

Isomorphism Check for 2^n Factorial Designs with Randomization Restrictions

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Abstract Factorial designs with randomization restrictions are often used in industrial experiments when a complete randomization of trials is impractical. In the statistics literature, the analysis, construction and isomorphism of factorial designs has been extensively investigated. Much of the work has been on a case-by-case basis – addressing completely randomized designs, randomized block designs, split-plot designs, etc. separately. In this paper we take a more unified approach, developing theoretical results and an efficient relabeling strategy to both construct and check the isomorphism of multi-stage factorial designs with randomization restrictions. The examples presented in this paper particularly focus on split-lot designs.

Keywords Finite Projective Geometry · Multi-stage factorial designs · Split-lot designs · $(t - 1)$ -Spread · Stars

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1 Introduction

Factorial designs are common in a wide variety of applications, however, complete randomization of trials is often impractical. This could be because some factors may be more expensive to change than others, the trials may need to be partitioned into homogeneous batches at each stage, the experimental units may need to be processed multiple times under different settings, and so on. Popular factorial designs with randomization restrictions include blocked designs, split-plot designs, strip-plot designs, split-lot designs, and combinations thereof. Though both the construction and the analysis of such designs have been active areas of research for decades, most of the literature focuses on a case-by-case basis. The literature started with the exploration of completely randomized designs (CRDs) and randomized block designs (RBDs) by R. A. Fisher and F. Yates. Later, Addelman (1964), Bingham and Sitter (1999) and many others investigated split-plot designs, Miller (1997) pioneered strip-plot designs, and Mee and Bates (1998) and Butler (2004) presented some fundamental results on split-lot designs. See Dean and Voss (1999), Mukerjee and Wu (2006), Wu and Hamada (2009), Hedayat et al. (2012), and Cheng (2016) for detailed references. In this paper, we focus on multi-stage factorial designs with randomization restrictions under a unified framework.

For easier understanding and more concise notation, we concentrate on two-level factorial designs, however, several results and algorithms presented in this paper can easily be extended for q -levels. Consider a factorial experiment investigating the significance of n basic factors and all of their interactions. Each r -factor interaction can be expressed as an n -dimensional vector composed of exactly r ones and $n - r$ zeros, with the r ones indicating which basic factors are present in the interaction term. We employ the following shorthand. Let the first n uppercase letters A, B, C, \dots denote the n basic factors in the experiment, and denote any interaction as a string of letters composed of the basic factors that are involved. For instance, $\{A, B, AB, C, \dots, ABCDE\}$ denotes all basic factors and their interactions for a 2^5 factorial experiment, with $AE = (1, 0, 0, 0, 1)$ representing a two-factor interaction between the first and the fifth basic factors.

Multi-stage factorial experiments are common in industrial applications, where all experimental units are processed at each stage, and the observations are taken at the end after the final stage. Some traditional designs like a RBD and a split-plot design can be thought of as multi-stage factorial designs with only one stage. A non-trivial example is a split-lot design (also referred to as *multiway split-unit design*), which consists of multiple processing stages with each stage using a split-plot design to partition the experimental units (Ryan, 2007). Popular applications include the laundry experiment for measuring wrinkles in Miller (1997) and Mee (2009), the fabrication of integrated circuits using silicon wafers in Mee and Bates (1998), and the plutonium alloy experiment in Bingham et al. (2008). See Section 2.1 for more details on some of these examples.

Over the decades, a handful of unifying methodologies have been developed for studying different factorial designs with randomization restrictions. For instance, Nelder (1965a,b) developed the notion of the simple block structure; Speed and Bailey (1982) and Tjur (1984) used association schemes to extend the simple block structure idea to orthogonal block structures which are more powerful and can characterize a wide variety of designs (see Bailey (2004) and Cheng and Tsai (2011) for more details). In this paper, we use the unified theory proposed by Ranjan (2007) which is inspired from the randomization group idea of Bingham et al. (2008). The comparison of different unified frameworks is outside the purview of this paper and we do not claim that the the unified theory considered here is more general or powerful.

The key idea behind the unified theory of Ranjan (2007) is to realize that the set of all factorial effects (main effects and all possible interactions) of a 2^n factorial design constitute an $(n-1)$ -dimensional finite projective geometry $\mathcal{P}_n := PG(n-1, 2)$ over $GF(2)$, which is the same as the n -dimensional vector space $V(2^n)$ over $GF(2)$ without the zero element (Bose, 1947). Furthermore, the randomization restrictions for any given stage of a multi-stage factorial design can be characterized by a projective subspace of \mathcal{P}_n . Such a subspace is referred to as a *randomization defining contrast subspace* (RDCSS). Note that a $(t-1)$ -dimensional projective subspace (also referred to as a $(t-1)$ -flat) of $PG(n-1, 2)$ is the same as a t -dimensional vector subspace of $V(2^n)$ excluding the zero element. In this approach, the overlapping pattern of the flats were exploited to construct useful split-lot designs. Ranjan et al. (2009) formalized the construction and analysis of split-lot designs that are derived from the set of disjoint flats of \mathcal{P}_n . In several real-life application, for instance, in the plutonium alloy experiment of Bingham et al. (2008), the overlap between two RDCSSs (or flats) cannot be avoided. Subsequently, Ranjan et al. (2010) proposed a new class of split-lot designs which is based on flats with a common overlap. Though the following work, Ranjan (2007), Ranjan et al. (2009) and Ranjan et al. (2010), have been frequently cited in this article, this is a standalone paper and, we have presented all necessary results for completeness and easy readability.

The construction and ranking of designs becomes important whenever there are potentially multiple candidate designs meeting the design requirements of a particular factorial experiment. In the design of experiments literature, one can find a plethora of research articles that focus on innovative techniques for constructing good designs, a variety of design ranking criteria (e.g., maximum resolution and minimum aberration), and methods of sorting through the candidates to find different or *non-isomorphic* designs. However, most of the literature operates on a case-by-case basis (e.g., Bingham and Sitter (1999), Ma et al. (2001), Cheng and Tang (2005), Lin and Sitter (2008)).

