcal{G}$	collection of groups
σ^2	variance of error
b	number of blocks
B_j	j^{th} block
c	constant
E	edge set
K	set of block sizes
k	block size
K_v	complete graph on v vertices
K_v^λ	λ-complete multigraph on v vertices
r	replication of treatment
V	vertex set
v	number of treatments
X	treatment set

ACKNOWLEDGEMENTS

I would like to thank:

My supervisors, Professors Peter Dukes and Julie Zhou, for persistent help through my master. The work in this thesis could not have been completed without your guidance, support, encouragement, and patience. The past two years have been a period of learning and building, I benefited a lot.

My family, for the endless love and moral support from my mother. I can not express how important it was to have your support and belief. I can not thank you enough.

My Friends, for all the unforgettable recollection we had together. You collectively have made my Masters a wonderfully experience being there whenever I needed someone to accompany.

The University of Victoria, for the beautiful, comfortable, homelike studying environment.

Chapter 1

Introduction

Experimental design is an essential tool in technology commercialization and product realization process. Since the results drawn from the experiment greatly depend on the method of data collection, a well-designed experiment is significantly important. The use of experimental design can substantially reduce development time and cost, greatly contribute on less variability, and enhance reliability (Montgomery, 2012). In some experiments, there are factors that may affect the results, but we are not interested in those factors and they are called nuisance factors. Randomization and blocking are design techniques to guard against such nuisance factors (Montgomery, 2012). Randomized complete block design (RCBD), where each block contains all the treatments, is widely used in industrial experiments. However, due to shortages of experimental equipment or constraints on block size, having all treatments in each block is not always possible. As a result, we use incomplete block design, where each block does not contain all the treatments. If randomized techniques are used, these designs are known as randomized incomplete block designs. If the number of times each pairs of treatments occur together within a block across the design is constant, then the design is called balanced incomplete block design (BIBD) (Montgomery, 2012). For a BIBD, it can be denoted by BIBD($v,\ r,\ k,\ b,\ \lambda$), where parameter v is the number of treatments, b denotes the number of blocks, λ is total number of times each pair of treatments appears in the same block, k stands for block size, and r

represents replication of each treatment. For a BIBD($v,\ r,\ k,\ b,\ \lambda$), the parameters satisfy that $vr = bk$ and $\lambda(v-1) = r(k-1)$. If $\lambda = \frac{r(k-1)}{(v-1)}$ is not an integer, then there does not exist BIBD($v,\ r,\ k,\ b,\ \lambda$) for this experiment. Since usually comparisons of each pair of treatments are equally important, we assume that the different treatment contrasts have the same variance. Thus, variance balanced has been introduced. Rao (1958), Raghavarao (1971) and Hedayat and Federer (1974) stated that a design such that all elementary contrasts in the treatment effects, which involving all the differences of the form $\theta_i - \theta_j$ for $i \neq j$, that are estimable with the same precision, is defined as variance balanced design (VBD). Here θ_i is the i^{th} treatment effect for $i = 1, 2, \ldots, v$. Among designs such that all elementary treatment contrasts are estimable (*connected design*), VBD has highest efficiency (Raghavarao, 1971).

It is known that BIBD is both variance balanced and pairwise balanced, and those two concepts are equivalent when block sizes are all equal (Hedayat and Stufken, 1989). Though we usually assume that all blocks are of the same size, designs with unequal block sizes are likely necessary in practical experiments in many fields including agriculture and biology. Experiments with unequal block sizes in biological problems were first examined by Pearce (1964). In addition, Kageyama (1976) also pointed out that block designs with unequal block sizes are getting useful in large experiments as the development of high speed computers (Gupta and Jones, 1983). Many theoretical results have been derived for those VBDs. Hedayat and Stufken (1989) found a construction method from pairwise balanced designs (PBDs) to VBDs with unequal block sizes. Gupta and Jones (1983) discussed the construction of VBDs with equal repilcates of each treatment (i.e. equirepliacted) from group divisible designs (GDDs).

In the following we provide details for the statistical model for block designs, and the research problems for this thesis.

1.1 Statistical Model for Block Design

The statistical model for a block design with fixed effects can be written as (Montgomery, 2012),

$$y_{ij} = \theta_i + \beta_j + \epsilon_{ij}, \quad i = 1, \ldots, v, \quad j = 1, \ldots, b, \tag{1.1}$$

where y_{ij} is the observed response of treatment i in block j, θ_i is the mean of the i^{th} treatment effect and β_j is the j^{th} block effect. Block effects satisfy $\sum_{j=1}^{b} \beta_j = 0$ so that model (1.1) is uniquely specified. The random errors ϵ_{ij} are uncorrelated with with mean zero and variance σ^2. Model (1.1) can also be written in matrix form as

$$\boldsymbol{y} = \boldsymbol{X}_1\boldsymbol{\theta} + \boldsymbol{X}_2\boldsymbol{\beta} + \boldsymbol{\epsilon},$$

where $\boldsymbol{y}^\top = (\bar{\boldsymbol{y}}_1^\top, \ldots, \bar{\boldsymbol{y}}_b^\top)$ with $\bar{\boldsymbol{y}}_j^\top$ being the vector containing all the observations in block j, $\boldsymbol{\theta}^\top = (\theta_1, \ldots, \theta_v)$, $\boldsymbol{\beta}^\top = (\beta_1, \ldots, \beta_b)$ and $\boldsymbol{X} = [\boldsymbol{X}_1|\boldsymbol{X}_2]$ is design matrix. Denote $\boldsymbol{N} = [n_{ij}]_{v\times b}$ to be an incidence matrix for a block design, which shows the relationship between treatments and blocks, and the entry in row i and column j is 1 if treatment i is in block j and 0 otherwise. Note that $\boldsymbol{N} = \boldsymbol{X}_1^\top \boldsymbol{X}_2$.

We use the least squares estimator (LSE) $\hat{\boldsymbol{\theta}}$ to estimate $\boldsymbol{\theta}$ by minimizing the sum of squared residuals, subject to $\sum_{j=1}^{b} \beta_j = 0$. Note that the regression gives information on block effect as well as treatment effect, but we are primarily interested in treatment effect. For model (1.1), we get

$$\hat{\boldsymbol{\theta}} = \boldsymbol{A}^{-1}\boldsymbol{B}\boldsymbol{y}, \tag{1.2}$$

where

$$\boldsymbol{A} = \boldsymbol{X}_1^\top \boldsymbol{X}_1 - \boldsymbol{N}(\boldsymbol{X}_2^\top \boldsymbol{X}_2)^{-1}\boldsymbol{N}^\top + \frac{1}{a}\boldsymbol{N}(\boldsymbol{X}_2^\top \boldsymbol{X}_2)^{-1}\mathbf{1}_b\mathbf{1}_b^\top(\boldsymbol{X}_2^\top \boldsymbol{X}_2)^{-1}\boldsymbol{N}^\top, \tag{1.3}$$

$$\boldsymbol{B} = \boldsymbol{X}_1^\top - \boldsymbol{N}(\boldsymbol{X}_2^\top \boldsymbol{X}_2)^{-1}\boldsymbol{X}_2^\top + \frac{1}{a}\boldsymbol{N}(\boldsymbol{X}_2^\top \boldsymbol{X}_2)^{-1}\mathbf{1}_b\mathbf{1}_b^\top(\boldsymbol{X}_2^\top \boldsymbol{X}_2)^{-1}\boldsymbol{X}_2^\top, \tag{1.4}$$

$a = \mathbf{1}_b^\top(\boldsymbol{X}_2^\top \boldsymbol{X}_2)^{-1}\mathbf{1}_b$, $\mathbf{1}_b$ is the vector of ones in $\mathbb{R}^b$.

Then the covariance matrix of $\hat{\boldsymbol{\theta}}$ is given by

$$\mathrm{Cov}(\hat{\boldsymbol{\theta}}) = \sigma^2\boldsymbol{A}^{-1}. \tag{1.5}$$

The random error terms are further assumed to be correlated. We assume that errors are correlated within block, and there is no correlation between the blocks. Thus, $\mathrm{Cov}(\boldsymbol{\epsilon}) = \sigma^2 \boldsymbol{V}$, where $\boldsymbol{V}$ is block diagonal matrix. When each block has the same correlated error structure, $\mathrm{Cov}(\boldsymbol{\epsilon}) = \sigma^2(\boldsymbol{V}_o \oplus \boldsymbol{V}_o \oplus \ldots \oplus \boldsymbol{V}_o)$, where $\sigma^2 \boldsymbol{V}_o$ is the covariance of the errors within block, and $\oplus$ denotes the direct sum of matrices, that is, $\boldsymbol{V}_o \oplus \boldsymbol{V}_o = \begin{bmatrix} \boldsymbol{V}_o & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{V}_o \end{bmatrix}$.

Then the covariance matrix of $\hat{\boldsymbol{\theta}}$ becomes

$$\begin{aligned} \mathrm{Cov}(\hat{\boldsymbol{\theta}}) &= \mathrm{Cov}(\boldsymbol{A}^{-1}\boldsymbol{B}\boldsymbol{y}) \\ &= \boldsymbol{A}^{-1}\boldsymbol{B}\,\mathrm{Cov}(\boldsymbol{y})\boldsymbol{B}^\top(\boldsymbol{A}^{-1})^\top \\ &= \sigma^2 \boldsymbol{A}^{-1}\boldsymbol{B}\boldsymbol{V}\boldsymbol{B}^\top\boldsymbol{A}^{-1}. \end{aligned} \tag{1.6}$$

In this thesis, we mainly use the covariance matrices in (1.5) and (1.6) to study VBDs and their construction methods.

1.2 Variance Balanced Design

We first introduce the definition of information matrix. Let the replication of the i^{th} treatment be r_i and block size of the j^{th} block be k_j. Define the information matrix, or $\boldsymbol{C}$-matrix, as

$$\begin{aligned} \boldsymbol{C} &= \boldsymbol{X}_1^\top \boldsymbol{X}_1 - \boldsymbol{N}(\boldsymbol{X}_2^\top \boldsymbol{X}_2)^{-1}\boldsymbol{N}^\top \\ &= \mathrm{Diag}[r_1, r_2, \cdots, r_v] - \boldsymbol{N}\,\mathrm{Diag}[k_1^{-1}, k_2^{-1}, \ldots, k_b^{-1}]\boldsymbol{N}^\top, \end{aligned} \tag{1.7}$$

where $\mathrm{Diag}[c_1, c_2, \ldots, c_v]$ denotes a diagonal matrix with diagonal elements being $c_1, \ldots, c_v$.

In statistics, it is important to study the amount of information that an observable random variable carries about an unknown parameter. If the constraint on block effect such that $\sum_{j=1}^{b} \beta_j = 0$ is removed, then $\mathrm{Cov}(\hat{\boldsymbol{\theta}})$ only depends on the $\boldsymbol{C}$-matrix. In this case, $\boldsymbol{C}$-matrix contained all information about estimating $\boldsymbol{\theta}$, so it is named as information matrix.

As mentioned above, VBD is defined as a design when all variances of the estimators of elementary treatment contrast are the same. In addition, Rao (1958) proves the following result (Raghavarao, 1971),

Theorem 1 (Rao)**.** *A block design is variance balanced if and only if all the nonzero eigenvalues of the information matrix $\boldsymbol{C}$ of the block design are the same.*

Specifically, if the nonzero eigenvalues of $\boldsymbol{C}$ are all equal to ζ, then the information matrix $\boldsymbol{C}$ is of the form

$$\boldsymbol{C} = \zeta(\boldsymbol{I}_v - v^{-1}\boldsymbol{J}_{v,v}),$$

where $\boldsymbol{J_{v,v}}$ denotes the all 1 matrix. If a matrix is in $\langle \boldsymbol{I}, \boldsymbol{J} \rangle$ algebra, then it is called *completely symmetric.* Note that

$$\langle \boldsymbol{I}, \boldsymbol{J} \rangle = \{c_1\boldsymbol{I} + c_2\boldsymbol{J} : c_1, c_2 \in \mathbb{R}\}.$$

It is obvious that $\langle \boldsymbol{I}, \boldsymbol{J} \rangle$ is closed under sum and scalar multiplication. Also, since $\boldsymbol{J}_{\boldsymbol{v,v}}^2 = v\boldsymbol{J}$, we have that it is closed under matrix multiplication. For this reason, it is called an *algebra* of matrices. Since $(c_1\boldsymbol{I} + c_2\boldsymbol{J})\left(\frac{1}{c_1}\boldsymbol{I} - \frac{1}{(v+1)c_2}\boldsymbol{J}\right) = \boldsymbol{I}$ and the uniqueness of matrix inverse, $(c_1\boldsymbol{I} + c_2\boldsymbol{J})^{-1} = \frac{1}{c_1}\boldsymbol{I} - \frac{1}{(v+1)c_2}\boldsymbol{J}$ is also in the algebra.

From Theorem 1, we conclude the following result.

Theorem 2. *A completely symmetric $\boldsymbol{C}$-matrix guarantees a VBD.*

We use VBD(v, K) to denote a VBD with v treatments and block sizes in set K.

Example 1. Consider a design with 5 treatments and 6 blocks in Table 1.1. Here $(k_1, \ldots, k_6) = (4, 4, 2, 2, 2, 2)$ and $(r_1, \ldots, r_5) = (3, 3, 3, 3, 4)$.

Block	Treatments
1	{1, 2, 3, 4}
2	{1, 2, 3, 4}
3	{1, 5}
4	{2, 5}
5	{3, 5}
6	{4, 5}

Table 1.1: VBD(5, $\{2, 4\}$)

The design matrix $\boldsymbol{X} = [\boldsymbol{X}_1|\boldsymbol{X}_2]$ and the incidence matrix are, respectively,

$$\boldsymbol{X} = [\boldsymbol{X}_1|\boldsymbol{X}_2] = \left[\begin{array}{ccccc|cccccc}
1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1
\end{array}\right]$$

and

$$\boldsymbol{N} = \begin{bmatrix} 1 & 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 & 1 & 0 \\ 1 & 1 & 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 1 & 1 & 1 \end{bmatrix},$$

.

From (1.7), we calculate the $\boldsymbol{C}$-matrix of the design in Table 1.1 and get $\boldsymbol{C} = 2.5\boldsymbol{I} - 0.5\boldsymbol{J}$. The $\boldsymbol{C}$-matrix is completely symmetric, so the design is a VBD. The LSE has covariance matrix,

$$\mathrm{Cov}(\hat{\boldsymbol{\theta}}) = \sigma^2 \begin{bmatrix} 0.425 & 0.025 & 0.025 & 0.025 & -0.042 \\ 0.025 & 0.425 & 0.025 & 0.025 & -0.042 \\ 0.025 & 0.025 & 0.425 & 0.025 & -0.042 \\ 0.025 & 0.025 & 0.025 & 0.425 & -0.042 \\ -0.042 & -0.042 & -0.042 & -0.042 & 0.292 \end{bmatrix}.$$

We also calculate the variance of the estimator of the contrast of each treatment pair from $\mathrm{Cov}(\hat{\boldsymbol{\theta}})$, which gives $\mathrm{Var}(\hat{\theta}_i - \hat{\theta}_l) = 0.8\sigma^2$ for all $i \neq l$. This also confirms that the design in Table 1.1 is a VBD.

