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Folded over non-orthogonal designs

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Abstract

In this article, we use the notion of minimal dependent sets (MDS) to introduce MDS-resolution and MDS-aberration as criteria for comparing non-orthogonal foldover designs, and discuss the ideas and their usefulness. We also develop a fast isomorphism check that uses a cyclic matrix defined on the design before it is folded over. By doing so, the speed of the check for comparing two isomorphic designs is increased relative to merely applying an isomorphism check to the foldover design. This relative difference becomes greater as the design size increases. Finally, we use the isomorphism check to obtain a catalog of minimum MDS-aberration designs for some useful n and k and discuss an algorithm for obtaining "good" larger designs.

Keywords: Aberration; Fractional factorial; Hadamard matrix; Minimal dependent sets; Plackett–Burman designs; Resolution; Isomorphism; Equivalence

1. Introduction

Screening experiments are used to sift through a set of candidate factors to identify those that impact the response—these factors are referred to as being "active". For this article we assume that the standard linear model assumptions are valid for the true model. Further we assume that the active factors can impact the response through either a main effect (ME) or a two-factor interaction (2FI) but that all interactions involving three or more factors are negligible. Thus the true model is a linear model that contains MEs and 2FIs formed using the active factors. The primary goal of a screening experiment is to identify the active factors but an important secondary goal is to provide a simple model that captures the essential features of the relationship between these active factors and the response, i.e., identify the active effects. Clearly, if an experiment is run that allows the true model to be correctly identified then both of these goals are achieved. Thus our approach is to evaluate screening designs with regard to their ability to correctly identify the true model (Plackett and Burman, 1946).

Margolin (1969) discussed resolution IV designs for k 2-level factors in $2k$ runs created by folding over minimal and efficient non-orthogonal 2-level resolution III designs. These designs have fewer runs than the competing orthogonal resolution IV designs and only a small efficiency loss in estimating MEs. The early literature on the construction of non-orthogonal resolution IV designs includes John (1962, 1964), Banerjee and Federer (1967) and Webb (1968).

Miller and Sitter (2005) explored the use of foldover non-orthogonal MEs-only designs for screening applications where the practitioner would like to be able to identify a small number of active 2FIs (if they exist) in addition to the

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active MEs (see also Miller and Sitter, 2001). In particular, designs that could accommodate 5 factors in 10 runs, 6 factors in 12 runs and 7 factors in 14 runs were investigated. Miller and Sitter (2005) used the idea of minimal dependent sets (MDS) to compare foldover non-orthogonal designs to their natural orthogonal competitors.

In this article, we first develop notation and context via discussion of results on resolvability due to Srivastava (1975) and their relationship to residual sums of squares (RSS), in Section 2. We then look at the relationship between MDS and resolvability and introduce the idea of minimum MDS-aberration (MDS-MA) as a method for ranking foldover non-orthogonal designs, in Section 3. In Section 4, we introduce what we refer to as a cyclic matrix and use it to develop an isomorphism check adapted from Clark and Dean (2001) to provide a fast method for determining whether two such designs are isomorphic, and use it to do an exhaustive search for smaller designs and together with a proposed search algorithm for larger designs, to obtain a catalog of good non-isomorphic non-orthogonal foldover designs with $n = 8, 12, \ldots, 24$ and between 4 and $n/2$ factors.

2. Resolvability and E(RSS)

Srivastava (1975) developed the idea of resolving power as a measure of the ability of a design to distinguish between competing linear models. To do so, he divided effects into three categories: (1) Effects that can be assumed negligible; (2) effects for which estimates are required; and (3) a group of candidate effects for which it is assumed that most are negligible but a few may be active. Define the h-candidate set to be all models that contain all of the category 2 effects and up to h category 3 effects. A design that can always identify the true model from this set, under the assumption of no error in the observations, is said to be strongly resolvable with resolving power h. Srivastava (1975) showed that a necessary and sufficient condition for strong resolvability is that every model consisting of all the effects from category 2 and $2h$ of the effects from category 3 must be estimable.

Suppose that the "no error" assumption is replaced by the standard linear model assumptions (normality, independence, constant variance) and that ordinary least squares are used to fit the competing models. Miller and Sitter (2004) showed that Srivastava's condition ensures that if the true model contains t category 3 effects where $t \leqslant h$, it will have an E(RSS) that is strictly less than that of any other model that contains $\leqslant t$ category 3 effects.

To lay the foundation for the discussion of MDSs and their use in ranking non-orthogonal fold-over designs that follows in Section 3, we will present a proof that Srivastava's condition is necessary and sufficient for strong resolvability—note that the proof given here is quite different from that in Srivastava (1975). Then we will briefly discuss (but not prove) the connection between strong resolvability and the "E(RSS) result."

Consider a vector representation of the linear model:

$$\mathbf{Y} = \boldsymbol{\mu} + \boldsymbol{\epsilon}, \quad \boldsymbol{\mu} = \mathbf{X}\boldsymbol{\beta}, \quad \boldsymbol{\epsilon} \sim \mathrm{N}(\mathbf{0}, \sigma^2 \mathbf{I}_n), \tag{1}$$

where $\mathbf{Y}$, $\boldsymbol{\mu}$ and $\boldsymbol{\epsilon}$ are vectors in $\mathbb{R}^n$, $\mathbf{X}$ is the model matrix and $\boldsymbol{\beta}$ is the vector of parameter values. Adopting Srivastava's framework, $\mathbf{X}$ must contain one column for each category 2 effect and may contain additional columns that correspond to category 3 effects. Srivastava's condition is based on the estimability of specific models. Using least squares, a model is estimable if and only if $\mathbf{X}'\mathbf{X}$ is non-singular. A consequence of this, which we exploit later, is that a model is estimable if and only if the dimension of colsp($\mathbf{X}$) is equal to the number of columns of $\mathbf{X}$.

Define the set of valid $\boldsymbol{\mu}$'s for a model matrix $\mathbf{X}$ as those that satisfy the following two conditions: (a) $\boldsymbol{\mu} \in \mathrm{colsp}(\mathbf{X})$ and (b) $\boldsymbol{\mu} \notin \mathrm{colsp}(\mathbf{X}_s)$ where $\mathbf{X}_s$ is a submatrix of $\mathbf{X}$ created by eliminating one or more columns of $\mathbf{X}$ that correspond to category 3 effects. Note that condition (b) arises from the requirement that all elements of $\boldsymbol{\beta}$ corresponding to category 3 effects must be non-zero. Under the assumption of no error we get to observe the exact $\boldsymbol{\mu}$ produced by the true model. Strong resolvability states that given the observed $\boldsymbol{\mu}$ we can always identify the true model. This implies that the sets of valid $\boldsymbol{\mu}$ for the h-candidate models must not overlap.

To see that Srivastava's condition is sufficient for strong resolvability, consider the intersection of the column spaces of the model matrices, $\mathbf{X}_1$ and $\mathbf{X}_2$ for any two h-candidate models. Note that condition (a) implies that any $\boldsymbol{\mu}$ that is valid for both models must be in this intersection. We will argue that if Srivastava's condition is true then any $\boldsymbol{\mu} \in \mathrm{colsp}(\mathbf{X}_1) \cap \mathrm{colsp}(\mathbf{X}_2)$ cannot satisfy condition (b) for both $\mathbf{X}_1$ and $\mathbf{X}_2$. To do this we use a result taken from Schott (1997, p. 68). If S_1 and S_2 are vector subspaces of $\mathbb{R}^n$, then

$$\dim(S_1 \cap S_2) = \dim(S_1) + \dim(S_2) - \dim(S_1 + S_2). \tag{2}$$