This paper concentrates on the problem of checking the isomorphism of 2^n multi-stage factorial designs under the unified framework characterized by the RDCSS structure. As per Ma et al. (2001), two fractional factorial designs are said to be isomorphic if one can be obtained from the other by relabeling the factors, reordering the runs, and switching the

levels of factors. For a multi-stage factorial experiment, Bingham et al. (2008) introduces an update to this definition by adding stage-wise restrictions.

In this paper, we present a formal definition of isomorphism using the RDCSS-based unified framework. If performed naively, checking for the isomorphism of designs can involve iterating over all possible relabelings and reorderings, which quickly becomes computationally infeasible for large designs. We present a bitstring representation of \mathcal{P}_n which helps in developing an efficient search algorithm. A new search strategy is also proposed which exploits the geometric structure of RDCSSs to significantly reduce the search space. We further apply known results from projective geometry (e.g. Soicher (2000); Topalova and Zhelezova (2010); Mateva and Topalova (2009)) to completely classify the isomorphism properties for several RDCSS-based designs (with small runsizes) that are useful from a practical standpoint. We also provide a new result which establishes that all RDCSS-based designs constructed using the cyclic method of Hirschfeld (1998) are isomorphic. These results are useful for determining when several isomorphism classes of designs must be considered. Furthermore, all proposed algorithms and important functions have been implemented in **R** and available on GitHub for easy access.

After reviewing the background theory, important existing results, and motivating examples for the RDCSS-based multi-stage factorial experiments in Section 2, the formal definition of equivalence and isomorphism are presented in Section 3. Sections 4 and 5 presents new theories and algorithms for reducing the search space and efficiently iterating through all possible relabelings for an isomorphism check. Section 6.1 reviews the classification of such designs from a practical standpoint, and Section 6.2 presents a theoretical result on the cyclic construction of RDCSSs. Finally, the concluding remarks are summarized in Section 7.

2 Background Review

A good design is often expected to facilitate efficient analysis. Daniel (1959) suggested that for unreplicated factorial experiments, the significance of factorial effects can be assessed using half-normal plots with the restriction that the effects appearing on the same plot must have the same error variance. Moreover, each half-normal plot should contain at least six or seven factorial effects for a meaningful inference. For an RDCSS-based multi-stage design, the variance of an estimator of a factorial effect is characterized by its presence in different RDCSSs. That is, if a multi-stage factorial design is defined by m RDCSSs and all RDCSSs are disjoint, then at most $m + 1$ half-normal plots are required for the significance assessment of factorial effects. On the other hand, if some of the m RDCSSs overlap then more than $m + 1$ separate half-normal plots would have to be used for the identification of significant factorial effects. As a result, it is desirable to construct RDCSSs that are big enough (with at least six or seven effects per half-normal plot) and disjoint. Section 2.1 presents a quick recap of two popular examples of multi-stage split-lot designs, and Section 2.2 reviews some

relevant results from the finite projective geometry literature, Ranjan (2007), Ranjan et al. (2009) and Ranjan et al. (2010), that are helpful for our discussion on isomorphism.

2.1 Examples of Multi-stage Experiments

In this section, we recap the silicon wafer example (Mee and Bates, 1998) and plutonium alloy experiment (Bingham et al., 2008)).

The fabrication of integrated circuits on silicon wafers goes through a sequence of processing steps. Mee and Bates (1998) discussed the construction and analysis of several split-plot designs for analyzing this process. Here, we present two designs for a 64-wafer experiment with nine processing stages and six basic factors. At each stage, all experimental units (i.e., 64 wafers) are processed and then passed on to the next stage. The measurements are taken at the end after the final stage, and the randomization of trials at each processing stage is guided by a set of restrictions defined by carefully chosen factors and factor interactions. The designs are given by $IC_1 = \{\langle A, EF, BCE \rangle, \langle B, AF, CDF \rangle, \langle C, AB, ADE \rangle, \langle D, BC, BEF \rangle, \langle E, CD, ACF \rangle, \langle F, DE, ABD \rangle, \langle BD, BF, ACE \rangle, \langle AC, CE, BDF \rangle, \langle AD, BE, CF \rangle\}$, and $IC_2 = \{\langle A, BD, CF \rangle, \langle B, AF, CE \rangle, \langle C, BF, DE \rangle, \langle D, AC, BE \rangle, \langle E, AB, DF \rangle, \langle F, AE, CD \rangle, \langle AD, BC, EF \rangle, \langle ACE, ADF, BEF \rangle, \langle ABC, ADE, CEF \rangle\}$, where $\langle \dots \rangle$ denotes the span of the vectors/effects within, e.g., $\langle A, EF, BCE \rangle = \{A, EF, AEF, BCE, ABCE, BCF, ABCF\}$. For both IC_1 and IC_2 , the nine RDCSSs are disjoint and each of size seven. Thus, the significance of all 63 factorial effects (excluding the null) can easily be assessed by nine half-normal plots. The question we address here is whether or not the two designs are isomorphic. Of course, the ranking of designs is a different question and we leave it for future research.

The so-called ‘‘plutonium alloy experiment’’ (in Bingham et al. (2008)) took place at Los Alamos National Laboratory (LANL), where the objective was to identify the significant factors and factor combinations involved in the process of manufacturing a plutonium alloy cookie which was to be used further for some classified experiments. This cookie-making-process involved five basic factors and had to go through three processing stages: casting and two different types of heat-treatments. Bingham et al. (2008) considered a 2^5 factorial split-plot design with 32 runs. Letting f_i^* denote the flat in \mathcal{P}_5 that characterizes the randomization of trials for the i -th processing stage, then as per Bingham et al. (2008), the restrictions are: $A, B \in f_1^*$, $C \in f_2^*$ and $D, E \in f_3^*$. Using a computer search, the authors found it impossible to construct disjoint RDCSSs which could facilitate meaningful half-normal plots. The design suggested at the end was, $PA_1 = \{\langle A, B, CDE \rangle, \langle C, AD, BE \rangle, \langle D, E, ABC \rangle\}$, which required four half-normal plots for the significance assessment of effects in f_1^*, f_2^*, f_3^* (excluding the common $ABCDE$) and $\mathcal{P}_5 \setminus \{f_1^*, f_2^*, f_3^*\}$. Later on, Ranjan et al. (2010) recommended an alternative design $PA_2 = \{\langle A, B, DE, ACD \rangle, \langle C, AB, DE, ACD \rangle, \langle D, E, AB, ACD \rangle\}$ for this experiment. As with the previous example, can we check if the two designs PA_1 and PA_2 are isomorphic?