1.3 Research Problem

We want to determine construction methods for VBDs with unequal block sizes by analyzing the $\boldsymbol{C}$-matrix to be completely symmetric. In addition, we want to explore effective methods for constructing block designs so that the covariance matrix of $\hat{\boldsymbol{\theta}}$ is completely symmetric. We verify that a VBD such that each treatment occurs equal number of times among blocks (*equireplicated, or an equireplicate design*) gives a covariance matrix in $\langle \boldsymbol{I}, \boldsymbol{J} \rangle$ algebra. There exist many construction methods of VBDs including PBDs and GDDs with unequal block sizes. The relations between

VBDs and PBDs (or GDDs) can contribute the existence and construction of VBDs. Tyagi (1979), Hedayat and Stufken (1989) and Khatri (1982) made contributions to the construction of VBDs with unequal block sizes and unequal replicates. Gupta and Jones (1983) developed some construction methods of equireplicated VBDs.

In this thesis, the construction methods of VBDs from known PBDs are reviewed in Chapter 2. In Chapter 3, we examine criteria of equireplicated variance balanced block designs and present constructions of the designs. In Chapters 2 and 3, we focus on the construction of VBDs with unequal block sizes from existing combinatorial designs including PBDs and GDDs. In Chapter 4, we address the problem of generating VBDs under the assumption that the errors within block are correlated. We investigate the covariance matrix under various correlated error structures, and explore construction methods of VBDs with completely symmetric covariance matrix. We use graph theory to illustrate correlations among the treatments within blocks, and develop construction methods via graph decomposition.

1.4 Main Contributions

Here is a summary of the main contributions in this thesis.

1. We study the conditions for constructing VBDs under the assumption of uncorrelated random errors, and further explore the properties for block designs with $\mathrm{Cov}(\hat{\boldsymbol{\theta}})$ to be completely symmetric. We study construction methods of such VBDs with equal or unequal block sizes.

2. We determine the conditions for constructing VBDs under the assumption that the random errors are correlated within block.

3. We extend the problem of constructing VBDs to the problem in graph decomposition.

4. We determine a general construction methods for VBDs under several structures of the error correlations.

Chapter 2

Construction of Variance Balanced Block Design

We review existing methods for constructing PBDs and VBDs and derive various properties of PBDs and VBDs for uncorrelated experimental errors. A relationship between PBDs and VBDs shows that the construction of VBD is equivalent to that of PBDs from Hedayat and Stufken (1989).

2.1 Pairwise Balanced Design

Definition 1. Let K be a set of positive integers, and let v and λ be two positive integers. Given a set X of v elements (treatments) and a collection $\mathcal{B}$ of blocks B_j, $j = 1, \ldots, b$, where B_j are subsets of X, then a *pairwise balanced design*, denoted by PBD(v, K, λ), satisfies the following properties:

- $k_j \in K$ for all $j = 1, \ldots, b$, where $|B_j| = k_j$ is the number of elements in B_j.
- Every pair of distinct elements in X is contained in exactly λ blocks.

If a PBD has $k_1 = k_2 = \ldots = k_b$, then it is also known as a BIBD. For more details on PBD and BIBD, the reader can see Stinson (2004).

We use the following theorem from Wilson (1972) to show necessary conditions for the existence of a PBD.

Theorem 3 (Wilson)**.** *Suppose* $K \subseteq \{n \in \mathbb{Z} : n \geq 2\}$ *and suppose that* $v \geq 3$ *is an integer, then there exists a* $\mathrm{PBD}(v,\ K,\ \lambda)$ *only if*

$$\lambda(v-1) \equiv 0 \,(\mathrm{mod}\ \alpha(K)) \tag{2.1}$$

$$\lambda v(v-1) \equiv 0 \,(\mathrm{mod}\ \beta(K)) \tag{2.2}$$

where we define $\alpha(K) = \gcd\,(k-1 : k \in K)$ *and* $\beta(K) = \gcd\,(k(k-1) : k \in K)$*.*

Proof. We first prove (2.1). Suppose $(X, \mathcal{B})$ is a $\mathrm{PBD}(v,\ K,\ \lambda)$, where $|X| = v$ and $\mathcal{B} = \{B_i : i \in I\}$ is the collection of blocks. Fix $z \in X$. Let N be the number of pairs (x, i) such that $x \neq z$, $\{x, z\} \subseteq B_i$, and N_{i_0} be the number of $x \neq z$ such that $\{x, z\} \subseteq B_{i_0}$ for $i_0 \in I$. If $z \in B_{i_0}$, there are $|B_{i_0}| - 1 \equiv 0\,(\mathrm{mod}\ \alpha(K))$ such pairs (x, i); if $z \notin B_{i_0}$, there is no such pair. Notice that $N = \sum\limits_{i_0 \in I} N_{i_0}$, thus $N \equiv 0\,(\mathrm{mod}\ \alpha(K))$. For each $x \neq z$, $\{x, z\}$ is contained in λ blocks, and there are $(v-1)$ such x. Thus $N = \lambda(v-1) \equiv 0\,(\mathrm{mod}\ \alpha(K))$.

For (2.2), let N' denote the number of (x, y, i) such that $x \neq y$ and $\{x, y\} \in B_i$. Fix $i_0 \in I$. The number N'_{i_0} of pairs (x, y) such that $x \neq y$ and $\{x, y\} \subseteq B_{i_0}$ is $|B_{i_0}|(|B_{i_0}| - 1) \equiv 0\,(\mathrm{mod}\ \beta(K))$. For each pair $\{x, y\}$ with $x \neq y$, it is contained in λ blocks, and there are $v(v-1)$ such pairs. Thus, $N' = \lambda v(v-1)$ and also notice that $N' = \sum\limits_{i_0 \in I} N'_{i_0} \equiv 0\,(\mathrm{mod}\ \beta(K))$, which implies $\lambda v(v-1) \equiv 0\,(\mathrm{mod}\ \beta(K))$.

□

2.2 Construction of Variance Balanced Designs

In this section we first derive conditions for constructing VBDs under the assumption of uncorrelated errors.

Assume there is a collection of b blocks $\mathcal{B} = \{B_1, \ldots, B_b\}$ with sizes from $K = \{k_1, \ldots, k_b\}$, and r_i is the replication of treatment i. According to Rao (1958), showing that the information matrix is completely symmetric suffices to obtain a variance balanced design.

Using the result in Rao (1958), we find a condition on block sizes and replicates to guarantee a completely symmetric $\boldsymbol{C}$-matrix, which is stated below.

Theorem 4. *A block design is variance balanced design if it satisfies the condition that the sum of reciprocals of all block sizes that contain treatments i and j are the same for all $i, j \in X$ with $i \neq j$.*

Proof. Suppose $\sum_{\substack{B_l \subset \mathcal{B} \\ \{i,j\} \in B_l}} \frac{1}{|B_l|} = c$ for each treatment pair $\{i, j\}$ such that $i \neq j$, where c is a constant. Then, the information matrix $\boldsymbol{C}$ in (1.7) has elements,

$$C_{ij} = -\sum_{l=1}^{b} n_{il} k_i^{-1} n_{lj} + r_i \delta_{ij}, \quad \text{where } \delta_{ij} = \begin{cases} 1 & i = j \\ 0 & i \neq j \end{cases}.$$

For $i \neq j$,

$$\begin{aligned} C_{ij} &= -\left(\sum_{\substack{B_l \subset \mathcal{B} \\ \{i,j\} \in B_l}} \frac{1}{|B_l|} \right) \\ &= -c. \end{aligned}$$

For $i = j$,

$$\begin{aligned}
C_{ii} &= r_i - \sum_{\substack{B_l \subset \mathcal{B} \\ i \in B_l}} \frac{1}{|B_l|} \\
&= \sum_{\substack{B_l \subset \mathcal{B} \\ i \in B_l}} \left(1 - \frac{1}{|B_l|}\right) \\
&= \sum_{j \neq i} \sum_{\substack{B_l \subset \mathcal{B} \\ \{i,j\} \subseteq B_l}} \frac{1 - \frac{1}{|B_l|}}{|B_l| - 1} \\
&= \sum_{j \neq i} \sum_{\substack{B_l \subset \mathcal{B} \\ \{i,j\} \subseteq B_l}} \frac{1}{|B_l|} \\
&= \sum_{j \neq i} c \\
&= (v-1)c.
\end{aligned}$$

Thus $\boldsymbol{C} = vc\boldsymbol{I} - c\boldsymbol{J}$. It is clear that $\sum_{\substack{B_l \subset \mathcal{B} \\ \{i,j\} \subseteq B_l}} \frac{1}{|B_l|} = c$ guarantees that $\boldsymbol{C}$ is completely symmetric. □

Remark. Notice that we want the sum of reciprocals of all block sizes that contain treatments i and j to be a constant. The condition indicates that, for a pair of treatments i and j, we can get more information if they occur in a small size block rather than a large size block.

From Example 1, the treatment pair, 1 and 2, occurs in two blocks of size 4, and treatment pair, 1 and 5, occurs only in one block of size 2. Since we get less information from block of size 4, we needed two copies of this block. For treatments 1 and 2, we get $\frac{1}{4} + \frac{1}{4} = \frac{1}{2}$, while for treatments 1 and 5 we have $\frac{1}{2}$. This is consistent with the result in Theorem 4.

The following construction is from Hedayat and Stufken(1989), and we provide a proof using our notation for completeness.

Theorem 5 (Hedayat and Stufken)**.** *Given a* PBD$(v,\ K = \{k_1, \ldots, k_t\},\ \lambda)$*, with treatment set* X *and a collection of blocks* $\mathcal{B} = \{B_l : l = 1, \ldots, s\}$*. Let's denote size* *of B_l be $k_{j(l)}$, where $k_{j(l)} = k_j \in K$. Obtain a new design by taking $\frac{ck_{j(l)}}{\eta}$ copies of block B_l, where $\eta = \gcd(k : k \in K)$, and c can be any positive integer. The resulting design is a* VBD$(v,\ K)$.

Proof. Given a PBD$(v,\ \{k_1, \ldots, k_t\},\ \lambda)$, let $\lambda^j_{i_p,i_q}$ denote the number of times that i_p, i_q pair appears in the blocks of size k_j, and $r^j_{i_p}$ be replicates of i_p in blocks with size k_j. Take $\frac{ck_{j(l)}}{\eta}$ copies of block of size k_j. Then we obtain the $\boldsymbol{C}$-matrix of the new design. We compute

$$\sum_{\substack{B_l \subset \mathcal{B} \\ \{i_p,i_q\} \subseteq B_l}} \frac{1}{|B_l|} = \sum_{\substack{B_l \subset \mathcal{B} \\ \{i_p,i_q\} \subseteq B_l}} \frac{ck_{j(l)}}{\eta} \frac{1}{k_{j(l)}} = \frac{c}{\eta} \left(\sum_{\substack{B_l \subset \mathcal{B} \\ \{i_p,i_q\} \subseteq B_l}} 1 \right) = \frac{c}{\eta} \lambda_{i_p,i_q} = \frac{c}{\eta} \lambda,$$

$$\text{and}\, r_{i_p} - \sum_{\substack{B_l \subset \mathcal{B} \\ i_p \in B_l}} \frac{1}{|B_l|} = \sum_{j=1}^{t} \left(\frac{ck_j}{\eta} r^j_{i_p} - \frac{ck_j}{\eta} \cdot \frac{r^j_{i_p}}{k_j} \right) = \frac{c}{\eta} \sum_{j=1}^{t} (k_j - 1) r^j_{i_p} = \frac{c}{\eta}(v-1)\lambda.$$

$$C_{i_p,i_q} = \begin{cases} -\frac{c\lambda}{\eta} & i \neq j, \\ \frac{c(v-1)\lambda}{\eta} & i = j \end{cases}. \tag{2.3}$$

From (2.3), notice that each entry of $\boldsymbol{C}$ depends only on whether $i_p = i_q$ and not on the treatments themselves. This implies we have a VBD. □

Example 2. Given a PBD$(5,\ \{2, 4\},\ 1)$ in Table 2.1, we want to construct a VBD based on Theorem 5.

Block	Treatments
1	{1, 2, 3, 4}
2	{1, 5}
3	{2, 5}
4	{3, 5}
5	{4, 5}

Table 2.1: PBD$(5,\ \{2, 4\},\ 1)$

Note that $|B_1| = 4$, and $|B_l| = 2$ for $l = 2, 3, 4, 5$. $\eta = \gcd(2, 4) = 2$, and we pick $c = 1$. Then we take two copies of B_1 and one copy of B_2, B_3, B_4, B_5 as our new design, which gives the design in Table 1.1. Thus the new design is a VBD, which is shown in Example 1. We verify that the construction from PBD to VBD works.

To show that any VBDs can be obtained as in Theorem 5, Hedayat and Stufken (1989) found a converse of Theorem 5.

Theorem 6 (Hedayat and Stufken)**.** *For a given* VBD$(v,\ \{k_1, \ldots, k_t\})$*, take* $\frac{\prod_{j \neq j_0} k_j}{\tau}$ *copies of each block of size* k_{j_0}*, where* $\tau = \gcd\left(\prod_{j \neq i} k_j : i = 1, 2, \ldots, t\right)$*. The resulting design is pairwise balanced.*

Proof. Denote λ_{i_p,i_q} as the number of times such that i_p and i_q occur in the same block.

$$\begin{aligned}
\lambda_{i_p,i_q} &= \sum_{j_0=1}^{t} \left(\frac{\prod_{j \neq j_0} k_j}{\tau} \right) \lambda_{i_p,i_q}^{j_0} \\
&= \frac{\prod_{j=1}^{t} k_j}{\tau} \cdot \sum_{j_0=1}^{t} \frac{\lambda_{i_p,i_q}^{j_0}}{k_{j_0}} \\
&= \frac{\prod_{j=1}^{t} k_j}{\tau} \cdot \sum_{\substack{B_l \subset \mathcal{B} \\ \{i_p,i_q\} \subseteq B_l}} \frac{1}{|B_l|}
\end{aligned}$$

Since the given design is a VBD, $\sum\limits_{\substack{B_l \subset \mathcal{B} \\ \{i_p,i_q\} \subseteq B_l}} \frac{1}{|B_l|}$ is constant for each pair of treatment. In addition, $\frac{\prod_{j=1}^{t} k_j}{\tau}$ is an integer under our construction, so λ_{i_p,i_q} is constant for all pair of treatments $i_p \neq i_q$. Thus the resulting design is pairwise balanced. □

Example 3. Consider a VBD$(8,\ \{k_1 = 2,\ k_2 = 6\})$ in Table 2.2. Apply Theorem 6 to the VBD$(8,\ \{2, 6\})$, $\prod\limits_{j \neq 1} k_j = k_2 = 6$ and $\prod\limits_{j \neq 2} k_j = k_1 = 2$, $\tau = \gcd(6,\ 2) = 2$. Thus, we obtain a new design by taking $\frac{2}{2} = 1$ copy of block with size 6 and $\frac{6}{2} = 3$ copies of blocks with size 2, and the resulting design is pairwise balanced. In fact it is a PBD$(8,\ \{2, 6\},\ 3)$.

Distinct Block	Treatment	Multiplicity for VBD	Multiplicity for PBD
1	{1,2,3,4,5,6}	3	3
2	{1,7}	1	3
3	{1,8}	1	3
4	{2,7}	1	3
5	{2,8}	1	3
6	{3,7}	1	3
7	{3,8}	1	3
8	{4,7}	1	3
9	{4,8}	1	3
10	{5,7}	1	3
11	{5,8}	1	3
12	{6,7}	1	3
13	{6,8}	1	3
14	{7,8}	1	3

Table 2.2: VBD(8, $\{2, 6\}$) and PBD(8, $\{2, 6\}$, 3)

Remark. We can divide by gcd of multiplicities of blocks in a PBD to reduce λ. From PBD(8, $\{2, 6\}$, 3), we can obtain PBD(8, $\{2, 6\}$, 1) by taking each distinct block in PBD(8, $\{2, 6\}$, 3) once.

