Design and Analysis of Experiments

Volume 2
Advanced Experimental Design

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Preface

The project of revising Kempthorne’s 1952 book *Design and Analysis of Experiments* started many years ago. Our desire was to not only make minor changes to what had become a very successful book but to update it and incorporate new developments in the field of experimental design. Our involvement in teaching this topic to graduate students led us soon to the decision to separate the book into two volumes, one for instruction at the MS level and one for instruction and reference at the more advanced level.

Volume 1 (Hinkelmann and Kempthorne, 1994) appeared as an *Introduction to Experimental Design*. It lays the philosophical foundation and discusses the principles of experimental design, going back to the ground-breaking work of the founders of this field, R. A. Fisher and Frank Yates. At the basis of this development lies the randomization theory as advocated by Fisher and the further development of these ideas by Kempthorne in the form of derived linear models. All the basic error control designs, such as completely randomized design, block designs, Latin square type designs, split-plot designs, and their associated analyses are discussed in this context. In doing so we draw a clear distinction among the three components of an experimental design: the error control design, the treatment design, and the sampling design.

Volume 2 builds upon these foundations and provides more details about certain aspects of error control and treatment designs and the connections between them. Much of the effort is concentrated on the construction of incomplete block designs for various types of treatment structures, including “ordinary” treatments, control and test treatments, and factorial treatments. This involves, by necessity, a certain amount of combinatorics and leads, almost automatically, to the notions of balancedness, partial balancedness, orthogonality, and uniformity. These, of course, are also generally desirable properties of experimental designs and aspects of their analysis.

In our discussion of ideas and methods we always emphasize the historical developments of and reasons for the introduction of certain designs. The development of designs was often dictated by computational aspects of the ensuing analysis, and this, in turn, led to the properties mentioned above. Even though
in the age of powerful computers and the wide availability of statistical com-
puter software these concerns no longer play the dominant feature, we remind
the reader that such properties have general statistical appeal and often serve as
starting points for new developments. Moreover, we caution the reader that not
all software can be trusted all the time when it comes to the analysis of data
from completely unstructured designs, apart from the fact that the interpretation
of the results may become difficult and ambiguous.

The development and introduction of new experimental designs in the last 50
years or so has been quite staggering, brought about, in large part, by an ever-
widening field of applications and also by the mathematical beauty and challenge
that some of these designs present. Whereas many designs had their origin in
agricultural field experiments, it is true now that these designs as well as modifica-
tions, extensions, and new developments were initiated by applications in almost
all types of experimental research, including industrial and clinical research. It
is for this reason that books have been written with special applications in mind.
We, on the other hand, have tried to keep the discussion in this book as general
as possible, so that the reader can get the general picture and then apply the
results in whatever area of application is desired.

Because of the overwhelming amount of material available in the literature, we
had to make selections of what to include in this book and what to omit. Many
special designs or designs for special cases (parameters) have been presented
in the literature. We have concentrated, generally speaking, on the more gen-
eral developments and results, providing and discussing methods of constructing
rather large classes of designs. Here we have built upon the topics discussed in
Kempthorne’s 1952 book and supplemented the material with more recent top-
ics of theoretical and applications oriented interests. Overall, we have selected
the material and chosen the depth of discussion of the various topics in order to
achieve our objective for this book, namely to serve as a textbook at the advanced
graduate level and as a reference book for workers in the field of experimen-
tal design. The reader should have a solid foundation in and appreciation of
the principles and fundamental notions of experimental design as discussed, for
example, in Volume 1. We realize that the material presented here is more than
can be covered in a one-semester course. Therefore, the instructor will have to
make choices of the topics to be discussed.

In Chapters 1 through 6 we discuss incomplete block and row–column designs
at various degrees of specificity. In Chapter 1 we lay the general foundation for
the notion and analysis of incomplete block designs. This chapter is essential
because its concepts permeate through almost every chapter of the book, in
particular the ideas of intra- and interblock analyses. Chapters 2 through 5 are
devoted to balanced and partially balanced incomplete block designs, their spe-
cial features and methods of construction. In Chapter 6 we present some other
types of incomplete block designs, such as $\alpha$-designs and control-test treatment
comparison designs. Further, we discuss various forms of row–column designs
as examples of the use of additional blocking factors.
In Chapters 7 through 13 we give a general discussion of the most fundamental and important ideas of factorial designs, beginning with factors at two levels (Chapters 7 through 9), continuing with the case of factors with three levels (Chapter 10) through the general case of symmetrical and asymmetrical factorial designs (Chapters 11 and 12), and concluding with the important concept of fractional factorial designs (Chapter 13). In these chapters we return often to the notion of incomplete block designs as we discuss various systems of confounding of interaction effects with block effects.