2.2 Projective Geometric Structures

The questions of the existence and construction of a pre-specified number of disjoint flats of $\mathcal{P}_n = PG(n-1, 2)$ with given sizes are non-trivial. The combinatorics literature contains some results on the existence and construction of spreads and maximal partial-spreads of \mathcal{P}_n .

A spread of \mathcal{P}_n is a set of disjoint flats that includes every element of \mathcal{P}_n . That is, a spread of \mathcal{P}_n is also a cover of \mathcal{P}_n . A *balanced $(t-1)$ -spread* ψ of \mathcal{P}_n consists of only $(t-1)$ -flats of \mathcal{P}_n . For simplicity, we do not consider the unbalanced spread case in this paper. A $(t-1)$ -spread ψ of \mathcal{P}_n contains $|\psi| = (2^n - 1)/(2^t - 1) = \sum_{i=1}^{n/t} 2^{(i-1)t}$ distinct $(t-1)$ -flats that can be used for constructing RDCSSs for different stages of randomization. For instance, in the silicon wafers example, IC_1 and IC_2 are two distinct 2-spreads of \mathcal{P}_6 . A necessary and sufficient condition for the existence of a balanced $(t-1)$ -spread of \mathcal{P}_n is that t divides n (André, 1954). For instance, in the silicon wafer example, the existence of a $(3-1)$ -spread of \mathcal{P}_6 is ensured as 3 divides 6.

If $t \nmid n$ (as in the plutonium example), then either a partial $(t-1)$ -spread or a non-overlapping set of RDCSSs have to be used for design construction. A partial spread is simply a set of disjoint flats of \mathcal{P}_n . Lemma 1 discusses the existence of a partial $(t-1)$ -spread of \mathcal{P}_n .

Lemma 1 (Eisfeld and Storme (2000)) *Let \mathcal{P}_n be a finite projective space $PG(n-1, 2)$, with $n = kt + r$ for $0 < r < t < n$. Then, there exists a partial $(t-1)$ -spread ψ of \mathcal{P}_n with $|\psi| = 2^r \frac{2^{kt}-1}{2^t-1} - 2^r + 1$.*

Assuming the overlap between two RDCSSs cannot be avoided, Ranjan et al. (2010) proposed a new geometric structure called a star¹ which requires all constituent flats to have a common overlap.

Definition 1 A *balanced star*, denoted by $\Omega = St(n, \mu, t, t_0)$, of \mathcal{P}_n is a set of μ rays ($(t-1)$ -flats) and a nucleus (one (t_0-1) -flat) in \mathcal{P}_n , such that the intersection of any two of the μ rays is the nucleus (so, $0 \leq t_0 < t < n$).

A star Ω is said to cover \mathcal{P}_n if the combined set of elements of all rays in Ω is equal to \mathcal{P}_n . For the purposes of this paper, all stars are balanced and covering. Thus a star $\Omega = St(n, \mu, t, t_0)$ provides $\mu = (2^{n-t_0} - 1)/(2^{t-t_0} - 1)$ overlapping RDCSSs of size $2^t - 1$ each. For instance, in the plutonium alloy experiment, PA_2 represents a $St(5, 3, 4, 3)$. Lemma 2 is taken from Ranjan et al. (2010, Lemma 3) which establishes the relationship between a spread and a star.

Lemma 2 *The existence of a balanced covering star $\Omega = St(n, \mu, t, t_0)$ of $\mathcal{P}_n = PG(n-1, 2)$ is equivalent to the existence of an $(h-1)$ -spread ψ of \mathcal{P}_u , where $u = n - t_0$, and $h = t - t_0$.*

¹ Stars were recently reinvented in a collection of works (Shaw and Topalova, 2014; McDonough et al., 2014) where they are referred to as book spreads.

The proof of Lemma 2 easily follows from the following construction steps. Let $\{f_1, \dots, f_\mu\}$ be the constituents of an $(h-1)$ -spread ψ of \mathcal{P}_u . Then there exists a (t_0-1) -flat π (referred to as the nucleus) in $\mathcal{P}_n \setminus \mathcal{P}_u$ such that $f_i^* = \langle f_i, \pi \rangle$ and $\{f_1^*, \dots, f_\mu^*\}$ form a covering star Ω of \mathcal{P}_n . For convenience, we denote such stars as $\Omega = \psi \times \pi$. In the plutonium alloy experiment, PA_2 satisfies this structure with $\pi = \langle AB, DE, ACD \rangle$ and $\psi = \{\{A\}, \{C\}, \{AC\}\}$. Here, ψ corresponds to a 0-spread of $\mathcal{P}_2 = \langle A, C \rangle$.

One of the most popular methods of constructing a balanced spread of a finite projective space in $GF(2)$ is the cyclic approach of Hirschfeld (1998). Suppose h and u are positive integers such that h divides u , and we wish to construct an $(h-1)$ -spread $\psi = \{f_1, \dots, f_\mu\}$ of \mathcal{P}_u , where $\mu = (2^u - 1)/(2^h - 1)$. The cyclic method for constructing ψ starts by writing the $2^u - 1$ nonzero elements of $GF(2^u)$ in cycles of length μ (Table 1). The nonzero elements of $GF(2^u)$ are written as $\{\omega^0, \omega^1, \dots, \omega^{2^u-2}\}$, where ω is a primitive element, and $\omega^i = \alpha_0\omega^0 + \alpha_1\omega^1 + \dots + \alpha_{u-1}\omega^{u-1}$, for $0 \leq i \leq 2^u - 2$, correspond to the vector representation $(\alpha_0, \dots, \alpha_{u-1})$ of elements in \mathcal{P}_u .