Chapter 3

Equireplicate Variance Balanced Block Design

In this Chapter, we focus on the construction of block designs such that the covariance matrix of the LSE $\hat{\boldsymbol{\theta}}$ is completely symmetric. By further analysis on the covariance matrix in (1.5), we find that equireplicate VBD is sufficient and necessary condition for obtaining a completely symmetric covariance matrix. Gupta and Jones (1983) provide several methods for constructing equireplicate VBDs with unequal block sizes using GDDs and present a table of 100 equireplicate VBDs. We review those methods and illustrate them with several examples.

3.1 Covariance and Information matrices

Theorem 7. *A VBD has completely symmetric covariance matrix* $\mathrm{Cov}(\hat{\boldsymbol{\theta}})$ *if and only if it is equireplicate.*

Proof. From (1.5), the covariance matrix of the LSE is proportional to the inverse of $\boldsymbol{A}$, where $\boldsymbol{A}$ is defined in (1.3). To obtain a completely symmetric covariance matrix, it is equivalent to obtain a completely symmetric matrix $\boldsymbol{A}$. Thus, we analyze matrix $\boldsymbol{A}$ and derive the conditions for the covariance matrix in $\langle \boldsymbol{I}, \boldsymbol{J} \rangle$ algebra. From (1.3) and (1.7), we find the relation between matrix $\boldsymbol{A}$ and the information matrix $\boldsymbol{C}$,

$$\boldsymbol{A} = \boldsymbol{C} + \frac{1}{a}\boldsymbol{N}(\boldsymbol{X}_2^\top \boldsymbol{X}_2)^{-1}\mathbf{1}_b\mathbf{1}_b^\top (\boldsymbol{X}_2^\top \boldsymbol{X}_2)^{-1}\boldsymbol{N}^\top,$$

and the elements of $\boldsymbol{A}$ are given by

$$A_{ij} = C_{ij} + \frac{\left(\sum\limits_{\substack{B_l \subset \mathcal{B} \\ i \in B_l}} \frac{1}{|B_l|}\right)\left(\sum\limits_{\substack{B_l \subset \mathcal{B} \\ j \in B_l}} \frac{1}{|B_l|}\right)}{\sum\limits_{B_l \subset \mathcal{B}} \frac{1}{|B_l|}}. \tag{3.1}$$

Since $\boldsymbol{C} \in \langle \boldsymbol{I}, \boldsymbol{J} \rangle$, from the proof of Theorem 4, $C_{ij} = \sum\limits_{\substack{B_l \subset \mathcal{B} \\ \{i,j\} \in B_l}} \frac{1}{|B_l|} = c$ is constant for $i \neq j$, and $C_{ii} = (v-1)c$. Also, from the proof of Theorem 4, we have $\sum\limits_{\substack{B_l \subset \mathcal{B} \\ i \in B_l}} \frac{1}{|B_l|} = C_{ii} + r_i$. Since $\sum\limits_{B_l \subset \mathcal{B}} \frac{1}{|B_l|}$ is independent of i and j, let $\sum\limits_{B_l \subset \mathcal{B}} \frac{1}{|B_l|} = \gamma$. Thus,

$$\begin{aligned} A_{ii} &= C_{ii} + \frac{1}{\sum\limits_{B_l \subset \mathcal{B}} \frac{1}{|B_l|}}(C_{ii} + r_i)(C_{ii} + r_i) \\ &= (v-1)c + \frac{1}{\gamma}((v-1)c + r_i)^2, \end{aligned}$$

and for $i \neq j$,

$$A_{ij} = c + \frac{1}{\gamma}((v-1)c + r_i)((v-1)c + r_j).$$

Let $r_i = r_j = r$ for $i \neq j$,

$$\boldsymbol{A} = ((v-2)c)\,\boldsymbol{I} + \left(c + \frac{1}{\gamma}((v-1)c + r)^2\right)\boldsymbol{J}.$$

Note that there are at least two treatments for comparison in a experiment, and if $v = 2$ then it is RCBD. In addition, block size is always positive integer. Thus $v > 2$ and $c > 0$ implies that $(v-2)c > 0$. The determinant of $\boldsymbol{A}$ is

$$\det(\boldsymbol{A}) = (v-2)c + \left(c + \frac{1}{\gamma}((v-1)c + r)^2\right)v > 0.$$

Thus $\boldsymbol{A}$ is always invertible when it is in $\langle \boldsymbol{I}, \boldsymbol{J} \rangle$ form. From (1.5), a completely symmetric $\boldsymbol{A}^{-1}$ implies a completely symmetric $\mathrm{Cov}(\hat{\boldsymbol{\theta}})$. $\square$

3.2 Group Divisible Design

Before reviewing this method of constructing equireplicate VBDs, we recall the definition of GDD.

Definition 2. Let X be a set of elements (treatments), and $\mathcal{G}$ be a partition of X into at least two nonempty subsets called groups. Let $\mathcal{B}$ denote a collection of subsets of X called blocks such that any $B_i \in \mathcal{B}$ has size greater than two. A group divisible design, abbreviated to GDD(X, $\mathcal{G}$, $\mathcal{B}$, λ_1, λ_2) has the property that every pair of treatments within the same group is contained in exactly λ_1 blocks, and every pair of treatments from distinct groups is contained in exactly λ_2 blocks.

Note that a PBD is a special case of GDD in which $\mathcal{G} = \{\{1\}, \ldots, \{v\}\}$, a partition into singletons. In this case, λ_1 is not used, and λ_2 becomes the usual parameter λ for a design. For more information on GDD, the reader can see Stinson (2004).

Example 4. The design in Table 3.1 is a GDD with group $\mathcal{G} = \{\{1, 4\}, \{2, 5\}, \{3, 6\}\}$. The pairs of treatments within group are $\{1, 4\}, \{2, 5\}, \{3, 6\}$, where each of those pairs is contained in exactly 2 blocks in $\mathcal{B}$. The rest of pairs are occurred in the same block exactly once.

Blocks	Treatments
1	{1, 2, 4}
2	{2, 3, 5}
3	{3, 4, 6}
4	{1, 4, 5}
5	{2, 5, 6}
6	{1, 3, 6}

Table 3.1: GDD$(\{1, \ldots, 6\}, \mathcal{G}, \mathcal{B}, \lambda_1 = 2, \lambda_2 = 1)$

3.3 Methods for Constructing Equireplicate VBD

Gupta and Jones (1983) contributed on methods for constructing equireplicate VBDs and presented a table of 100 equireplicate VBDs from partially balanced incomplete block designs (PBIBD) provided by Clatworthy (1973), John, Wolock and David (1974) and Hall and Jarrett (1981).

Theorem 8 (Gupta and Jones)**.** *Given* G_j= GDD$(X,\ \mathcal{G},\ \mathcal{B}_j,\ \lambda_{1j},\ \lambda_{2j})$ *for* $j = 1, \ldots, s$*, where* $\mathcal{B}_j$ *is collection of* b_j *blocks with uniform block size* k_j*,* $\mathcal{G}$ *is collection of* m *groups with uniform group size* n*. If* $\sum\limits_{j\in\{1,\ldots,s\}} \frac{\lambda_{1j}}{k_j} = \sum\limits_{j\in\{1,\ldots,s\}} \frac{\lambda_{2j}}{k_j}$*, then there exists design* D *obtained by taking all blocks of* $\{G_j : j = 1, \ldots, s\}$ *is a VBD.* D *is a VBD on* $v = |X|$ *treatments with replication number* $r = \sum\limits_{j\in\{1,\ldots,s\}} r_j$*, and block sizes taken from* $K = \{k_1, \cdots, k_s\}$*.*

Theorem 9 (Gupta and Jones)**.** *Suppose* D_1 = BIBD$(v_1,\, r_1,\, k_1,\, b_1,\, \lambda_1)$*, if there exists a* D_2 = BIBD$(v_2 = r_1,\, r_2,\, k_2,\, b_2,\, \lambda_2)$*, where* $\lambda_2 = \frac{ck_2(k_2-1)(k_1-1)}{k_1(r_1-k_2)}$ *for some integer* c*, then there exists an equireplicate variance balanced block design with block sizes from* $K = \{k_1, (k_1-1)k_2\}$

Proof. The proof gives a construction method for equireplicate VBD from a GDD.

Given a design D = BIBD$(v_1,\, r_1,\, k_1,\, b_1,\, \lambda)$, omit a treatment $p \in \{1, \ldots, v\}$ and all the blocks containing p; this method was proposed by Bose (1953). We get GD_1= GDD$(X = \{1, \ldots, v_1 - 1\},\, \mathcal{G}_1,\, \mathcal{B}_1,\, \lambda_{11} = 0,\, \lambda_{21} = 1)$, where $\mathcal{G}_1$ consists of r_1 groups such that each group size equals to $k_1 - 1$ and $\mathcal{B}_1$ consists of $c(b_1 - r_1)$ blocks such that each block size equals to k_1.

Given BIBD$(r_1,\ r_2,\ k_2,\ b_2,\ \lambda_2)$, we find isomorphic function from $\{1, \cdots, r_1\}$ to $\mathcal{G}_2$, and we can obtain a GD_2= GDD$(v_1 - 1 = (k_1 - 1)r_1,\, \mathcal{G}_2 = \mathcal{G}_1,\, \mathcal{B}_2,\, \lambda_{12} = r_2,\, \lambda_{22} = \lambda_2)$ where $\mathcal{B}_2$ consists of b_2 blocks such that each block size equals to $(k_1 - 1)k_2$.

Obtaining a new design D by taking c copies of GD_1 and one copy of GD_2. We have

$$\begin{aligned}
\sum_{j\in\{1,\dots,c+1\}} \frac{\lambda_{1j}}{k_j} &= c\frac{\lambda_{11}}{k_1} + \frac{\lambda_{21}}{(k_1-1)k_2} = \frac{r_2}{(k_1-1)k_2} \quad \text{and} \\
\sum_{j\in\{1,\dots,c+1\}} \frac{\lambda_{2j}}{k_j} &= c\frac{\lambda_{12}}{k_1} + \frac{\lambda_{22}}{(k_1-1)k_2} = \frac{c}{k_1} + \frac{\lambda_2}{(k_1-1)k_2} \\
&= \frac{\lambda_2 k_1(r_1-k_2)}{k_2(k_2-1)(k_1-1)} \cdot \frac{1}{k_1} + \frac{\lambda_2}{(k_1-1)k_2} \\
&= \frac{\lambda_2(r_1-k_2)+\lambda_2(k_2-1)}{k_2(k_2-1)(k_1-1)} \\
&= \frac{\lambda_2(r_1-1)}{k_2(k_2-1)(k_1-1)} = \frac{r_2}{(k_1-1)k_2}.
\end{aligned}$$

By Theorem 8, D is a VBD with replication number $c(r_1-1)+r_2$. □

Example 5. Given D_1 =BIBD(13, 6, 3, 26, 1) and D_2 =BIBD(6, 5, 2, 15, 1), we apply Theorem 9 to D_1 and D_2. Since $c = \frac{\lambda_2 k_1(r_1-k_2)}{k_2(k_2-1)(k_1-1)} = 3$, we can obtain VBD($v = 12,\ K = \{3, 6\}$) by taking 3 copies of GD_1 and 1 copy of GD_2 as in Table 3.2, where GD_1 and GD_2 are obtained by the methods in the proof of Theorem 9.

Distinct Block	Multiplicity	Distinct Block	Multiplicity
B_1={1,3,9}	3	B_{19}={2,3,12}	3
B_2={2,4,10}	3	B_{20}={1,4,5}	3
B_3={3,5,11}	3	B_{21}={6,7,11,15}	1
B_4={4,6,12}	3	B_{22}={2,7,8,15}	1
B_5={1,6,8}	3	B_{23}={7,9,12,15}	1
B_6={2,7,9}	3	B_{24}={1,7,10,15}	1
B_7={3,8,10}	3	B_{25}={3,4,7,15}	1
B_8={4,9,11}	3	B_{26}={2,6,8,11}	1
B_9={5,10,12}	3	B_{27}={6,9,11,12}	1
B_{10}={1,7,12}	3	B_{28}={1,6,10,11}	1
B_{11}={2,5,6}	3	B_{29}={3,4,6,11}	1
B_{12}={3,6,7}	3	B_{30}={2,8,9,12}	1
B_{13}={4,7,8}	3	B_{31}={1,2,8,10}	1
B_{14}={5,8,9}	3	B_{32}={2,3,4,8}	1
B_{15}={6,9,10}	3	B_{33}={1,9,10,12}	1
B_{16}={7,10,11}	3	B_{34}={3,4,9,12}	1
B_{17}={8,11,12}	3	B_{35}={1,3,4,10}	1
B_{18}={1,2,11}	3		

Table 3.2: VBD($v = 12$, $K = \{3, 4\}$)

Theorem 10 (Gupta and Jones). *Consider a* GDD($\{1, \ldots, mn\}$, $\mathcal{G}_1$, $\mathcal{B}_1$, $\lambda_{11} = 0$, λ_{21})*, where replication number* $r_1 = n\lambda_{21}$, $|\mathcal{B}_1| = b_1 = n^2\lambda_{21}$*, and block size* $k_1 = m$*. Then the existence of* BIBD($m,\ r_2,\ k_2,\ b_2,\ \lambda_2$) *with* $\lambda_2 = \frac{cnk_2(k_2-1)\lambda_{21}}{m(m-k_2)}$ *implies the existence of a* VBD(nm, $\{k_1, nk_2\}$) *with equal replication number* $r = cr_1 + r_2$*.*

Proof. Given a GD_1=GDD($\{1, \ldots, mn\}$, $\mathcal{G}_1$, $\mathcal{B}_1$, $\lambda_{11} = 0$, λ_{21}). If there exists a BIBD($m,\ r_2,\ k_2,\ b_2,\ \lambda_2$) such that $\lambda_2 = \frac{cnk_2(k_2-1)\lambda_{21}}{m(m-k_2)}$, replacing treatments $\{1, \cdots, m\}$ by groups in $\mathcal{G}_1$ yields GD_2= GDD($\{1, \ldots, mn\}$, $\mathcal{G}_1$, $\mathcal{B}_2$, $\lambda_{12} = r_2$, $\lambda_{22} = \lambda_2$), where

$\mathcal{B}_2$ contains b_2 blocks of size nk_2. We obtaining a new design D by taking c copies of GD_1 and one copy of GD_2. We compute

$$\begin{aligned}
\sum_{j\in\{1,\ldots,\alpha+1\}} \frac{\lambda_{1j}}{k_j} &= \frac{r_2}{nk_2} \quad \text{and} \\
\sum_{j\in\{1,\ldots,\alpha+1\}} \frac{\lambda_{2j}}{k_j} &= \alpha\frac{\lambda_{21}}{m} + \frac{\lambda_2}{nk_2} \\
&= \frac{\lambda_2 m(m-k_2)}{nk_2(k_2-1)\lambda_{21}}\frac{\lambda_{21}}{m} + \frac{\lambda_2}{nk_2} \\
&= \frac{\lambda_2(m-k_2)+\lambda_2(k_2-1)}{nk_2(k_2-1)} \\
&= \frac{\lambda_2(m-1)}{nk_2(k_2-1)} = \frac{r_2}{nk_2}.
\end{aligned}$$

By Theorem 8, D is a VBD with replication number $r = cr_1 + r_2$. $\square$

Example 6. Given GD_1= GDD($\{1,\ldots,6\}$, $\mathcal{G}$, $\mathcal{B}_1$, $\lambda_{11}=0$, $\lambda_{21}=1$), where $\mathcal{G}=\{g_1=\{1,4\}, g_2=\{2,5\}, g_3=\{3,6\}\}$ and $\mathcal{B}_1=\{\{1,2,3\},\{1,5,6\},\{2,4,6\},\{3,4,5\}\}$. For a BIBD($m=3$, $r_2=2$, $k_2=2$, $b_2=3$, $\lambda_2=1$), replacing treatment $i\in\{1,2,3\}$ by g_i, then we obtain GD_2= GDD($\{1,\ldots,6\}$, $\mathcal{G}$, $\mathcal{B}_2$, $\lambda_{12}=2$, $\lambda_{22}=1$), where $\mathcal{B}_2=\{(\{1,4,2,5\},\{2,5,3,6)\},\{1,4,3,6\}\}$. Since $\lambda_2=\frac{cnk_2(k_2-1)\lambda_{21}}{m(m-k_2)} \implies c=\frac{3(3-2)}{2\cdot2\cdot(2-1)}=\frac{3}{4}$, we obtain VBD($v=6$, $K=\{3,4\}$) by taking 3 copies of GD_1 and 4 copies of GD_2.