Additional topics involving factorial designs are taken up in Chapters 14 through 17. In Chapter 14 we discuss the important concept of main effect plans and their construction. This notion is then extended to supersaturated designs (Chapter 15) and incorporated in the ideas of search designs (Chapter 16) and robust-design or Taguchi experiments (Chapter 17). We continue with an extensive chapter about lattice designs (Chapter 18), where the notions of factorial and incomplete block designs are combined in a unique way. We conclude the book with a chapter on crossover designs (Chapter 19) as an example where the ideas of optimal incomplete row–column designs are complemented by the notion of carryover effects.

In making a selection of topics for teaching purposes the instructor should keep in mind that we consider Chapters 1, 7, 8, 10, and 13 to be essential for the understanding of much of the material in the book. This material should then be supplemented by selected parts from the remaining chapters, thus providing the student with a good understanding of the methods of constructing various types of designs, the properties of the designs, and the analyses of experiments based on these designs. The reader will notice that some topics are discussed in more depth and detail than others. This is due to our desire to give the student a solid foundation in what we consider to be fundamental concepts.

In today’s computer-oriented environment there exist a number of software programs that help in the construction and analysis of designs. We have chosen to use the *Statistical Analysis System* (SAS) for these purposes and have provided throughout the book examples of input statements and output using various procedures in SAS, both for constructing designs as well as analyzing data from experiments based on these designs. For the latter, we consider, throughout, various forms of the analysis of variance to be among the most important and informative tools.

As we have mentioned earlier, Volume 2 is based on the concepts developed and described in Volume 1. Nevertheless, Volume 2 is essentially self-contained. We make occasional references to certain sections in Volume 1 in the form (I.xx.yy) simply to remind the reader about certain notions. We emphasize again that the entire development is framed within the context of randomization theory and its approximation by normal theory inference. It is with this fact in mind that we discuss some methods and ideas that are based on normal theory.

There exist a number of books discussing the same types of topics that we exposit in this book, some dealing with only certain types of designs, but perhaps present more details than we do. For some details we refer to these books
in the text. A quite general, but less detailed discussion of various aspects of experimental design is provided by Cox and Reid (2000).

Even though we have given careful attention to the selection of material for this book, we would be remiss if we did not mention that certain areas are completely missing. For example, the reader will not find any discussion of Bayesian experimental design. This is, in part, due to our philosophical attitude toward the Bayesian inferential approach (see Kempthorne, 1984; Hinkelmann, 2001). To explain, we strongly believe that design of experiment is a Bayesian experimentation process, *not* a Bayesian inference process, but one in which the experimenter approaches the experiment with some beliefs, to which he accommodates the design. It is interesting to speculate whether precise mathematical formulation of informal Bayesian thinking will be of aid in design. Another area that is missing is that of sequential design. Here again, we strongly believe and encourage the view that most experimentation is sequential in an operational sense. Results from one, perhaps exploratory, experiment will often lead to further, perhaps confirmatory, experimentation. This may be done informally or more formally in the context of sequential probability ratio tests, which we do not discuss explicitly. Thus, the selection and emphases are to a certain extent subjective and reflect our own interests as we have taught over the years parts of the material to our graduate students.

As mentioned above, the writing of this book has extended over many years. This has advantages and disadvantages. My (K.H.) greatest regret, however, is that the book was not completed before the death of my co-author, teacher, and mentor, Oscar Kempthorne. I only hope that the final product would have met with his approval.

This book could not have been completed without the help from others. First, we would like to thank our students at Virginia Tech, Iowa State University, and the University of Dortmund for their input and criticism after being exposed to some of the material. K.H. would like to thank the Departments of Statistics at Iowa State University and the University of Dortmund for inviting him to spend research leaves there and providing him with support and a congenial atmosphere to work. We are grateful to Michele Marini and Ayca Ozol-Godfrey for providing critical help with some computer work. Finally, we will never be able to fully express our gratitude to Linda Breeding for her excellent expert word-processing skills and her enormous patience in typing the manuscript, making changes after changes to satisfy our and the publisher’s needs. It was a monumental task and she did as well as anybody possibly could.