Table 1 The elements of $GF(2^u)$ in cycles of length $\mu = (2^u - 1)/(2^h - 1)$.

f_1	f_2	\dots	f_μ
ω^0	ω^1	\dots	$\omega^{\mu-1}$
ω^μ	$\omega^{\mu+1}$	\dots	$\omega^{2\mu-1}$
\vdots	\vdots	\ddots	\vdots
$\omega^{2^u-\mu-1}$	$\omega^{2^u-\mu}$	\dots	ω^{2^u-2}

Hirschfeld (1998) showed that the f_i 's are $(h-1)$ -flats and $\psi = \{f_1, \dots, f_\mu\}$ partitions the set of all nonzero elements of $GF(2^u)$, i.e., ψ is an $(h-1)$ -spread of \mathcal{P}_u . For a quick reference, Table 2 shows the 2-spread ψ of \mathcal{P}_6 generated using the primitive polynomial $\omega^6 + \omega + 1$ and primitive element ω . Here, $\mu = (2^6 - 1)/(2^3 - 1) = 9$ disjoint 2-flats $\{f_1, \dots, f_9\}$ can be used to construct different RDCSSs as required.

Table 2 The 2-spread obtained using the cyclic construction.

f_1	f_2	f_3	f_4	f_5	f_6	f_7	f_8	f_9
F	E	D	C	B	A	EF	DE	CD
BC	AB	AEF	DF	CE	BD	AC	BEF	ADE
CDEF	BCDE	ABCD	ABCEF	ABDF	ACF	BF	AE	DEF
CDE	BCD	ABC	ABEF	ADF	CF	BE	AD	CEF
BDE	ACD	BCEF	ABDE	ACDEF	BCDF	ABCE	ABDEF	ACDF
BCF	ABE	ADEF	CDF	BCE	ABD	ACEF	BDF	ACE
BDEF	ACDE	BCDEF	ABCDE	ABCDEF	ABCDF	ABCF	ABF	AF

3 Isomorphism of RDCSS-based Designs

In this paper, we only consider the spread- and star-based designs, and for simplicity, we also assume that all RDCSSs of a design are of the same size (so the resulting structure is balanced). Let d_1 and d_2 be two 2^n multi-stage factorial designs with μ stages of randomization, and let the respective RDCSSs be represented by $d_1 = \{f_1, \dots, f_\mu\}$ and $d_2 = \{g_1, \dots, g_\mu\}$. In spirit of Bingham et al. (2008), the two designs are said to be isomorphic (denoted by $d_1 \cong d_2$) if one can be obtained from the other by applying some sort of relabeling of factors and factor levels and/or reordering of effects within the RDCSSs. We formalize this definition by first bundling up the reordering and rearrangement-type operations together in one concept called “equivalence” and then addressing the relabeling step.

Definition 2 Two 2^n RDCSS-based factorial designs $d_1 = \{f_1, \dots, f_\mu\}$ and $d_2 = \{g_1, \dots, g_\mu\}$ are said to be *equivalent* (denoted by, $d_1 \equiv d_2$) if and only if, for every $f_i \in d_1$, there is a unique $g_j \in d_2$ such that $\{f_i\} = \{g_j\}$ (set equality), for $1 \leq i, j \leq \mu$.

This notion of equivalence will not only take care of rearrangement of factor combinations within a given RDCSS, but also account for reordering of the RDCSSs themselves. Let $\mathcal{E}(d_1)$ be the set of all such 2^n designs in μ -stages that are equivalent to d_1 (i.e., $\mathcal{E}(d_1)$ denotes the equivalence class of d_1). If $|f_i| = 2^t - 1$ for each $f_i \in d_1$, then,

$$|\mathcal{E}(d_1)| = \mu! \cdot [(2^t - 1)!]^\mu. \quad (1)$$

Assuming the existence of a $(t - 1)$ -spread or a covering star $St(n, \mu, t, t_0)$ of \mathcal{P}_n involved in the construction of the 2^n design, the maximum value of μ is $(2^n - 1)/(2^t - 1)$ or $(2^{n-t_0} - 1)/(2^{t-t_0} - 1)$, respectively. When n is large, checking the equivalence of two designs by naively iterating through the entire equivalence class of one of them is too computationally intensive, e.g., in the plutonium alloy experiment, $|\mathcal{E}(PA_2)| = 6(15!)^3 \approx 1.37 \times 10^{37}$. However, the computational burden can be reduced through a combination of sorting and the following *bitstring representation* scheme.

Each element of \mathcal{P}_n can be represented as a unique binary string of $2^n - 1$ bits with exactly one nonzero entry. For instance, following the Yates Order (Box et al., 1978) of \mathcal{P}_3 , the bitstring representations of the elements of $\mathcal{P}_3 = \{A, B, AB, C, AC, BC, ABC\}$ are $A \rightarrow 1000000$, $B \rightarrow 0100000$, ..., $ABC \rightarrow 0000001$. In this representation, the contents of any RDCSS f can now be uniquely identified by the sum of the bitstring representations of its elements. For instance, $f = \{AB, AC, BC\}$ is now uniquely identified by the representation 0010110. After converting to this representation, checking the equivalence of two RDCSSs amounts to checking the equality of two bitstrings. Furthermore, checking the equivalence of two RDCSS-based designs becomes equivalent to checking the equality of two sets of bitstrings, which is straightforward if one sorts them first. Note that this new bitstring representation is typically more advantageous for spreads with larger values of t . For smaller t (say, 2 or 3), simply sorting the elements in each RDCSS is sufficient.