Chapter 4

Variance Balanced Design Under Correlated Errors

In model (1.1), the errors ϵ_{ij} are usually considered to be uncorrelated if we allocate the treatments randomly within blocks. However, for some experiments, there are correlations among the errors. Using the error correlation information in designing an experiment can help make more precise inferences for $\boldsymbol{\theta}$ (Gill and Shukla, 1985). In this chapter, we investigate the construction of VBDs under the assumption that the errors are correlated. In particular, we develop the conditions for constructing VBDs such that the covariance matrix of the LSE is completely symmetric.

4.1 Statistical Model Under Correlated Error

While conducting experiments in field plots or over time, the observations are often correlated, such as serial correlation over time and spatial correlation over field plots (Mann, Edwards and Zhou, 2015). We give an example of spatial correlation among observations in Example 7, while Example 8 discusses serial correlation over time.

Example 7. The treatment means may be influenced by the geographical location of the experimental plots (Peterson, 2017). Consider an $m \times n$ array of field plots in Figure 4.1, where lag 1 represents plots that are immediate neighbors of plot O, and lag 2 represents plots that are in the same row or column with plot O. The spatial correlations can be modelled as a function of lag distance and are expected to approach zero when lag distance goes to infinitely (Taye and Njuho, 2007).

4	3	2	3	4
3	1	1	1	3
2	1	O	1	2
3	1	1	1	3
4	3	2	3	4

Figure 4.1: Lag distance between plot O and the other plots

Example 8. Temporal variation occurs in experiments with repeated measurements. In ecological experiments, repeated measurements over time on groups of samples subjected to different treatments are frequently used (Gurevitch and Chester, 1986). When an individual sample is measured repeatedly, there are often correlations among those measurements, and higher correlation occurs on measurements taken more closely in time (Gurevitch and Chester, 1986).

To address those variations raising from spatial and temporal variability, correlated error structure is considered in the model. Then $\text{Cov}(\hat{\boldsymbol{\theta}})$ depends on the covariance of the errors. There exists many theoretical papers working on evaluation of covariance of the errors, for example, Wiebe (1935) investigated the variation and correlation in grain yield among 1500 wheat nursery plots.

In (1.1), we assume that the errors are correlated with $Cov(\boldsymbol{\epsilon}) = \sigma^2\boldsymbol{V}$, where $\boldsymbol{V}$ is an $n \times n$ correlation matrix. Also, we assume that errors between different blocks are considered to be independent, and there are only correlations among the errors within each block. Let $\boldsymbol{V}_j$ be the error correlation matrix within each block. Then $\boldsymbol{V}$ is a block diagonal matrix i.e., $\boldsymbol{V} = \bigoplus_{j=1}^{b} \boldsymbol{V}_j$. To explore the influence of the error correlation on the covariance matrix of $\hat{\boldsymbol{\theta}}$, we recall (1.6) and get $\mathrm{Cov}(\hat{\boldsymbol{\theta}}) = \sigma^2 \boldsymbol{A}^{-1}\boldsymbol{B}\boldsymbol{V}\boldsymbol{B}^\top \boldsymbol{A}^{-1}$.

Notice that the structure of $\mathrm{Cov}(\hat{\boldsymbol{\theta}})$ depends on $\boldsymbol{A}^{-1}$ and $\boldsymbol{B}\boldsymbol{V}\boldsymbol{B}^\top$. We have analyzed the structure of $\boldsymbol{A}$ in Chapter 3 and obtained the result in Theorem 7. In the following, we analyze matrix $\boldsymbol{B}\boldsymbol{V}\boldsymbol{B}^\top$ and derive several results using graph theory. These results will help us construct VBDs.

4.2 Definitions from Graph Decomposition

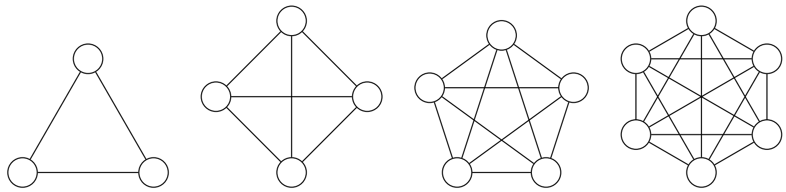
To show various correlations among observations in each block, we use graphs to represent blocks and vertices to represent treatments. If the observations at two treatments in the same block are correlated, then there is an edge to connect the two treatments (vertices). First, we present several definitions in graph theory.

Definition 3. A graph is denoted by $G{=}(V, E)$, where G contains a vertex set V connected by a set of edges $E \subseteq \binom{V}{2} = \{\{a, b\} : a, b \in V, a \neq b\}$.

Graph theory is a large subject in discrete mathematics. For more information on graphs, the reader can see West (1996). For complements, we introduce the important definitions and notations for our purpose.

Definition 4. The degree of a vertex x of a graph G is the number of edges adjacent to x, denoted by $\deg_x(G)$. When every vertex has the same degree, then it is a regular graph.

Definition 5. The complete graph $K_v = (V, E)$ is a simple undirected graph and each pair of distinct vertices in V are connected by a unique edge in E, where v is the number of vertices in V.



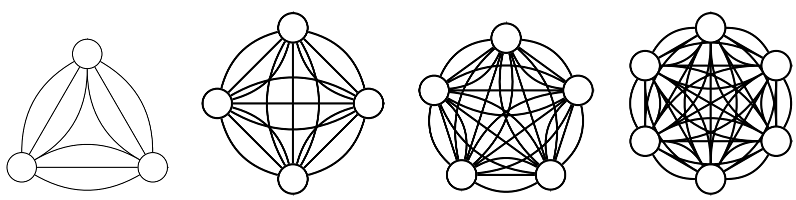
K_3 K_4 K_5 K_6

Figure 4.2: Complete graphs K_v with $v = 3, 4, 5$ and 6

In a multigraph, we permit multiple edges, that is, two vertices may be connected by more than one edge.

Definition 6. The λ-complete multigraph on v vertices is a multigraph in which there are exactly λ edges between each pair of vertices, and denoted by K_v^λ.

Figures 4.2 and 4.3 show complete graphs and 3-complete multigraphs with $v = 3, 4, 5$ and 6.



K_3^3 K_4^3 K_5^3 K_6^3

Figure 4.3: 3-complete multigraphs K_v^3 with $v = 3, 4, 5$ and 6

Definition 7. An *isomorphism* of graphs G and H is a bijection function $f : V(G) \to V(H)$ such that for any two vertices $u, v \in V(G)$, $uv \in E(G)$ if and only if $f(u)f(v) \in E(H)$. If there exists isomorphism between G and H, then G is isomorphic to H. An *automorphism* of a graph G is a graph isomorphism from G to itself.

Example 9. Labeling vertices of Figures 4.5a and 4.5b by $\{v_1, \ldots, v_7\}$ and $\{1, \ldots, 7\}$ respectively, we can find an isomorphism between G_1 and G_2 in Table 4.1. Note that G_1, G_2 and G_3 are all isomorphic to a cycle on 7 vertices, which is denoted as C_7.

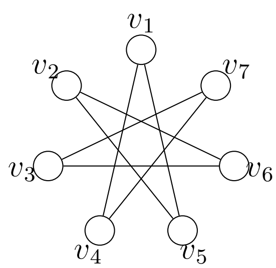
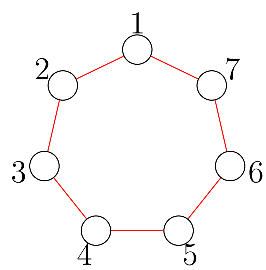
<table>
<tr><th>Graph G_1</th><th>Graph G_2</th><th>An isomorphism between G_1 and G_2</th></tr>
<tr><td rowspan="7"></td><td rowspan="7"></td><td>$f(v_1) = 1$</td></tr>
<tr><td>$f(v_2) = 3$</td></tr>
<tr><td>$f(v_3) = 5$</td></tr>
<tr><td>$f(v_4) = 7$</td></tr>
<tr><td>$f(v_5) = 2$</td></tr>
<tr><td>$f(v_6) = 4$</td></tr>
<tr><td>$f(v_7) = 6$</td></tr>
</table>

Table 4.1: Isomorphism between G_1 and G_2

In addition, G_1 has seven nontrivial automorphisms $\{\pi_i : i = 1\ldots,7\}$, which are illustrated in Figure 4.4. The set of all automorphisms of an G_1 forms a group, call the *automorphism group*, and $\mathrm{Aut}(G_1) = 7$.

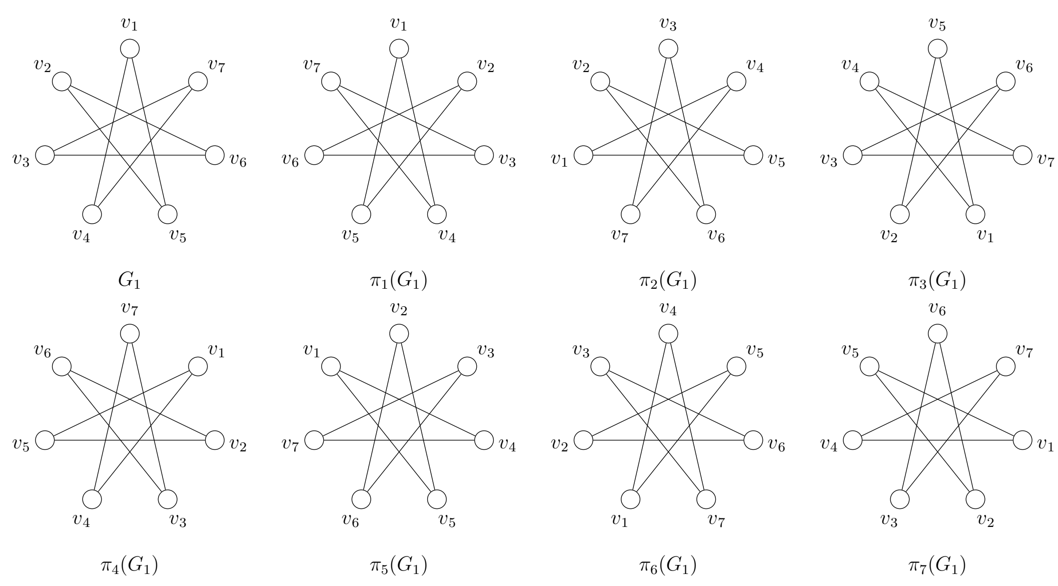
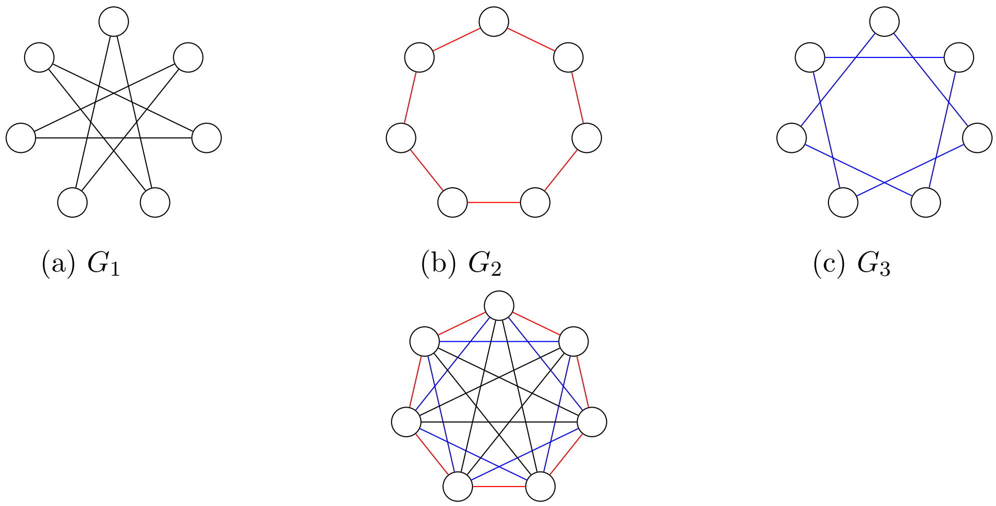


Figure 4.4: Automorphism group of G_1

Definition 8. A *decomposition* of a graph G is a collection of subgraphs of G, $G_1, G_2, \ldots, G_k$ of G, such that for each edge $e \in G$, the sum of multiplicity of edge e over all subgraphs in the collection including an edge e equals to the multiplicity of

e in G. A decomposition in which each subgraph G_i is isomorphic to a fixed graph H, is called an H-decomposition of G.

Example 10. Figure 4.5 shows that a complete graph K_7 can be decomposed into G_1, G_2 and G_3. Note that G_1, G_2, G_3 are all isomorphic to C_7, so it is a C_7-Decomposition of K_7.



(a) G_1 (b) G_2 (c) G_3

(d) K_7

Figure 4.5: A decomposition of K_7

Definition 9. The *complement* of a graph G, denoted as $\overline{G}$, is a graph on $V(G)$ such that each edge $e \in E(\overline{G})$ if and only if $e \notin E(G)$. A *self complementary graph* is a graph G such that G is isomorphic to its complement $\overline{G}$.

Example 11. Figure 4.6 shows the complement of G_1 in Figure 4.5a.

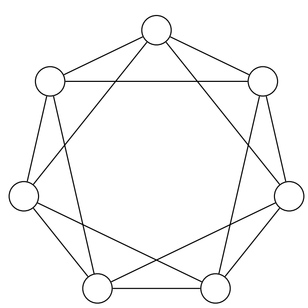


Figure 4.6: Complement of G_1

4.3 Relation between Graphs and Block Designs

For a block design $(X, \mathcal{B})$, where X contains v treatments and $\mathcal{B}$ is a collection of b blocks on X. Then $\mathcal{B} = \{B_i\}$ can be represented by a collection of graphs $\mathcal{G} = \{G_i\}$ by taking the treatments in B_i as vertices in $V(G_i)$, and any correlated pair of treatments within block are considered as edge between their corresponding vertices in $E(G_i)$. That is, each block $B_i \in \mathcal{B}$ can be drawn as a graph G_i, where $V(G_i) = B_i$.

For a BIBD(v, r, k, b, λ), each block contains k treatments, such that every pair of distinct treatments contained in the same block exactly λ times. In addition, since we assume random errors are independent, observations on each pair of treatments within block are uncorrelated. Thus, the graph representing each block is a graph G of k isolated vertices, and we have collection $\mathcal{G}$ containing b graphs isomorphic to G. The composition of complement of each graph in $\mathcal{G}$ is a λ-complete multigraph. Thus, the construction of BIBD can be easily seen as construction of K_k - decomposition of the λ-complete multigraph on order v.