Klaus Hinkelmann

Blacksburg, VA

May 2004
CHAPTER 1

General Incomplete Block Design

1.1 INTRODUCTION AND EXAMPLES

One of the basic principles in experimental design is that of reduction of experimental error. We have seen (see Chapters I.9 and I.10) that this can be achieved quite often through the device of blocking. This leads to designs such as randomized complete block designs (Section I.9.2) or Latin square type designs (Chapter I.10). A further reduction can sometimes be achieved by using blocks that contain fewer experimental units than there are treatments.

The problem we shall be discussing then in this and the following chapters is the comparison of a number of treatments using blocks the size of which is less than the number of treatments. Designs of this type are called incomplete block designs (see Section I.9.8). They can arise in various ways of which we shall give a few examples.

In the case of field plot experiments, the size of the plot is usually, though by no means always, fairly well determined by experimental and agronomic techniques, and the experimenter usually aims toward a block size of less than 12 plots. If this arbitrary rule is accepted, and we wish to compare 100 varieties or crosses of inbred lines, which is not an uncommon situation in agronomy, we will not be able to accommodate all the varieties in one block. Instead, we might use, for example 10 blocks of 10 plots with different arrangements for each replicate (see Chapter 18).

Quite often a block and consequently its size are determined entirely on biological or physical grounds, as, for example, a litter of mice, a pair of twins, an individual, or a car. In the case of a litter of mice it is reasonable to assume that animals from the same litter are more alike than animals from different litters. The litter size is, of course, restricted and so is, therefore, the block size. Moreover, if one were to use female mice only for a certain investigation, the block size would be even more restricted, say to four or five animals. Hence,
comparing more than this number of treatments would require some type of incomplete block design.

Suppose we wish to compare seven treatments, $T_1, T_2, T_3, T_4, T_5, T_6, T_7$, say, using female mice, and suppose we have several litters with four females. We then could use the following incomplete block design, which, as will be explained later, is a balanced incomplete block design:

<table>
<thead>
<tr>
<th>Animal</th>
<th>Litter</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1</td>
</tr>
<tr>
<td>1</td>
<td>$T_1$</td>
</tr>
<tr>
<td>2</td>
<td>$T_3$</td>
</tr>
<tr>
<td>3</td>
<td>$T_7$</td>
</tr>
<tr>
<td>4</td>
<td>$T_1$</td>
</tr>
<tr>
<td>5</td>
<td>$T_2$</td>
</tr>
<tr>
<td>6</td>
<td>$T_5$</td>
</tr>
<tr>
<td>7</td>
<td>$T_2$</td>
</tr>
</tbody>
</table>

Notice that with this arrangement every treatment is replicated four times, and every pair of treatments occurs together twice in the same block; for example, $T_1$ and $T_2$ occur together in blocks 3 and 4.

Many sociological and psychological studies have been done on twins because they are “alike” in many respects. If they constitute a block, then the block size is obviously two. A number of incomplete block designs are available for this type of situation, for example, Kempthorne (1953) and Zoellner and Kempthorne (1954).

Blocks of size two arise also in some medical studies, when a patient is considered to be a block and his eyes or ears or legs are the experimental units.

With regard to a car being a block, this may occur if we wish to compare brands of tires, using the wheels as the experimental units. In this case one may also wish to take the effect of position of the wheels into account. This then leads to an incomplete design with two-way elimination of heterogeneity (see Chapters 6 and I.10).

These few examples should give the reader some idea why and how the need for incomplete block designs arises quite naturally in different types of research. For a given situation it will then be necessary to select the appropriate design from the catalogue of available designs. We shall discuss these different types of designs in more detail in the following chapters along with the appropriate analysis.

Before doing so, however, it seems appropriate to trace the early history and development of incomplete block designs. This development has been a remarkable achievement, and the reader will undoubtedly realize throughout the next chapters that the concept of incomplete block designs is fundamental to the understanding of experimental design as it is known today.
The origins of incomplete block designs go back to Yates (1936a) who introduced the concept of balanced incomplete block designs and their analysis utilizing both intra- and interblock information (Yates, 1940a). Other incomplete block designs were also proposed by Yates (1936b, 1937a, 1940b), who referred to these designs as quasi-factorial or lattice designs. Further contributions in the early history of incomplete block designs were made by Bose (1939, 1942) and Fisher (1940) concerning the structure and construction of balanced incomplete block designs. The notion of balanced incomplete block design was generalized to that of partially balanced incomplete block designs by Bose and Nair (1939), which encompass some of the lattice designs introduced earlier by Yates. Further extensions of the balanced incomplete block designs and lattice designs were made by Youden (1940) and Harshbarger (1947), respectively, by introducing balanced incomplete block designs for eliminating heterogeneity in two directions (generalizing the concept of the Latin square design) and rectangular lattices some of which are more general designs than partially balanced incomplete block designs. After this there has been a very rapid development in this area of experimental design, and we shall comment on many results more specifically in the following chapters.