We use a collineation of \mathcal{P}_n to express the relabelings of factors and factor combinations (Coxeter, 1969). A *collineation* of \mathcal{P}_n is a mapping of the points from \mathcal{P}_n to \mathcal{P}_n such that $(t - 1)$ -flats gets mapped to $(t - 1)$ -flats for all $1 \leq t \leq n$. A collineation of \mathcal{P}_n can be characterized by a full rank $n \times n$ matrix \mathcal{C} over $GF(2)$, referred to as the *collineation matrix* (Batten, 1997), where the j -th column of \mathcal{C} is the image of the j -th basic factor (say) F_j (i.e., the factorial effect in \mathcal{P}_n that F_j gets mapped to). For instance, the 3×3 collineation matrix

$$\mathcal{C} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 1 \\ 0 & 0 & 1 \end{bmatrix}$$

relabels the basic factors as $A \rightarrow A$, $B \rightarrow B$ and $C \rightarrow BC$. See Appendix C for easy implementation in R. We interchangeably use the terms ‘‘collineation’’ and ‘‘collineation matrix’’ to refer to the same linear mapping. Let \mathcal{C}_n be the set of all collineations of $\mathcal{P}_n = PG(n - 1, 2)$, then the size of \mathcal{C}_n is given by

$$|\mathcal{C}_n| = \prod_{j=1}^n (2^n - 2^{j-1}). \quad (2)$$

The proof of (2) follows by simply counting the total number of linearly independent images of F_j . That is, given that the images of F_1, \dots, F_j have already been selected, the total number of possible images for F_{j+1} is $2^n - 2^j$.

Suppose we wish to construct a collineation \mathcal{C} which defines the mapping between $\{x_1, \dots, x_n\}$ and $\{y_1, \dots, y_n\}$, i.e., $\mathcal{C}(x_i) = y_i$, for $i = 1, \dots, n$. One intuitive method of constructing such a collineation matrix is to solve a system of n equations with n unknown over $GF(2)$. As discussed in Algorithm 1 of Section 4, this equation solving approach could be computationally expensive for checking isomorphism. Thus, we propose a two-step alternative approach. First construct a collineation matrix $\mathcal{C}_{x,B}$ that canonicalize $\{x_1, \dots, x_n\}$, i.e., $x_1 \rightarrow A$, $x_2 \rightarrow B$, and so on, and then construct $\mathcal{C}_{B,y}$ that maps the canonical basis elements to y_j 's, i.e., $A \rightarrow y_1$, $B \rightarrow y_2$, etc. As a result the desired collineation matrix is $\mathcal{C} = \mathcal{C}_{B,y} \cdot \mathcal{C}_{x,B}$.

For instance, for the silicon wafers example, let $x_1 = A$, $x_2 = EF$, $x_3 = BCE$, $x_4 = B$, $x_5 = AF$, $x_6 = CDF$ be the effects from RDCSSs in IC_1 , and $y_1 = A$, $y_2 = BD$, $y_3 = CF$, $y_4 = B$, $y_5 = AF$, $y_6 = CE$ be chosen from RDCSSs in IC_2 . Then, $\mathcal{C}_{x,B}$ can be constructed by writing x_i 's as column vectors and then inverting the matrix, i.e.,

$$\mathcal{C}_{x,B} = \begin{bmatrix} 1 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 1 & 1 \end{bmatrix}^{-1} = \begin{bmatrix} 1 & 0 & 1 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 & 1 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 1 & 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 \end{bmatrix}.$$

From an implementation standpoint the inversion of a matrix M over $GF(2)$ can easily be done in R (R Core Team, 2014) using the code: `solve(M)%%2`. As highlighted in Algorithm 1,

spread-based designs (with disjoint RDCSSs), and the star-based designs, where all RDCSSs have a common overlap.

4 Search Algorithm for Spread-based Designs

When undertaken naively, determining if two RDCSS-based designs on \mathcal{P}_n are isomorphic involves exhaustively searching over the entire space \mathcal{C}_n — as enumerated by (2)— to check if any are IECs. Depending on the value of n , this full search space can be prohibitively large, meaning an exhaustive search would be computationally intractable. We propose a strategy that exploits the structure of IECs to reduce the size of this search space. Here, we motivate and describe our strategy as it applies to RDCSS-based designs with no overlap. In Section 5, we extend this approach to RDCSSs that share a common overlap (i.e., star-based designs).

From the definition of isomorphism (Definition 3), a collineation \mathcal{C} can be considered as an IEC if and only if, for all $i \in \{1, 2, \dots, \mu\}$, the RDCSS f_i in d_1 is relabeled by \mathcal{C} to g_j in d_2 for some $j \in \{1, 2, \dots, \mu\}$. We refer to this as the *full RDCSS mapping property* (FRMP) of an IEC. The FRMP characterizes which collineations to consider when searching for an IEC. For example, if \mathcal{C} is an IEC from IC_1 to IC_2 for the silicon wafers example in Section 2.1, then we know that $\mathcal{C}(A)$, $\mathcal{C}(EF)$, and $\mathcal{C}(BCE)$ must all fall within the same RDCSS of IC_2 ; we need not consider any \mathcal{C} for which $\mathcal{C}(A)$ and $\mathcal{C}(EF)$ belong to different RDCSSs, such as $\mathcal{C}(A) = B$ and $\mathcal{C}(EF) = C$. Furthermore, because A and B are in different RDCSSs in IC_1 , we know that A and B must be mapped to different RDCSSs in IC_2 ; we can rule out any other collineation, such as those for which $A \rightarrow BD$ and $B \rightarrow A$, when searching for an IEC.