Theorem 11. *The construction of* BIBD(v, r, k, b, λ) *is equivalent to K_k decomposition of λ-complete multigraph K_v^λ.*

Example 12. We illustrate Theorem 11 by showing an example that we construct a BIBD(4, 3, 3, 4, 2) by finding a K_3 decomposition of K_4 in Figure 4.7, where each graph is the complement of the graph representing block in BIBD(4, 3, 3, 4, 2).

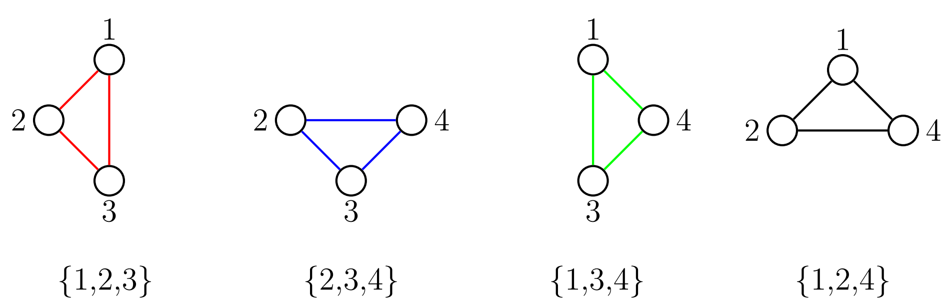


Figure 4.7: Complement of Graph representing block in BIBD(4, 3, 3, 4, 2)

The composition of the four graphs in Figure 4.7 is a 2-complete multigraph K_4^2, as shown in Figure 4.8.

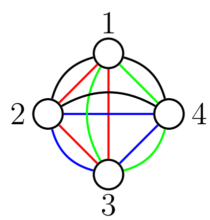


Figure 4.8: Composition of graph in Figure 4.7

Example 13. For correlated errors, if there is correlation between the observations on the pair of treatments i and j within block B, then i and j are adjacent in G, that is, $ij \in E(G)$, and G is the corresponding graph of B. Consider a block design with 5 blocks on 5 treatments and each block containing 3 treatments as in Figure 4.9, and the error covariance matrix is given by

$$\mathrm{Cov}(\boldsymbol{\epsilon}) = \sigma^2 \bigoplus_{j=1}^{5} \begin{bmatrix} 1 & \rho & 0 \\ \rho & 1 & \rho \\ 0 & \rho & 1 \end{bmatrix}. \tag{4.1}$$

Note that the treatments are list as $\{1, 2, 4\}, \{2, 3, 5\}, \{3, 4, 1\}, \{4, 5, 2\}, \{5, 1, 3\}$. If treatments in each block are permuted, then $\mathrm{Cov}(\boldsymbol{\epsilon})$ in (4.1) may be presents differently.

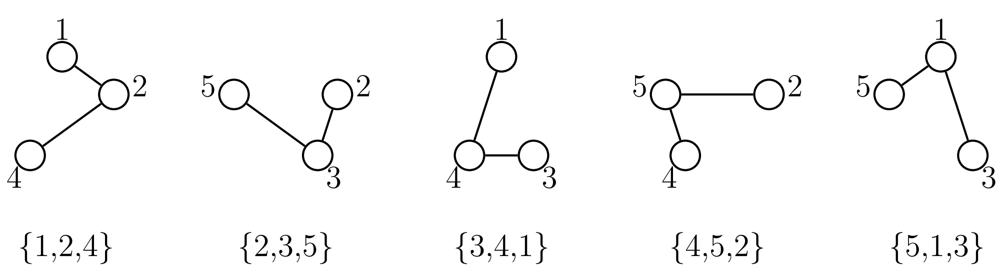


Figure 4.9: Block design under correlated error

In the following section, we will explore general sufficient conditions for obtaining a design under correlated errors such that $\mathrm{Cov}(\hat{\boldsymbol{\theta}})$ is in $\langle \boldsymbol{I}, \boldsymbol{J} \rangle$ form.

4.4 Sufficient Conditions

In this section, we want to determine sufficient conditions for designs to have $\mathrm{Cov}(\hat{\boldsymbol{\theta}})$ in $\langle \boldsymbol{I}, \boldsymbol{J} \rangle$ form. We will focus on the case that the error correlation is either ρ or 0 within block. For example,

$$V_1 = \begin{bmatrix} 1 & \rho & 0 \\ \rho & 1 & \rho \\ 0 & \rho & 1 \end{bmatrix} \tag{4.2}$$

for a block with size 3. From the previous section, we present each block by drawing an undirected graph. Edges in the graph represent pairwise dependencies among errors.

We can further analyze $\boldsymbol{B}\boldsymbol{V}\boldsymbol{B}^\top$ by using (1.4). We get

$$\begin{aligned}
&\boldsymbol{B}\boldsymbol{V}\boldsymbol{B}^\top = \boldsymbol{X}_1^\top \boldsymbol{V}\boldsymbol{X}_1 - \boldsymbol{X}_1^\top \boldsymbol{V}\boldsymbol{X}_2(\boldsymbol{X}_2^\top \boldsymbol{X}_2)^{-1}\boldsymbol{N}^\top - (\boldsymbol{X}_1^\top \boldsymbol{V}\boldsymbol{X}_2(\boldsymbol{X}_2^\top \boldsymbol{X}_2)^{-1}\boldsymbol{N}^\top)^\top \\
&+ \frac{1}{a}\boldsymbol{X}_1^\top \boldsymbol{V}\boldsymbol{X}_2(\boldsymbol{X}_2^\top \boldsymbol{X}_2)^{-1}\mathbf{1}_b\mathbf{1}_b^\top(\boldsymbol{X}_2^\top \boldsymbol{X}_2)^{-1}\boldsymbol{N}^\top \\
&+ \frac{1}{a}(\boldsymbol{X}_1^\top \boldsymbol{V}\boldsymbol{X}_2(\boldsymbol{X}_2^\top \boldsymbol{X}_2)^{-1}\mathbf{1}_b\mathbf{1}_b^\top(\boldsymbol{X}_2^\top \boldsymbol{X}_2)^{-1}\boldsymbol{N}^\top)^\top \\
&+ \boldsymbol{N}(\boldsymbol{X}_2^\top \boldsymbol{X}_2)^{-1}\boldsymbol{X}_2^\top \boldsymbol{V}\boldsymbol{X}_2(\boldsymbol{X}_2^\top \boldsymbol{X}_2)^{-1}\boldsymbol{N}^\top \\
&- \frac{1}{a}\boldsymbol{N}(\boldsymbol{X}_2^\top \boldsymbol{X}_2)^{-1}\boldsymbol{X}_2^\top \boldsymbol{V}\boldsymbol{X}_2(\boldsymbol{X}_2^\top \boldsymbol{X}_2)^{-1}\mathbf{1}_b\mathbf{1}_b^\top(\boldsymbol{X}_2^\top \boldsymbol{X}_2)^{-1}\boldsymbol{N}^\top \\
&- \frac{1}{a}(\boldsymbol{N}(\boldsymbol{X}_2^\top \boldsymbol{X}_2)^{-1}\boldsymbol{X}_2^\top \boldsymbol{V}\boldsymbol{X}_2(\boldsymbol{X}_2^\top \boldsymbol{X}_2)^{-1}\mathbf{1}_b\mathbf{1}_b^\top(\boldsymbol{X}_2^\top \boldsymbol{X}_2)^{-1}\boldsymbol{N}^\top)^\top \\
&+ (\frac{1}{a})^2\boldsymbol{N}(\boldsymbol{X}_2^\top \boldsymbol{X}_2)^{-1}\mathbf{1}_b\mathbf{1}_b^\top(\boldsymbol{X}_2^\top \boldsymbol{X}_2)^{-1}\boldsymbol{X}_2^\top \boldsymbol{V}\boldsymbol{X}_2(\boldsymbol{X}_2^\top \boldsymbol{X}_2)^{-1}\mathbf{1}_b\mathbf{1}_b^\top(\boldsymbol{X}_2^\top \boldsymbol{X}_2)^{-1}\boldsymbol{N}^\top.
\end{aligned} \tag{4.3}$$

There are nine terms in (4.3), and we examine each term as follows. The first term is straightforward.

$$\boldsymbol{X}_1^\top \boldsymbol{V}\boldsymbol{X}_1 = \begin{pmatrix} \boldsymbol{X}_{11} \\ \vdots \\ \boldsymbol{X}_{1b} \end{pmatrix}^\top \Big(\boldsymbol{V}_1 \oplus \boldsymbol{V}_2 \oplus \cdots \oplus \boldsymbol{V}_b\Big) \begin{pmatrix} \boldsymbol{X}_{11} \\ \vdots \\ \boldsymbol{X}_{1b} \end{pmatrix}$$

$$= \boldsymbol{X}_{11}^\top \boldsymbol{V}_1 \boldsymbol{X}_{11} + \cdots + \boldsymbol{X}_{1b}^\top \boldsymbol{V}_b \boldsymbol{X}_{1b},$$

which gives

$$\Big[\boldsymbol{X}_1^\top \boldsymbol{V}\boldsymbol{X}_1\Big]_{ij} = \sum_{H\in\mathcal{H}} \begin{cases} 1, & i=j \\ \rho, & ij \in E(H) \\ 0, & o.w. \end{cases} \tag{4.4}$$

For the second and third terms, we have

$$\boldsymbol{X}_1^\top \boldsymbol{V}\boldsymbol{X}_2(\boldsymbol{X}_2^\top \boldsymbol{X}_2)^{-1}\boldsymbol{N}^\top = \begin{pmatrix} \boldsymbol{X}_{11} \\ \vdots \\ \boldsymbol{X}_{1b} \end{pmatrix}^\top \Big(\boldsymbol{V}_1 \oplus \cdots \oplus \boldsymbol{V}_b\Big) \begin{pmatrix} \boldsymbol{X}_{21} \\ \vdots \\ \boldsymbol{X}_{2b} \end{pmatrix} (\boldsymbol{X}_2^\top \boldsymbol{X}_2)^{-1}\boldsymbol{N}^\top$$

$$= \Big(\boldsymbol{X}_{11}^\top \boldsymbol{V}_1 \boldsymbol{X}_{21} + \cdots + \boldsymbol{X}_{1b}^\top \boldsymbol{V}_b \boldsymbol{X}_{2b}\Big)\Big(\tfrac{1}{k_1} \oplus \cdots \oplus \tfrac{1}{k_b}\Big)\boldsymbol{N}^\top.$$

Thus, $\Big[\boldsymbol{X}_1^\top \boldsymbol{V}\boldsymbol{X}_2(\boldsymbol{X}_2^\top \boldsymbol{X}_2)^{-1}\boldsymbol{N}^\top\Big]_{ij} = \sum_{l=1}^{v} \frac{N_{il} + \rho \deg_{H_l}(i)}{k_l} N_{il}$

$$= \begin{cases} \sum_{i\in V(H_l)} \frac{1+\rho\deg_{H_l}(i)}{k_l}, & i=j \\ \sum_{i,j\in V(H_l)} \frac{1+\rho\deg_{H_l}(i)}{k_l}, & i\neq j. \end{cases} \tag{4.5}$$

The forth term can be computed as

$$\boldsymbol{X}_1^\top \boldsymbol{V}\boldsymbol{X}_2(\boldsymbol{X}_2^\top \boldsymbol{X}_2)^{-1}\mathbf{1}_b\mathbf{1}_b^\top(\boldsymbol{X}_2^\top \boldsymbol{X}_2)^{-1}\boldsymbol{N}^\top = \Big[N_{ij} + \rho\deg_{H_j}(i)\Big]\Big[k_i k_j\Big]\Big[N_{ji}\Big]$$

$$\Big[\boldsymbol{X}_1^\top \boldsymbol{V}\boldsymbol{X}_2(\boldsymbol{X}_2^\top \boldsymbol{X}_2)^{-1}\mathbf{1}_b\mathbf{1}_b^\top(\boldsymbol{X}_2^\top \boldsymbol{X}_2)^{-1}\boldsymbol{N}^\top\Big]_{ij} = \sum_{i\in V(H_l)} \frac{1+\rho\deg_{H_l}(i)}{k_l} \sum_{j\in V(H_h)} \frac{1}{k_h}. \tag{4.6}$$

The fifth term is the transpose of the forth term.

Next, we obtain a diagonal matrix depending on k, ρ and $|E(H)|$.

$$\boldsymbol{X}_2^\top \boldsymbol{V} \boldsymbol{X}_2 = \begin{pmatrix} \boldsymbol{X}_{21} \\ \vdots \\ \boldsymbol{X}_{2b} \end{pmatrix}^\top \Big(\boldsymbol{V}_1 \oplus \boldsymbol{V}_2 \oplus \cdots \oplus \boldsymbol{V}_b \Big) \begin{pmatrix} \boldsymbol{X}_{21} \\ \vdots \\ \boldsymbol{X}_{2b} \end{pmatrix}$$
$$= \boldsymbol{X}_{21}^\top \boldsymbol{V}_1 \boldsymbol{X}_{21} + \cdots + \boldsymbol{X}_{2b}^\top \boldsymbol{V}_b \boldsymbol{X}_{2b}$$
$$\Big[\boldsymbol{X}_2^\top \boldsymbol{V} \boldsymbol{X}_2 \Big]_{ij} = \begin{cases} k + 2\rho|E(H)|, & i = j \\ 0, & i \neq j. \end{cases}$$

The sixth term is

$$\begin{aligned} &\boldsymbol{N}(\boldsymbol{X}_2^\top \boldsymbol{X}_2)^{-1} \boldsymbol{X}_2^\top \boldsymbol{V} \boldsymbol{X}_2 (\boldsymbol{X}_2^\top \boldsymbol{X}_2)^{-1} \boldsymbol{N}^\top \\ &= \rho|E(H)| \boldsymbol{N}(\boldsymbol{X}_2^\top \boldsymbol{X}_2)^{-1} (\boldsymbol{X}_2^\top \boldsymbol{X}_2)^{-1} \boldsymbol{N}^\top. \end{aligned} \tag{4.7}$$

The 8$^{\text{th}}$ term is the transpose of the 7$^{\text{th}}$ term, and the 7$^{\text{th}}$ is computed as

$$\begin{aligned} &\boldsymbol{N}(\boldsymbol{X}_2^\top \boldsymbol{X}_2)^{-1} \boldsymbol{X}_2^\top \boldsymbol{V} \boldsymbol{X}_2 (\boldsymbol{X}_2^\top \boldsymbol{X}_2)^{-1} \mathbf{1}_b \mathbf{1}_b^\top (\boldsymbol{X}_2^\top \boldsymbol{X}_2)^{-1} \boldsymbol{N}^\top \\ &= (1 + \rho|E(H)|) \boldsymbol{N}(\boldsymbol{X}_2^\top \boldsymbol{X}_2)^{-1} (\boldsymbol{X}_2^\top \boldsymbol{X}_2)^{-1} \mathbf{1}_b \mathbf{1}_b^\top (\boldsymbol{X}_2^\top \boldsymbol{X}_2)^{-1} \boldsymbol{N}^\top. \end{aligned} \tag{4.8}$$

The last term is

$$\begin{aligned} &\boldsymbol{N}(\boldsymbol{X}_2^\top \boldsymbol{X}_2)^{-1} \mathbf{1}_b \mathbf{1}_b^\top (\boldsymbol{X}_2^\top \boldsymbol{X}_2)^{-1} \boldsymbol{X}_2^\top \boldsymbol{V} \boldsymbol{X}_2 (\boldsymbol{X}_2^\top \boldsymbol{X}_2)^{-1} \mathbf{1}_b \mathbf{1}_b^\top (\boldsymbol{X}_2^\top \boldsymbol{X}_2)^{-1} \boldsymbol{N}^\top \\ &= (1 + \rho|E(H)|) \boldsymbol{N}(\boldsymbol{X}_2^\top \boldsymbol{X}_2)^{-1} \mathbf{1}_b \mathbf{1}_b^\top (\boldsymbol{X}_2^\top \boldsymbol{X}_2)^{-1} (\boldsymbol{X}_2^\top \boldsymbol{X}_2)^{-1} \mathbf{1}_b \mathbf{1}_b^\top (\boldsymbol{X}_2^\top \boldsymbol{X}_2)^{-1} \boldsymbol{N}^\top. \end{aligned} \tag{4.9}$$