1.2 GENERAL REMARKS ON THE ANALYSIS OF INCOMPLETE BLOCK DESIGNS

The analysis of incomplete block designs is different from the analysis of complete block designs in that comparisons among treatment effects and comparisons among block effects are no longer orthogonal to each other (see Section I.7.3). This is referred to usually by simply saying that treatments and blocks are not orthogonal. This nonorthogonality leads to an analysis analogous to that of the two-way classification with unequal subclass numbers. However, this is only partly true and applies only to the analysis that has come to be known as the intrablock analysis.

The name of the analysis is derived from the fact that contrasts in the treatment effects are estimated as linear combinations of comparisons of observations in the same block. In this way the block effects are eliminated and the estimates are functions of treatment effects and error (intrablock error) only. Coupled with the theory of least squares and the Gauss–Markov theorem (see I.4.16.2), this procedure will give rise to the best linear unbiased intrablock estimators for treatment comparisons. Historically, this has been the method first used for analyzing incomplete block designs (Yates, 1936a). We shall derive the intrablock analysis in Section 1.3.

Based upon considerations of efficiency, Yates (1939) argued that the intrablock analysis ignores part of the information about treatment comparisons, namely that information contained in the comparison of block totals. This analysis has been called recovery of interblock information or interblock analysis.
Yates (1939, 1940a) showed for certain types of lattice designs and for the balanced incomplete block design how these two types of analyses can be combined to yield more efficient estimators of treatment comparisons. Nair (1944) extended these results to partially balanced incomplete block designs, and Rao (1947a) gave the analysis for any incomplete block design showing the similarity between the intrablock analysis and the combined intra- and interblock analysis.

The intrablock analysis, as it is usually presented, is best understood by assuming that the block effects in the underlying linear model are fixed effects. But for the recovery of interblock information the block effects are then considered to be random effects. This leads sometimes to confusion with regard to the assumptions in the combined analysis, although it should be clear from the previous remark that then the block effects have to be considered random effects for both the intra- and interblock analysis. To emphasize it again, we can talk about intrablock analysis under the assumption of either fixed or random block effects. In the first case ordinary least squares (OLS) will lead to best linear unbiased estimators for treatment contrasts. This will, at least theoretically, not be true in the second case, which is the reason for considering the interblock information in the first place and using the Aitken equation (see I.4.16.2), which is also referred to as generalized (weighted) least squares.

We shall now derive the intrablock analysis (Section 1.3), the interblock analysis (Section 1.7), and the combined analysis (Section 1.8) for the general incomplete block design. Special cases will then be considered in the following chapters.

1.3 THE INTRABLOCK ANALYSIS

1.3.1 Notation and Model

Suppose we have \( t \) treatments replicated \( r_1, r_2, \ldots, r_t \) times, respectively, and \( b \) blocks with \( k_1, k_2, \ldots, k_b \) units, respectively. We then have

\[
\sum_{i=1}^{t} r_i = \sum_{j=1}^{b} k_j = n
\]

where \( n \) is the total number of observations.

Following the derivation of a linear model for observations from a randomized complete block design (RCBD), using the assumption of additivity in the broad sense (see Sections I.9.2.2 and I.9.2.6), an appropriate linear model for observations from an incomplete block design is

\[
y_{ij\ell} = \mu + \tau_i + \beta_j + e_{ij\ell} \tag{1.1}
\]

\((i = 1, 2, \ldots, t; \quad j = 1, 2, \ldots, b; \quad \ell = 0, 1, \ldots, n_{ij})\), where \( \tau_i \) is the effect of the \( i \)th treatment, \( \beta_j \) the effect of the \( j \)th block, and \( e_{ij\ell} \) the error associated with the
observation $y_{ij\ell}$. As usual, the $e_{ij\ell}$ contain both experimental and observational (sampling) error, that is, using notation established in Volume 1,

$$e_{ij\ell} = \epsilon_{ij\ell} + \eta_{ij\ell}$$

with $\epsilon_{ij\ell}$ representing experimental error and $\eta_{ij\ell}$ representing observational error. Also, based on previous derivations (see I.6.3.4), we can treat the $e_{ij\ell}$ as i.i.d. random variables with mean zero and variance $\sigma^2_e = \sigma^2_\epsilon + \sigma^2_\eta$. Note that because $n_{ij}$, the elements of the incidence matrix $N$, may be zero, not all treatments occur in each block which is, of course, the definition of an incomplete block design.