Unfortunately, we are not aware of any constructive approaches for isolating collineations that completely satisfy the FRMP. For this reason, we introduce a relaxed version of the FRMP — called the *partial RDCSS mapping property* (PRMP) — that does admit a constructive approach. A collineation \mathcal{C} satisfies the PRMP for points $x_1, \dots, x_n \in \mathcal{P}_n$ if it meets the following requirement: for all $i, j : 1 \leq i, j \leq n$, there exist unique k, l ($1 \leq k \neq l \leq \mu$) such that, $x_i, x_j \in f_k$ if and only if $\mathcal{C}(x_i), \mathcal{C}(x_j) \in g_l$. That is, a collineation \mathcal{C} satisfies the PRMP for x_1, \dots, x_n if x_i, x_j being co-members of an RDCSS in d_1 occurs if and only if $\mathcal{C}(x_i)$ and $\mathcal{C}(x_j)$ are co-members of an RDCSS in d_2 .

Our reasons for defining the PRMP in this manner are two-fold. Firstly, the constraints imposed by the PRMP are a strict subset of the constraints imposed by the FRMP. As a result, any collineation satisfying the FRMP (i.e. IECs) will also satisfy the PRMP for any given x_1, \dots, x_n ; our reduction of the search space does not ignore any possible IECs. Secondly, because the constraints in the PRMP involve just n points, the collineations satisfying the PRMP are now straightforward to construct.

Recall that for linearly independent x_1, \dots, x_n , any collineation \mathcal{C} is characterized by the images $y_1 = \mathcal{C}(x_1), \dots, y_n = \mathcal{C}(x_n)$ with the corresponding collineation matrix being easily determined using the algorithm provided in Section 3. Thus, the entire search space for IECs

given by a PRMP can be constructed by iterating through the possible options for y_1, \dots, y_n in d_2 that match the RDCSS co-membership structure of x_1, \dots, x_n in d_1 . The remainder of this section describes an approach that efficiently iterates through the collineation matrices in this class to look for IECs. We can then check the equivalence of $\mathcal{C}(d_1)$ and d_2 — via the bitstring representation — for every \mathcal{C} in this class.

We now develop some theory to provide guidance on how to choose the basis set $x_1, \dots, x_n \in \mathcal{P}_n$. Proposition 1 presents an upper bound on the number of collineations satisfying the PRMP for a basis $\{x_1, \dots, x_n\}$. Appendix A provides a proof of this result, as well as a comment explaining why it is only an upper bound.

Proposition 1 *Let $d_1 = \{f_1, \dots, f_\mu\}$ and $d_2 = \{g_1, \dots, g_\mu\}$ be two 2^n RDCSS-based designs obtained from balanced $(t-1)$ -spreads of \mathcal{P}_n . Let $\{x_1, \dots, x_n\}$ be a basis of \mathcal{P}_n , $m_i = |f_i \cap \{x_1, \dots, x_n\}|$ for $i = 1, \dots, \mu$, and ℓ be the number of nonzero m_i 's. Then, the number of collineations \mathcal{C} from d_1 to d_2 which satisfy the PRMP for x_1, \dots, x_n is bounded above by*

$$\frac{\mu!}{(\mu - \ell)!} \prod_{i=1}^{\ell} \left(\prod_{j=1}^{m_i} (2^t - 2^{j-1}) \right). \quad (3)$$

Recall that a balanced $(t-1)$ -spread of \mathcal{P}_n exists if and only if t divides n . Therefore, the upper bound (3) from Proposition 1 is minimized for $\ell = n/t$, which further implies either $m_i = t$ or zero. Proposition 2 guarantees the existence of such a basis for any set of RDCSSs obtained from a balanced $(t-1)$ -spread of \mathcal{P}_n (see Appendix A for the proof).

Proposition 2 *For any balanced $(t-1)$ -spread based multi-stage design $d_1 = \{f_1, \dots, f_\mu\}$ in \mathcal{P}_n , there exists $\ell_0 = n/t$ distinct RDCSSs $f_{u_1}, \dots, f_{u_{\ell_0}}$ from d_1 , with $1 \leq u_1, \dots, u_{\ell_0} \leq \mu$, such that $\langle \cup_{i=1}^{\ell_0} f_{u_i} \rangle = \mathcal{P}_n$.*

Subsequently, there exist a set x_1, \dots, x_n such that the maximum number of collineations that satisfy PRMP can be reduced to

$$\frac{\mu!}{(\mu - n/t)!} \left(\prod_{j=1}^t (2^t - 2^{j-1}) \right)^{n/t}. \quad (4)$$

As compared to the naive approach (enumerated in (2)), the proposed approach corresponds to a reduction of the search space by 7 orders of magnitude for checking the isomorphism of 2-spreads of \mathcal{P}_6 . For 1-spreads and 4-spreads of \mathcal{P}_{10} , the search space is reduced by 13 orders and 12 orders of magnitude, respectively. For larger n , the improvements are even greater.

For checking the isomorphism of $d_1 = \{f_1, \dots, f_\mu\}$ and $d_2 = \{g_1, \dots, g_\mu\}$ in \mathcal{P}_n , we follow a systematic approach to search for the IEC by iterating through the candidate collineations. First, choose $\ell_0 = n/t$ out of μ RDCSSs in d_1 that can generate a basis $\{x_1, \dots, x_n\}$ for \mathcal{P}_n such that each of the ℓ_0 RDCSSs contributed t points to the basis (as in Proposition 2). Then, construct a collineation matrix $\mathcal{C}_{x,B}$ to transform the x 's to a canonical basis with basic factors, $\{A, B, \dots\}$ (as demonstrated in Section 3). Note that the isomorphism of $\mathcal{C}_{x,B}(d_1)$ and

d_2 implies the isomorphism of d_1 and d_2 . Now, iterate through all possible sets of ℓ_0 RDCSSs from d_2 to construct the basis set $\{y_1, \dots, y_n\}$ in d_2 and the corresponding collineation matrix $\mathcal{C}_{B,y}$ that maps the canonical basis to y 's. If $\mathcal{C}_{B,y}(\mathcal{C}_{x,B}(d_1))$ is equivalent to d_2 , then we have found the IEC. The step-by-step algorithm is summarized in Algorithm 1. Note that two subscripts for the x 's and y 's are introduced to keep track of their RDCSS membership in d_1 and d_2 , respectively. Let F_1, \dots, F_n be an alternative notation for the basic factors, with the assumption that $F_1 := A$, $F_2 := B$, and so on.