If each block has equal size k, then we can rewrite $(\boldsymbol{X}_2^\top \boldsymbol{X}_2)^{-1}$ as $\frac{1}{k}\boldsymbol{I}$. Notice that $\boldsymbol{N}\boldsymbol{N}^\top = r_1 \oplus r_2 \oplus \cdots \oplus r_v$ and $\boldsymbol{N}\mathbf{1}_b\mathbf{1}_b^\top \boldsymbol{N}^\top = \Big[r_i r_j \Big]_{ij}$. As a result, (4.7) - (4.9) are completely symmetric if the design has equal replication for each treatment, and we obtain

$$
\begin{aligned}
(4.4) &= \begin{cases} r, & i = j \\ \sum\limits_{ij \in E(H)} \rho, & i \neq j, \end{cases} \\
(4.6) &= \frac{2r}{ak^2} \sum_{i \in V(H_l)} 1 + \rho \deg_{H_l}(i), \\
(4.7) &= \frac{\rho|E(H)|}{k^2} \boldsymbol{N}\boldsymbol{N}^\top, \\
(4.8) &= \frac{1 + \rho|E(H)|}{k^3} \boldsymbol{N}\mathbf{1}_b\mathbf{1}_b^\top \boldsymbol{N}^\top, \\
(4.9) &= \frac{b(1 + \rho|E(H)|)}{k^4} \boldsymbol{N}\mathbf{1}_b\mathbf{1}_b^\top \boldsymbol{N}^\top.
\end{aligned}
$$

If we assume the design is equalreplicate and equal block size, then the diagonal elements of (4.4) are the same. The off diagonal element of (4.4) depend on $\sum\limits_{ij \in E(H)} \rho$, which is number of edges between each pair of vertices in the composition of all subgraphs. Structure of (4.6) only depends on $\sum\limits_{i \in V(H_l)} \deg_{H_l}(i)$. Notice that (4.5) is hard to be completely symmetric, we calculate the sum of itself and its transpose as (4.10). The diagonal of (4.10) depends on $\sum\limits_{i \in V(H_l)} \deg_{H_l}(i)$, and the off diagonal depends on $\sum\limits_{\{i,j\} \in V(H_l)} \deg_{H_l}(i) + \deg_{H_l}(j)$. If $\sum\limits_{\{i,j\} \in V(H_l)} \deg_{H_l}(i) + \deg_{H_l}(j)$ are the same for each pair of treatments, then $\sum\limits_{i \in V(H_l)} \deg_{H_l}(i) = (v-1)\left(\sum\limits_{\{i,j\} \in V(H_l)} \deg_{H_l}(i) + \deg_{H_l}(j)\right)$ is also the same for each treatment i. Therefore,

$$
\begin{aligned}
&\boldsymbol{X}_1^\top \boldsymbol{V} \boldsymbol{X}_2 (\boldsymbol{X}_2^\top \boldsymbol{X}_2)^{-1} \boldsymbol{N}^\top + (\boldsymbol{X}_1^\top \boldsymbol{V} \boldsymbol{X}_2 (\boldsymbol{X}_2^\top \boldsymbol{X}_2)^{-1} \boldsymbol{N}^\top)^\top \\
&= \begin{cases} \frac{2}{k} \sum\limits_{i \in V(H_l)} 1 + \rho \deg_{H_l}(i), & i = j \\ \frac{1}{k} \sum\limits_{\{i,j\} \in V(H_l)} 2 + \rho(\deg_{H_l}(i) + \deg_{H_l}(j)), & i \neq j. \end{cases}
\end{aligned} \tag{4.10}
$$

From (1.6), the covariance matrix depends on $\boldsymbol{A}^{-1}$ and $\boldsymbol{B}\boldsymbol{V}\boldsymbol{B}^\top$. From Theorem 7, we know that a VBD with equal replication for each treatment guarantees that $\boldsymbol{A}$ is completely symmetric. Furthermore, together with the analysis of $\boldsymbol{B}\boldsymbol{V}\boldsymbol{B}^\top$, we obtain sufficient conditions below for $\mathrm{Cov}(\hat{\boldsymbol{\theta}})$ to be in $\langle \boldsymbol{I}, \boldsymbol{J} \rangle$ form.

Theorem 12. *Consider equal-size block designs D under the assumption that* $\mathrm{Cov}(\boldsymbol{\epsilon}) = \sigma^2\boldsymbol{V}$*. Suppose a collection $\mathcal{H}$ represents the blocks of D. D has a completely symmetric* $\mathrm{Cov}(\hat{\boldsymbol{\theta}})$ *if it satisfies the following conditions:*

- $\{V(H) : H \in \mathcal{H}\}$ *is the block collection of a* $\mathrm{BIBD}(v,\, r = \frac{bk}{v},\, k,\, b,\, \lambda)$.
- $|E(H)|$ *is constant for all* $H \in \mathcal{H}$.
- *The composition of all $H \in \mathcal{H}$ is a λ_1-complete multigraph, where $\lambda_1 \leq \lambda$.*
- $\sum\limits_{\substack{H:\{i,j\}\in V(H)\\ H\in\mathcal{H}}} \deg_H(i) + \deg_H(j)$ *is constant for each treatment pair, i and j.*

Example 14. Consider a design where each block has three treatments and each pair of treatment within block are considered as concurrence if they are neighbours. Recall the 5 blocks in Figure 4.9, we note that it is not a VBD. We add 5 more blocks try to make it balanced as shown in Figure 4.10. The red dashed edge represents there is no correlation between the pair of treatments, and black edge represents there is correlation between the pair. The correlation matrix within each block is $\boldsymbol{V}_1$, given in (4.2).

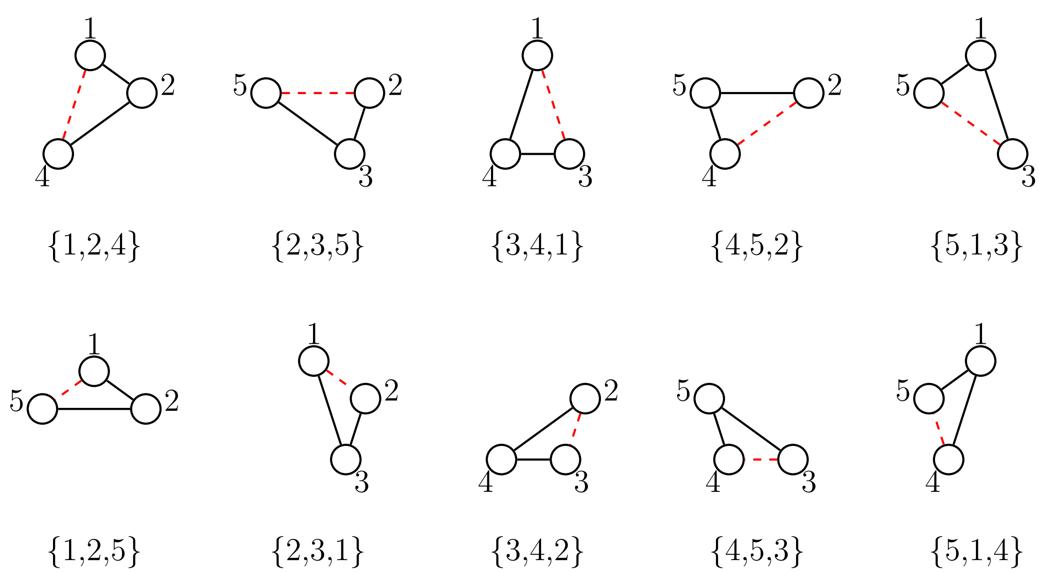


Figure 4.10: VBD with $v = 5$, $b = 10$, $k = 3$, $r = 6$ and $\lambda = 3$

(a) Composition of H in Figure 4.10 (K_5^2) (b) Composition of $\overline{H}$ in Figure 4.10 (K_5)

Figure 4.11: Composition of H and $\overline{H}$ in Figure 4.10 respectively

It is obvious that the design is equilreplicate, and each graph contains two edges. Treatment pair 1 and 2, are in blocks $\{1,2,4\}$, $\{1,2,5\}$, $\{2,3,1\}$, and treatment pair, 1 and 3, are in blocks $\{1,4,3\}$, $\{3,1,5\}$, $\{2,3,1\}$. Thus, $\sum_{\{1,2\}\in V(H)} \deg_H(1)+\deg_H(2) = (1+2)+(1+2)+(1+1) = 8 = (1+1)+(2+1)+(1+2) = \sum_{\{1,3\}\in V(H)} \deg_H(1)+\deg_H(3)$. We assume $\rho = 0.1$ and calculate the covariance matrix of LSE of $\boldsymbol{\theta}$, which gives $\mathrm{Cov}(\hat{\boldsymbol{\theta}}) = \sigma^2(0.18667\boldsymbol{I} + 0.00044\boldsymbol{J})$. Thus, the design is VBD, and in particular, its $\mathrm{Cov}(\hat{\boldsymbol{\theta}})$ is completely symmetric.

4.5 Construction Methods

In this section, we construct VBDs with completely symmetric $\mathrm{Cov}(\hat{\boldsymbol{\theta}})$ by finding graphs that satisfy the conditions in Theorem 12. Notice that we want equal block size, that is, each graph that representing the block has the same number of vertices. In addition, the number of edges is the same for each graph. In the following examples, we assume $\rho = 0.1$ for calculating $\mathrm{Cov}(\hat{\boldsymbol{\theta}})$.

Given a block design $D = (X, \mathcal{B})$ on v treatments, each graph that represents a block in $\mathcal{B}$ is a subgraph of K_{k_B}, where k_B is the size of the block.

From Example 14, we notice that the design satisfies the condition that both the composition of all graphs and the composition of all complements of the graphs as shown in Figure 4.11 are λ_1-complete multigraphs and λ_2-complete multigraphs respectively. However, this condition does not imply the degree summation condition of Theorem 12. The following is a counterexample.

Example 15. Consider an experiment with $v = 11, b = 11$, and $k = 5$. Define a difference set $D = \{1, 3, 4, 5, 9\}(\text{mod } 11)$. Every nonzero integer (mod 11) is a difference of two elements of D in exactly 2 ways, that is, every pair of distinct elements of D occurs 2 times. Let each edge coloured by distance which is the difference of their vertex numbers in the complete graph on $\{1, 3, 4, 5, 9\}$ as in Figure 4.12.

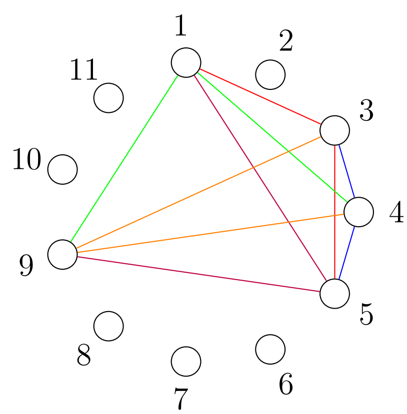


Figure 4.12: K_5 on $\{1, 3, 4, 5, 9\}$

Suppose that the covariance matrix within block is

$$V_1 = \begin{bmatrix} 1 & 0 & 0 & \rho & \rho \\ 0 & 1 & 0 & \rho & 0 \\ 0 & 0 & 1 & \rho & \rho \\ \rho & \rho & \rho & 1 & 0 \\ \rho & 0 & \rho & 0 & 1 \end{bmatrix}.$$

Blocks can be represented by graphs as shown in Figure 4.13, and their treatments are listed as: $\{1, 3, 4, 5, 9\}$, $\{2, 4, 5, 6, 10\}$, $\{3, 4, 5, 6, 11\}, \ldots, \{11, 2, 3, 4, 8\}$.

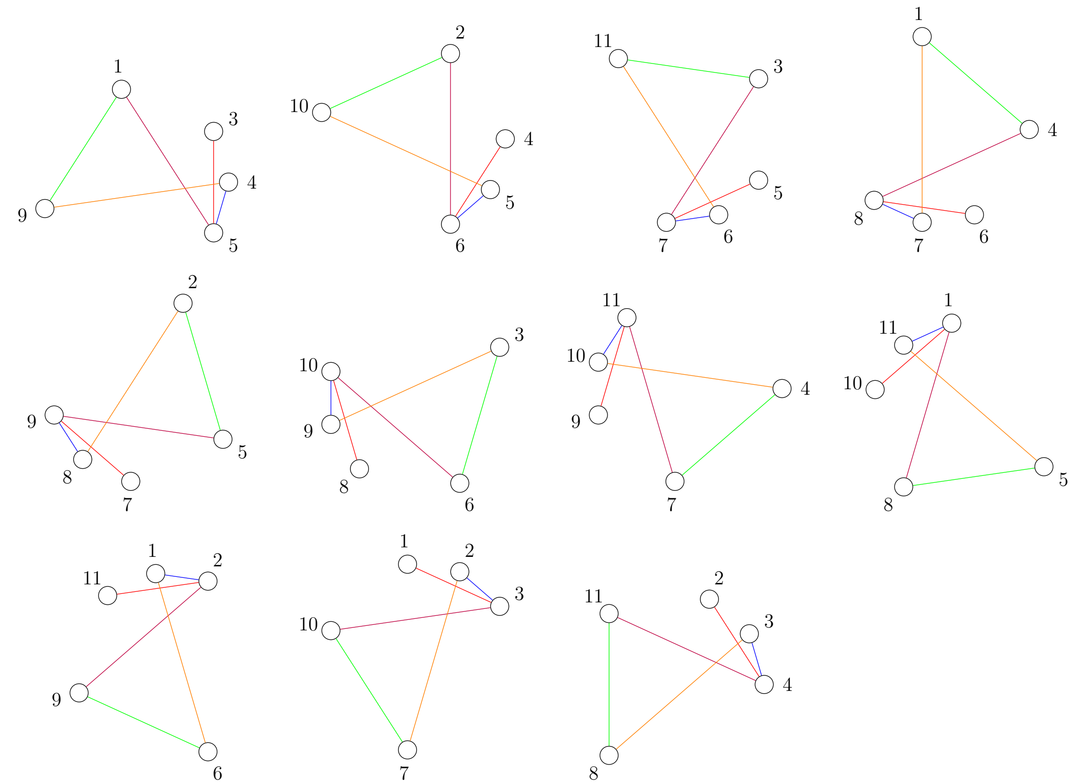


Figure 4.13: An example of block design under the assumption of correlated error

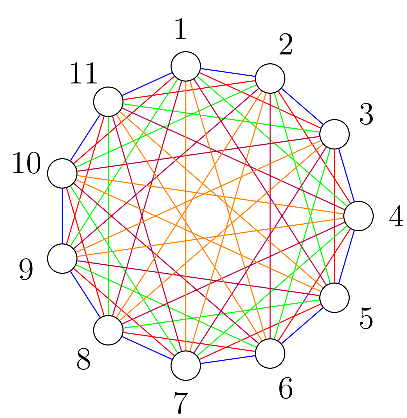


Figure 4.14: Composition of all graphs in Figure 4.13

If we choose any subgraph H of K_5 on 5 edges so that it has exactly one edge of each colour and same graph apply on translates of vertices of $V(K_5)$ (mod 11) as in Figure 4.13, the composition of those graphs and composition of their complements are both complete graph K_{11}. However, for pair of vertices $\{i,j\}$ with distance $min((i-j)(\text{mod } v),(j-i)(\text{mod } v))$ equal to two, say $\{i,j\}=\{1,3\}$, $\sum\limits_{\{1,3\}\in V(H)} \deg_H(1)+\deg_H(3)=(1+2)+(1+3)=7$; for the pair of vertices with distance equal to four, say $\{1,5\}$, $\sum\limits_{\{1,5\}\in V(H)} \deg_H(1)+\deg_H(5)=(2+3)+(2+3)=10$. As a result, it does not satisfies the defree sum condition in Theorem 12. Also, it is easy to compute $\text{Cov}(\hat{\boldsymbol{\theta}})$ as follows,