Model (1.1) can also be written in matrix notation as

$$y = \mu I + X\tau + X_\beta\beta + e$$

where $I$ is a column vector consisting of $n$ unity elements, $X_\beta$ is the observation-block incidence matrix

$$X_\beta = \begin{bmatrix} J_{k_1} & J_{k_2} & \ldots & J_{k_b} \end{bmatrix}$$

with $J_{kj}$ denoting a column vector of $k_j$ unity elements ($j = 1, 2, \ldots, b$) and

$$X_\tau = (x_1, x_2, \ldots, x_t)$$

is the observation-treatment incidence matrix, where $x_i$ is a column vector with $r_i$ unity elements and $(n - r_i)$ zero elements such that $x'_i x_i = r_i$ and $x'_i x_{i'} = 0$ for $i \neq i' (i, i' = 1, 2, \ldots, t)$.

1.3.2 Normal and Reduced Normal Equations

The normal equations (NE) for $\mu$, $\tau_i$, and $\beta_j$ are then

$$n\hat{\mu} + \sum_{i=1}^{t} r_i \hat{\tau}_i + \sum_{j=1}^{b} k_j \hat{\beta}_j = G$$

$$r_i \hat{\mu} + r_i \hat{\tau}_i + \sum_{j=1}^{b} n_{ij} \hat{\beta}_j = T_i \quad (i = 1, 2, \ldots, t)$$

$$k_j \hat{\mu} + \sum_{i=1}^{t} n_{ij} \hat{\tau}_i + k_j \hat{\beta}_j = B_j \quad (j = 1, 2, \ldots, b)$$
where
\[ T_i = \sum_{j\ell} y_{ij\ell} = i \text{th treatment total} \]
\[ B_j = \sum_{i\ell} y_{ij\ell} = j \text{th block total} \]
\[ G = \sum_i T_i = \sum_j B_j = \text{overall total} \]

Equations (1.3) can be written in matrix notation as
\[
\begin{pmatrix}
    J_n'J_n & J_n'X_\tau & J_n'X_\beta \\
    X_\tau'J_n & X_\tau'X_\tau & X_\tau'X_\beta \\
    X_\beta'J_n & X_\beta'X_\tau & X_\beta'X_\beta
\end{pmatrix}
\begin{pmatrix}
    \hat{\mu} \\
    \hat{\tau} \\
    \hat{\beta}
\end{pmatrix}
= \begin{pmatrix}
    J_n'y \\
    X_\tau'y \\
    X_\beta'y
\end{pmatrix}
\tag{1.4}
\]

which, using the properties of \( J, X_\tau, X_\beta \), can be written as
\[
\begin{bmatrix}
    J_n'J_n & J_n'R & J_b'RK \\
    RJ_\tau & R & N \\
    KJ_b & N' & K
\end{bmatrix}
\begin{bmatrix}
    \hat{\mu} \\
    \hat{\tau} \\
    \hat{\beta}
\end{bmatrix}
= \begin{bmatrix}
    G \\
    T \\
    B
\end{bmatrix}
\tag{1.5}
\]

where
\[ R = \text{diag} \,(r_i) \quad t \times t \]
\[ K = \text{diag} \,(k_j) \quad b \times b \]
\[ N = (n_{ij}) \quad t \times b \quad (\text{the incidence matrix}) \]
\[ T' = (T_1, T_2, \ldots, T_t) \]
\[ B' = (B_1, B_2, \ldots, B_b) \]
\[ \tau' = (\tau_1, \tau_2, \ldots, \tau_t) \]
\[ \beta' = (\beta_1, \beta_2, \ldots, \beta_b) \]

and the \( J \)'s are column vectors of unity elements with dimensions indicated by the subscripts. From the third set of equations in (1.5) we obtain
\[
\hat{\mu}J_b + \hat{\beta} = K^{-1}(B - N'\hat{\tau}) \tag{1.6}
\]