Algorithm 1 Isomorphism check between two $(t-1)$ -spread based designs in \mathcal{P}_n .

1. Choose $\ell_0 = n/t$ out of μ RDCSSs from $d_1 = \{f_1, \dots, f_\mu\}$, that satisfy Proposition 2. Let these be $\{f_{u_1}, \dots, f_{u_{\ell_0}}\}$ for $1 \leq u_1, \dots, u_{\ell_0} \leq \mu$.
 2. For $i = 1, \dots, \ell_0$, specify $\{x_{i,1}, \dots, x_{i,t}\} \in f_{u_i}$ such that $f_{u_i} = \langle x_{i,1}, \dots, x_{i,t} \rangle$.
 3. Construct the collineation matrix $\mathcal{C}_{x,B}$ which maps the x 's in Step 2 to the canonical basis $\{A, B, \dots\}$ such that each $x_{i,j}$ is mapped to $F_{t(i-1)+j}$.
 4. (a) Choose ℓ_0 out of μ RDCSSs from $d_2 = \{g_1, \dots, g_\mu\}$ for mapping f_{u_i} 's (note that ordering is important). Let that be $\{g_{v_1}, \dots, g_{v_{\ell_0}}\}$ for $1 \leq v_1, \dots, v_{\ell_0} \leq \mu$. If $|\langle g_{v_1} \cup \dots \cup g_{v_{\ell_0}} \rangle| < 2^n - 1$, proceed to the next choice for $\{g_{v_1}, \dots, g_{v_{\ell_0}}\}$.
 - (b) For $i = 1, \dots, \ell_0$, choose a $\{y_{i,1}, \dots, y_{i,t}\} \in g_{v_i}$ such that $g_{v_i} = \langle y_{i,1}, \dots, y_{i,t} \rangle$.
 - (c) Choose one of the $(\ell_0)!$ permutations of the elements $1, \dots, \ell_0$, say σ_k , for $k = 1, \dots, (\ell_0)!$.
 - (d) Construct $\mathcal{C}_{B,y}$ which maps the canonical basis elements to y 's such that $F_{t(i-1)+j}$ is mapped to $y_{\sigma_k(i),j}$.
 - (e) If $\mathcal{C}_{B,y}(\mathcal{C}_{x,B}(d_1))$ is equivalent to d_2 (as per the bitstring method in Section 3), then, $d_1 \cong d_2$, and report $\mathcal{C} = \mathcal{C}_{B,y} \cdot \mathcal{C}_{x,B}$ as an IEC and exit; otherwise, continue.
 - (f) Go to Step 4(c) and choose another ordering σ_k if possible, otherwise, continue.
 - (g) Go to Step 4(b) and choose another basis if possible, otherwise, continue.
 - (h) Go to Step 4(a) and choose another set of RDCSSs if possible, otherwise report that d_1 and d_2 are non-isomorphic.
-

A few quick remarks worth noting. From an implementation standpoint, the stages in Step 4 are nested, making it straightforward to parallelize at any stage of the hierarchy. The matrix inversion is required only for Step 3, and the factorization $\mathcal{C} = \mathcal{C}_{B,y} \cdot \mathcal{C}_{x,B}$ avoids the need to repeatedly solve that systems of linear equations associated with $\mathcal{C}(x_{i,j}) = y_{\sigma_k(i),j}$. Moreover, Algorithm 1 iterates through all possible collineations satisfying the PRMP for a particular chosen set $\{x_1, \dots, x_n\}$. As discussed above, the set of collineations satisfying a PRMP is a superset of the collineations satisfying the FRMP (which contains all possible IECs). Therefore, by exhausting the set of collineations for one chosen set $\{x_1, \dots, x_n\}$, we are guaranteed to have already visited all possible IECs.

In terms of algorithmic complexity, the speed-up of moving from the naive search method to Algorithm 1 is proportional to the reduction in the search space size from (2) to (4). The complexity of the equivalence check algorithm (as described in Section 3) is $O(n^2 2^n)$. We have also implemented this algorithm in R (see Appendix C for illustration).

Example: To demonstrate Algorithm 1, we will illustrate a run to check the isomorphism of IC_1 and IC_2 (in the silicon wafers experiment) below. Recall that $IC_1 = \{f_1 = \langle A, EF, BCE \rangle, f_2 = \langle B, AF, CDF \rangle, f_3 = \langle C, AB, ADE \rangle, f_4 = \langle D, BC, BEF \rangle, f_5 = \langle E, CD, ACF \rangle, f_6 = \langle F, DE, ABD \rangle, f_7 = \langle BD, BF, ACE \rangle, f_8 = \langle AC, CE, BDF \rangle, f_9 = \langle AD, BE, CF \rangle\}$, and $IC_2 = \{g_1 = \langle A, BD, CF \rangle, g_2 = \langle B, AF, CE \rangle, g_3 = \langle C, BF, DE \rangle, g_4 = \langle D, AC, BE \rangle, g_5 = \langle E, AB, DF \rangle, g_6 = \langle F, AE, CD \rangle, g_7 = \langle AD, BC, EF \rangle, g_8 = \langle ACE, ADF, BEF \rangle, g_9 = \langle ABC, ADE, CEF \rangle\}$. The following represents an iteration of Step 4 for which an ICE from IC_1 to IC_2 is found.