$$\text{Cov}(\hat{\boldsymbol{\theta}})=\sigma^2\begin{bmatrix}
0.21810 & 0.00219 & 0.00322 & 0.00219 & 0.00012 & 0.00322 & 0.00322 & 0.00012 & 0.00219 & 0.00322 & 0.00219\\
0.00219 & 0.21810 & 0.00219 & 0.00322 & 0.00219 & 0.00012 & 0.00322 & 0.00322 & 0.00012 & 0.00219 & 0.00322\\
0.00322 & 0.00219 & 0.21810 & 0.00219 & 0.00322 & 0.00219 & 0.00012 & 0.00322 & 0.00322 & 0.00012 & 0.00219\\
0.00219 & 0.00322 & 0.00219 & 0.21810 & 0.00219 & 0.00322 & 0.00219 & 0.00012 & 0.00322 & 0.00322 & 0.00012\\
0.00012 & 0.00219 & 0.00322 & 0.00219 & 0.21810 & 0.00219 & 0.00322 & 0.00219 & 0.00012 & 0.00322 & 0.00322\\
0.00322 & 0.00012 & 0.00219 & 0.00322 & 0.00219 & 0.21810 & 0.00219 & 0.00322 & 0.00219 & 0.00012 & 0.00322\\
0.00322 & 0.00322 & 0.00012 & 0.00219 & 0.00322 & 0.00219 & 0.21810 & 0.00219 & 0.00322 & 0.00219 & 0.00012\\
0.00012 & 0.00322 & 0.00322 & 0.00012 & 0.00219 & 0.00322 & 0.00219 & 0.21810 & 0.00219 & 0.00322 & 0.00219\\
0.00219 & 0.00012 & 0.00322 & 0.00322 & 0.00012 & 0.00219 & 0.00322 & 0.00219 & 0.21810 & 0.00219 & 0.00322\\
0.00322 & 0.00219 & 0.00012 & 0.00322 & 0.00322 & 0.00012 & 0.00219 & 0.00322 & 0.00219 & 0.21810 & 0.00219\\
0.00219 & 0.00322 & 0.00219 & 0.00012 & 0.00322 & 0.00322 & 0.00012 & 0.00219 & 0.00322 & 0.00219 & 0.21810
\end{bmatrix}.$$

This result shows that $\text{Cov}(\hat{\boldsymbol{\theta}})$ is not in the $\langle \boldsymbol{I}, \boldsymbol{J}\rangle$ form.

From Example 15, we claim that graphs in Figure 4.13 and complements of those graphs decompose λ_1-complete multigraph and λ_2-complete multigraph, respectively. However, the design is not a VBD. To construct a VBD, if there is a regular subgraph of K_5 on vertices $\{1,3,4,5,9\}$ such that contains each colour the same number of times, then this subgraph and its translates should satisfy the degree summation condition. We illustrate it in Example 16.

Example 16. Figure 4.15 represents block $B_1=\{1,3,4,5,9\}$ with error correlation matrix within block as

$$V_1=\begin{bmatrix}
1 & 0 & 0 & \rho & \rho\\
0 & 1 & \rho & \rho & 0\\
0 & \rho & 1 & 0 & \rho\\
\rho & \rho & 0 & 1 & 0\\
\rho & 0 & \rho & 0 & 1
\end{bmatrix}.$$

As in Example 15, each colour (distance) of edges occurs exactly once. The composition of graph in Figure 4.15 and its translates is K_{11} as in Figure 4.14. The design is obvious equal replicate. For each pair, $\sum_{\{i,j\}\in V(H)} \deg_H(i) + \deg_H(j) = (2+2)\cdot 2 = 8$. Thus this design satisfies all conditions in Theorem 12. By taking B_1 and its translates, we can obtain a VBD with completely symmetric $\mathrm{Cov}(\hat{\boldsymbol{\theta}})$. We calculate that $\mathrm{Cov}(\hat{\boldsymbol{\theta}}) = \sigma^2(0.21591\boldsymbol{I} + 0.00219\boldsymbol{J})$.

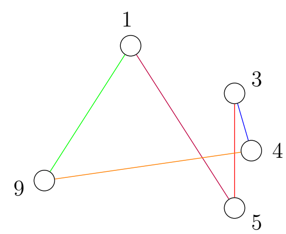


Figure 4.15: A cycle of K_5 on $\{1, 3, 4, 5, 9\}$

Definition 10. Let $(G, +)$ be a finite group of order v with identity 0. A (v, k, λ) - *difference set* is a nonempty proper subset $D \subset G$, such that D has k elements, and the multiset of differences $\{i - j : i, j \in D \,\&\, i \neq j\}$ contains every element in $G \setminus \{0\}$ exactly λ times.

Definition 11. Let $q \equiv 3 (\mathrm{mod}\ 4)$ be a prime integer and let $(\mathbb{Z}_q, +)$ be the additive group of integers modulo q. The *Paley Difference Set* in this group is the subset D of quadratic residues modulo q.

Example 17. Consider a $(19, 9, 4)$ Paley difference set, we obtain a BIBD(19, 9, 9, 19, 4) by taking $\{1, 4, 5, 6, 7, 9, 11, 16, 17\}$ and its translates as blocks. Similarly with the previous examples, different edge colour represent the different distance between the pair of vertices. For the complete graph K_9 on vertices $\{1, 4, 5, 6, 7, 9, 11, 16, 17\}$ as in Figure 4.16, there exists a $(1, 4, 5, 7, 11, 17, 9, 16, 6, 1)$-cycle such that each colour using exactly once. Blocks can be represented by graphs as in Figure 4.18, and treatments in each block are listed as: $\{1, 4, 5, 7, 11, 17, 9, 16, 6\}$, $\{2, 5, 6, 8, 12, 18, 10, 17, 7\}$,

$\{3, 6, 7, 9, 13, 19, 11, 18, 8\}, \ldots, \{19, 3, 4, 6, 10, 16, 8, 15, 5\}$. Then

$$V_1 = \begin{bmatrix} 1 & \rho & 0 & 0 & 0 & 0 & 0 & 0 & \rho \\ \rho & 1 & \rho & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \rho & 1 & \rho & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \rho & 1 & \rho & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \rho & 1 & \rho & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \rho & 1 & \rho & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \rho & 1 & \rho & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \rho & 1 & \rho \end{bmatrix}.$$

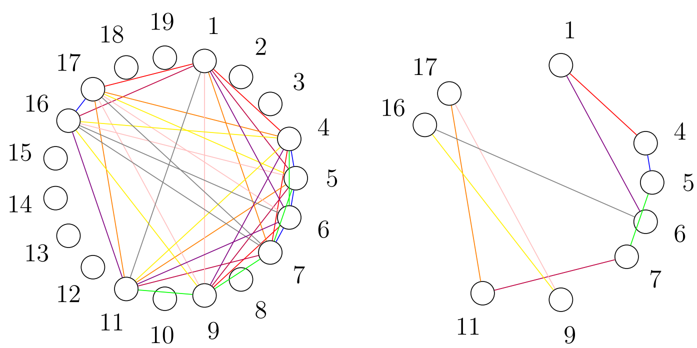


Figure 4.16: K_9 on $\{1, 4, 5, 6, 7, 9, 11, 16, 17\}$

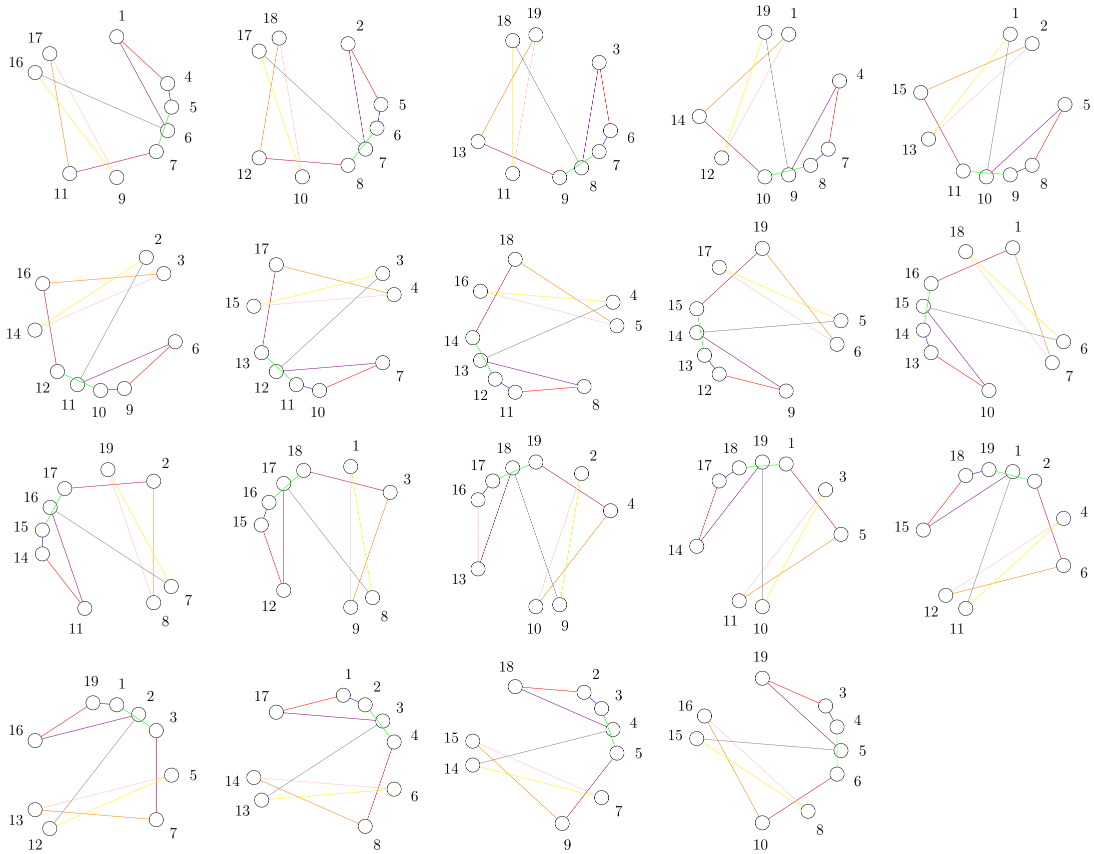


Figure 4.17: Cycles representing 19 blocks

The same with translates of $\{1, 4, 5, 6, 7, 9, 11, 16, 17\}$, then we obtain 19 graphs shown in Figure 4.17, which gives $\text{Cov}(\hat{\boldsymbol{\theta}}) = \sigma^2(0.11546\boldsymbol{I} + 0.00094\boldsymbol{J})$. The composition of all cycles in Figure 4.17 is a K_{19} in Figure 4.18.

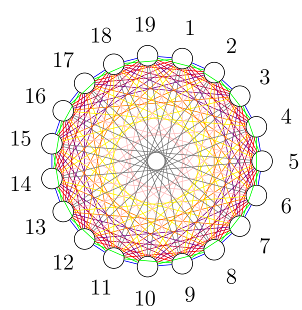


Figure 4.18: Composition of all cycles in Figure 4.17 is a K_{19}

Theorem 13. *For a difference set $D = (v, k, \lambda)$, it can be drawn as a complete* *graph K_k, denote it K_D, and label $V(K_D)$ by the integer in D. Let $E(K_D)$ coloured by distance between the incident vertices. If there exists a regular graph on $V(K_D)$ such that each colour of edges occurs equal times, then this graph and graphs on its translates modulo v represent a block design under error structure, and this block design is variance balanced.*

Theorem 14. *Suppose K_v can be decomposed into b copies of a d-regular graph G on k vertices, and there exists a* $\mathrm{BIBD}(v,\, r = \frac{v-1}{d},\, k,\, b,\, \lambda = \frac{k-1}{d})$*. Then there exists a block design on v treatments under error structure corresponding to G such that* $\mathrm{Cov}(\hat{\boldsymbol{\theta}})$ *is completely symmetric.*

Proof. Given a graph G-decomposition of K_v such that G is d-regular graph on k vertices, and $\mathrm{BIBD}(v,\, r,\, k,\, b,\, \lambda) = (X, \mathcal{B})$. We construct an isomorphism from $V(G)$ to B_i for each $B_i \in \mathcal{B}$. Thus, $b = \frac{\lambda v(v-1)}{k(k-1)} = \frac{v(v-1)}{dk} \implies \lambda = \frac{k-1}{d}$ and $r = \frac{\lambda(v-1)}{k-1} = \frac{v-1}{d}$. Then it automatically satisfies first three conditions in Theorem 12. Since G is regular, thus $\sum_{H:\{i,j\} \in V(H)} \deg_H(i) + \deg_H(j) = 2\lambda \deg_G(i)$ which is obviously constant. $\square$

Remark. Suppose there exists a H-decomposition of G, where H represents a block of size k under correlated error structure. Then, there exists a block design on v treatments under error structure corresponding to H such that $\mathrm{Cov}(\hat{\boldsymbol{\theta}})$ is completely symmetric.

Remark. For a given block $B \in \mathcal{B}$ and its corresponding graph H on k vertices, where H is a regular graph, we colour $E(H)$ by colour 1. Use colour 2 to colour $E(K_k)$, and let G be the composition of coloured H and coloured K_k. We define an edge-2-coloured complete graphs $K_{1,2}^{\lambda_1,\lambda_2}$ as an composition of $K_v^{\lambda_1}$ coloured by colour 1 and $K_v^{\lambda_2}$ coloured by colour 2. The construction of block design with completely symmetric covariance can be addressed to construction of G-decomposition of $K_{1,2}^{\lambda_1,\lambda_2}$.

Example 18. Recall Example 15, there exists a self complementary subgraph G as Figure 4.19a of K_5 as Figure 4.12. We can obtain a desired design by taking G and $\overline{G}$ and their translates as blocks, and $\mathrm{Cov}(\hat{\boldsymbol{\theta}}) = \sigma^2(0.01079\boldsymbol{I} + 0.09826\boldsymbol{J})$.

(a) G (b) $\overline{G}$

Figure 4.19: a self-complementary graph

Remark. Suppose there exists a BIBD(X, $\mathcal{B}$) where $|X| = v$, $|\mathcal{B}| = b$, and each block $B_i \in \mathcal{B}$ contains k treatments. There exists a VBD if the correlated error structure within each block corresponds to a self complementary subgraph G of K_k. The design can be constructed by taking each block in $\mathcal{B}$ twice, and treatments within block are experimented as in Example 18.

In most experiments, we can not control the error produced from experiment. As a result, a general method to construct a VBD is worth studying.

Theorem 15. *If there exists a BIBD $= (X, \mathcal{B})$ with each block of size k, and the correlated error structure within block corresponds to graph G. If each block in $\mathcal{B}$ is replaced by all $\frac{k!}{|Aut(G)|}$ distinct copies of G on the treatments of that block, then the resulting design is variance balanced.*

Knowing that for a graph G with n vertices, there are $\frac{n!}{|Aut(G)|}$ distinct graphs in total that are automorphic to G. For a graph with trivial automorphism group, there are $n!$ graphs needed.

Theorem 16. *Given G with $V(G) = q$, where q is a prime power, label its vertex set with $\mathbb{F}_q$. Then the collection of $q(q-1)$ blocks $\{a \cdot G + b : a, b \in \mathbb{F},\ a \neq 0\}$ is a VBD with completely symmetric* $\mathrm{Cov}(\hat{\boldsymbol{\theta}})$.

Example 19. To illustrate Theorem 16, assume there is a error structure represented as a graph in Figure 4.20. We want to determine a variance balance design under this error structure. We shift the treatment i to $a \cdot i \pmod 7$ for each treatment, where $a = 1, \ldots, 6$ as shown. For each graph in Figure 4.20, we also take the additive shifts, that is, shift the treatment i to $i + b \pmod 7$, where $b \in \mathbb{Z}_7$. There are $7(7-1) = 42$ blocks in total, which is much better than $7!$.

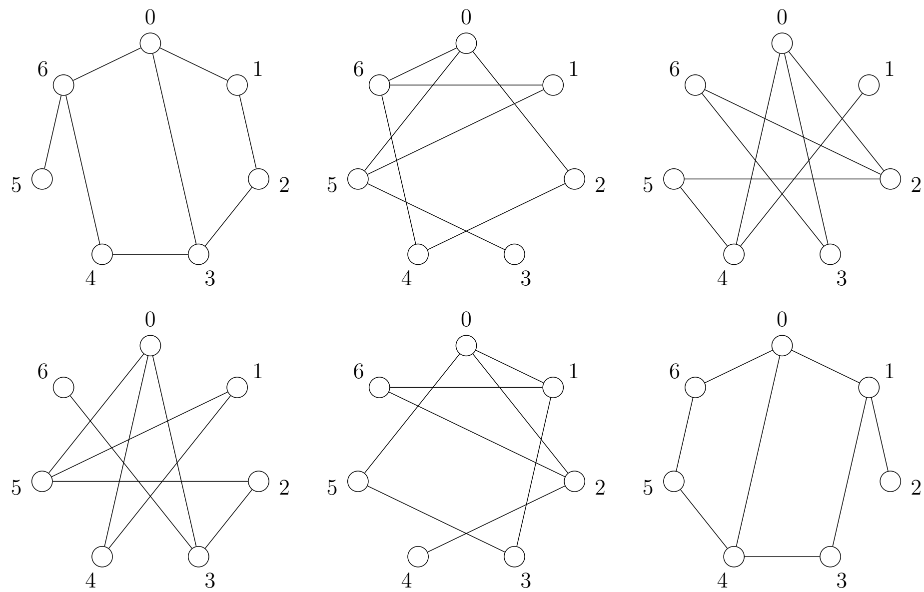


Figure 4.20: aG, $a = 1, \ldots, 6$

Also, for some specific given error structures, the only way to make the degree sum to be constant is to take all non-automorphic graphs.

Example 20. Assume that the correlation structure within block as in (4.11), which its corresponding graph is shown as Figure 4.21, and it can be imagined as field plots such that neighbour plots are correlated in field experiment. Notice that there are two kinds of vertices, $\deg(1) = \deg(2) = \deg(3) = \deg(4) = 1$ and $\deg(5) = 4$, where we think of 5 as a center vertex. To balance the degree sum, the best way is to make each vertex (treatment) be the center once.

$$V_1 = \begin{bmatrix} 1 & 0 & 0 & 0 & \rho \\ 0 & 1 & 0 & 0 & \rho \\ 0 & 0 & 1 & 0 & \rho \\ 0 & 0 & 0 & 1 & \rho \\ \rho & \rho & \rho & \rho & 1 \end{bmatrix}. \tag{4.11}$$

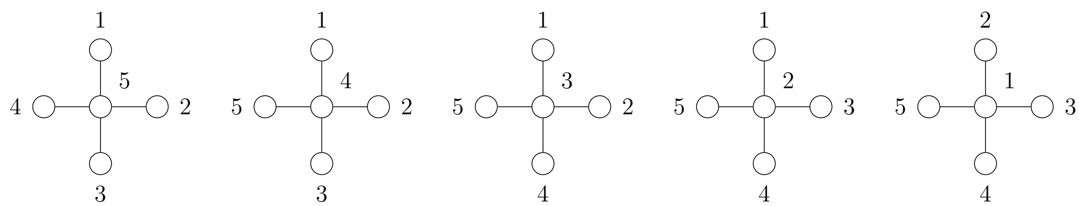


Figure 4.21: VBD with $v = 5$, $b = 5$, $k = 5$, $r = 5$ and $\lambda = 5$

We calculate that $\mathrm{Cov}(\hat{\boldsymbol{\theta}}) = \sigma^2(0.192\boldsymbol{I} + 0.008\boldsymbol{J})$.

Theorem 17 (Wilson)**.** *Given a graph G, K_v can be G-decomposed for all sufficiently large integers v for which v satisfies conditions:*

- $v(v-1) \equiv 0 (\mathrm{mod}\ 2m_G)$
- $v - 1 \equiv 0 (\mathrm{mod}\ g_G)$

where $m_G = |E(G)|$, and $g_G = \gcd\left(\deg_G(v_i) : v_i \in V(G)\right)$.

Theorem 17 from Wilson (1975) gives conditions for existence of D-decomposition of K_v for sufficiently large v.

Theorem 18. *For a VBD D_1 on k treatments under certain error structure, where D_1 satisfies all conditions in Theorem 12, if there exists an $D_2 = \mathrm{BIBD}(v, r, k, b, \lambda)$, then we can construct a VBD with completely symmetric $\mathrm{Cov}(\hat{\boldsymbol{\theta}})$ on v treatments by performing design D_1 on each block in the D_2.*

Example 21. Given a BIBD(8, 7, 4, 14, 3) containing blocks in Table 4.2 and a VBD D as in the Figure 4.22. For the design D on four vertices, it is obvious that the design satisfies Theorem 12.

{1,2,3,5}	{1,2,6,8}	{1,3,4,8}	{1,3,6,7}	{1,5,7,8}	{1,2,4,7}	{1,4,5,6}
{4,6,7,8}	{3,4,5,7}	{2,5,6,7}	{2,4,5,8}	{2,3,4,6}	{3,5,6,8}	{2,3,7,8}

Table 4.2: BIBD(8, 7, 4, 14, 3)

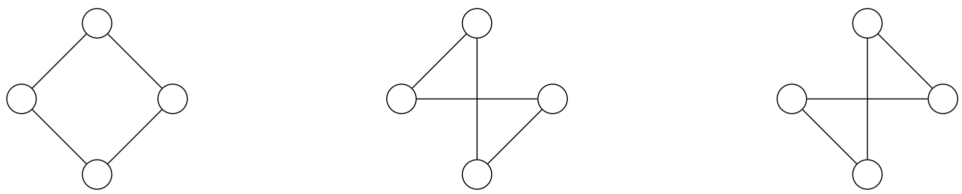


Figure 4.22: A VBD D with $v = 4$, $b = 3$, $k = 4$, $r = 3$ and $\lambda = 3$

We construct a new block design by applying the design D to each blocks in Table 4.2. For example, for block $\{1, 2, 3, 5\}$, if we apply the design D to those four treatments then we have three blocks as shown in Figure 4.23.

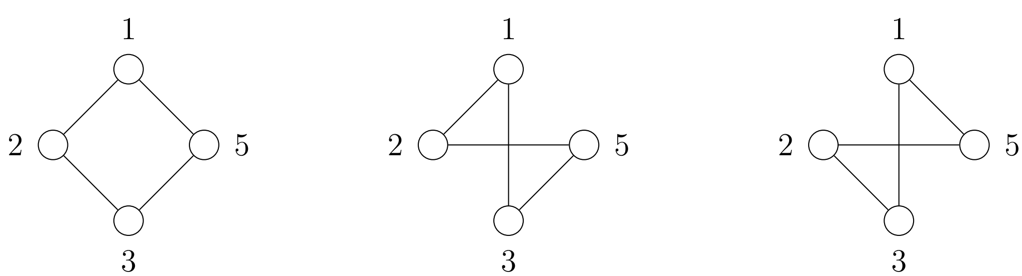


Figure 4.23: Apply D on block $\{1, 2, 3, 5\}$

As a result, there are $14 \times 3 = 42$ blocks in total. We can obtain that $\mathrm{Cov}(\hat{\boldsymbol{\theta}}) = \sigma^2(0.005185\boldsymbol{I} + 0.00066\boldsymbol{J})$.

Chapter 5

Discussion

We introduced variance balanced designs (VBD) and the associated statistical model in the first chapter. Then we reviewed several existing construction methods of VBD under the assumption that the errors within each block are independent. In addition, we derived theoretical properties for constructing a block design such that its covariance matrix of LSE of treatment effect ($\mathrm{Cov}(\hat{\boldsymbol{\theta}})$) is completely symmetric (in the algebra $\langle \boldsymbol{I}, \boldsymbol{J} \rangle$ form) and reviewed construction methods of such design. Furthermore, we studied the criteria for constructing a block design with completely symmetric $\mathrm{Cov}(\hat{\boldsymbol{\theta}})$ under the assumption that errors within blocks are correlated. To illustrate the construction methods, we modelled the correlation structure using graph theory and extended the problem of construction of block designs as a graph decomposition problem.

Assuming errors are independent, if the block sizes are equal, then a VBD is simply a BIBD. We determined the conditions of VBD if block sizes are unequal, and reviewed the construction method from PBD to VBD. Furthermore, we determined the conditions for block design such that $\mathrm{Cov}(\hat{\boldsymbol{\theta}})$ is completely symmetric, which is just equilreplicate VBD.

When we analyzed the $\mathrm{Cov}(\hat{\boldsymbol{\theta}})$ of design under correlated error structure within each block, we determined designs with equal block size, and $\mathrm{Cov}(\hat{\boldsymbol{\theta}})$ is completely symmetric. We determined general construction methods for particular error structures represented by regular graphs. Since we want to balance the degree sum for each pair of treatments as stated in Theorem 12, weighted-edge or edge-coloured graph decompositions may be helpful for developing construction methods under more irregular error structures.

We recall that a VBD is defined as a design such that the variance of all elementary contrasts are the same. Having a completely symmetric $\mathrm{Cov}(\hat{\boldsymbol{\theta}})$ is not a necessary condition that block design be variance balanced. A question worth further study is the determination of necessary and sufficient conditions for existence of variance balanced designs under correlated error. Moreover, if the block sizes are unequal, the $\mathrm{Cov}(\hat{\boldsymbol{\theta}})$ will be much more complicated, and such design criteria have not been studied to this point. The case of unequal block sizes merits further work, both for correlated and uncorrelated error.

Appendix A

R Code

A.1 Main function

```
The function is used to compute the covariance matrix of the least squares
    estimator. You should set up incidence matrix and covariance matrix of
    error first and then use the function.
```

```
Input variables:
N - incidence matrix
v - the number of treatment
b - the number of block
Error - covariance matrix of errors

Output:
Information matrix C
Covariance matrix Cov
```

```
getcov<-function(N,v,b,Error){#Get covariance matrix
    n=sum(N)
    p=v+b
```

```
    X=matrix(0,nrow=n,ncol=p)
    V=diag(rep(1,v))
    B=diag(rep(1,b))
    L=0
    for (j in c(1:b)){
        for (i in c(1:v)){
            if (N[i,j]==1){
                L=L+1
                X[L,]=c(V[i,],B[j,])
            }
        }
    }
    X1=X[,c(1:v)]
    X2=X[,c((v+1):p)]
    invX2=solve(t(X2)%*%X2)
    a=sum(invX2)
    Ib=rep(1,b)%*%t(rep(1,b))
    A=t(X1)%*%X1-N%*%invX2%*%t(N)+N%*%invX2%*%Ib%*%invX2%*%t(N)/a
    B=t(X1)-N%*%invX2%*%t(X2)+N%*%invX2%*%Ib%*%invX2%*%t(X2)/a
    C=t(X1)%*%X1-N%*%invX2%*%t(N)
    Cov=solve(A)%*%B%*%Error%*%t(B)%*%t(solve(A))
    my_list <- list("Information.matrix" = C, "Covariance.matrix" =
        round(Cov,3))
    return(my_list)
}
```

Bibliography

[1] Clatworthy, W.H. (1973). *Tables of two-associate-class partially balanced designs.* [Washington, D.C.: U.S.] National Bureau of Standards.

[2] Gill, P.S., & Shukla, G.K. (1985). Efficiency of nearest neighbour balanced block designs for correlated observations. *Biometrika, 72*(3), 539-544.

[3] Gupta, S.C., & Jones, B. (1983). Equireplicate balanced block designs with unequal block sizes. *Biometrika, 70*(2), 433-440.

[4] Gurevitch, J., & Chester, S. (1986). Analysis of repeated measures experiments. *ecology, 67*(1), 251-255.

[5] Hall, W. B., & Jarrett, R. G. (1981). Nonresolvable incomplete block designs with few replicates. *Biometrika, 68*(3), 617-627.

[6] Hedayat, A., & Federer, W.T. (1974). Pairwise and variance balanced incomplete block designs. *Annals of the Institute of Statistical Mathematics*, 26, 331-338.

[7] Hedayat, A., & Stufken, J. (1989). A relation between pairwise balanced and variance balanced block designs. *Journal of the American Statistical Association, 84*(407), 753-755.

[8] John, J.A., Wolock, F.W., & David, H. A. (1974). Cyclic designs. *Technometrics, 16*(1), 138-138.

[9] Khatri, C. (1982). A note on variance balanced designs. *Journal of Statistical Planning and Inference, 6*(2), 173-177.

[10] Mann, R.K., Edwards, R., & Zhou, J. (2015). Robust designs for experiments with blocks. *Communications in Statistics - Theory and Methods, 45*(18), 5363-5379.

[11] Montgomery, D.C. (2012). *Design and Analysis of Experiments.* New York : John Wiley.

[12] Pearce, S.C. (1964). Experimenting with blocks of natural size. *Biometrics, 20*(4), 699-706.

[13] Petersen, R.G. (2017). *Agricultural field experiments: Design and analysis.* New York: M. Dekker.

[14] Raghavarao, D. (1971). *Constructions and Combinatorial Problems in Design of Experiments.* New York: J. Wiley & Sons.

[15] Rao, V.R. (1958). A note on balanced designs. *Annals of the Institute of Mathematical Statistics, 29*(1), 290-294.

[16] Stinson, D.R. (2004). *Combinatorial Designs Constructions and Analysis.* New York: Springer.

[17] Taye, G., & Njuho, P. (2007). An improvement on the papadakis covariate to account for spatial variation. *Journal of Agricultural, Biological, and Environmental Statistics, 12*(3), 397-413.

[18] Tyagi, B. (1979). On a class of variance balanced block designs. *Journal of Statistical Planning and Inference, 3*(4), 333-336.

[19] West, D.B. (1996). *Introduction to Graph Theory.* Upper Saddle River: Prentice Hall.

[20] Wiebe, G.A. (1935). Variation and correlation in grain yield among 1500 wheat nursery plots. *Journal of Agricultural Research 50*(4), 331-357.

[21] Wilson, R.M. (1972). An existence theory for pairwise balanced designs II. The structure of PBD-closed sets and the existence conjectures. *Journal of Combinatorial Theory, Series A*, *13*(2), 246-273.

[22] Wilson, R.M. (1975). Decompositions of complete graphs into subgraphs isomorphic to a given graph. In Nash-Williams, C. S. (Eds.), *Proceedings of the Fifth British Combinatorial Conference.*(pp. 647-659). Winnipeg: Utilitas Mathematica.