1. Here, $\ell_0 = 2$ with $f_{u_1} = \langle A, EF, BCE \rangle$ and $f_{u_2} = \langle B, AF, CDF \rangle$.
2. Let $x_{1,1} = A, x_{1,2} = EF, x_{1,3} = BCE$, and $x_{2,1} = B, x_{2,2} = AF, x_{2,3} = CDF$.
3. The collineation matrix $\mathcal{C}_{x,B}$ that canonicalize these x 's has been presented in Section 3.
4. Here, we calculate the total number of options at each stage, and then demonstrate their values when the first IEC found.
 - (a) There are $9!/(9-2)! = 72$ choices for $\{v_1, v_2\} \subset \{1, \dots, 9\}$. Our first choice of $\{v_1, v_2\} = \{1, 2\}$ leads to an IEC.
 - (b) There are $(2^3 - 1) \cdot (2^3 - 2) \cdot (2^3 - 2^2) = 7 \cdot 6 \cdot 4 = 168$ choices for linearly independent $y_{1,1}, y_{1,2}, y_{1,3} \in g_1$, and 168 choices for linearly independent $y_{2,1}, y_{2,2}, y_{2,3} \in g_2$. Out of $(168)^2$ iterations, we found an IEC in the 359th step of our search. The y 's that led to the first IEC are $y_{1,1} = A, y_{1,2} = BD, y_{1,3} = BCDF, y_{2,1} = B, y_{2,2} = ABCEF, y_{2,3} = ABF$.
 - (c) There are two options for the permutation: $\sigma_1 = (1, 2)$ or $\sigma_2 = (2, 1)$. Our first IEC was found using σ_1 .
 - (d) Here,

$$\mathcal{C}_{B,y} = \begin{bmatrix} 1 & 0 & 0 & 0 & 1 & 1 \\ 0 & 1 & 1 & 1 & 1 & 1 \\ 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 & 1 \end{bmatrix}.$$

- (e) A run of the equivalence check algorithm verifies that $\mathcal{C}_{B,y}(\mathcal{C}_{x,B}(d_1))$ is equivalent to d_2 (details omitted for space). Thus, $d_1 \cong d_2$, and

$$\mathcal{C} = \mathcal{C}_{B,y} \cdot \mathcal{C}_{x,B} = \begin{bmatrix} 1 & 0 & 0 & 0 & 1 & 1 \\ 0 & 1 & 1 & 1 & 1 & 1 \\ 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 1 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 & 1 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 1 & 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 & 1 & 1 \end{bmatrix}$$

is an IEC. We can exit the algorithm.

5 Search Algorithm for Star-based Designs

Recall that a balanced star-based design refers to a multi-stage factorial design with equal sized RDCSSs that share a common overlap. As per Lemma 1, a star $\Omega = St(n, \mu, t, t_0)$ can be expressed as $\Omega = \psi \times \pi$, where ψ is a $((t-t_0)-1)$ -spread of \mathcal{P}_{n-t_0} , and π is (t_0-1) -dimensional subspace in $\mathcal{P}_n \setminus \mathcal{P}_{n-t_0}$. As earlier, let $u = n - t_0$ and $h = t - t_0$. Thus, the isomorphism check between two star-based designs d_1 and d_2 (with (t_0-1) -dimensional nuclei) can be reduced to checking isomorphism between two $(h-1)$ -spreads of \mathcal{P}_{n-t_0} by iterating through the elements of \mathcal{C}_{n-t_0} instead of \mathcal{C}_n . Even for small nuclei (e.g. $t_0 = 1$ or 2), this corresponds to a large reduction in the search space.

Algorithm 2 summarizes the steps of how Algorithm 1 can be used to search for an IEC between d_1 and d_2 based on $\Omega_1 = \psi_1 \times \pi_1$ and $\Omega_2 = \psi_2 \times \pi_2$, respectively.

Algorithm 2 Isomorphism check between two $St(n, \mu, t, t_0)$ -based designs d_1 and d_2 , which correspond to stars $\Omega_1 = \psi_1 \times \pi_1$ and $\Omega_2 = \psi_2 \times \pi_2$, respectively.

1. Determine two bases $\{p_{1,1}, \dots, p_{1,t_0}\}$ and $\{p_{2,1}, \dots, p_{2,t_0}\}$ of the nuclei π_1 and π_2 , respectively.
 2. Construct a collineation matrix $\mathcal{C}_{\pi_1, B}$ mapping $\{p_{1,1}, \dots, p_{1,t_0}\}$ to the t_0 trailing basic factors F_{n-t_0+1}, \dots, F_n . The pre-images of F_1, \dots, F_{n-t_0} can be chosen as an arbitrary linearly independent set from $\mathcal{P}_n \setminus \pi_1$.
 3. Similarly, construct a collineation matrix $\mathcal{C}_{\pi_2, B}$ mapping $\{p_{2,1}, \dots, p_{2,t_0}\}$ to the t_0 trailing basic factors F_{n-t_0+1}, \dots, F_n .
 4. Extract designs d_1^* and d_2^* on \mathcal{P}_{n-t_0} corresponding to the spreads $\mathcal{C}_{\pi_1, B}(\psi_1)$ and $\mathcal{C}_{\pi_2, B}(\psi_2)$.
 5. Run Algorithm 1 on d_1^* and d_2^* . If we come across a \mathcal{C}^* that is an IEC, then an IEC for d_1 and d_2 is given by $\mathcal{C} = \mathcal{C}_{\pi_2, B}^{-1} \cdot \mathcal{C}^* \cdot \mathcal{C}_{\pi_1, B}$. Otherwise, d_1 and d_2 are non-isomorphic.
-

Note that in Algorithm 2, Steps 1-4 relabel the $(h-1)$ -spreads ψ_1 and ψ_2 of \mathcal{P}_{n-t_0} such that their points are within the span of the first $n-t_0$ canonical factors F_1, \dots, F_{n-t_0} (or A, B, \dots). This relabeling allows Algorithm 1 to be run using a search space of collineations over \mathcal{P}_{n-t_0} rather than over \mathcal{P}_n , as all effects involving the last t_0 basic factors are discarded along with the nuclei. This reduction of the search space decreases both the number of collineations that need to be considered as well as the dimension of the structures involved.

Similar to Algorithm 1, the computational complexity of Algorithm 2 improves over the naive method proportionally to the reduction in the search space from (2) evaluated at n to (4) evaluated at $n - t_0$. Furthermore, the complexity of each equivalence check decreases from $O(n^2 2^n)$ to $O(n^2 2^{n-t_0})$ because the objects being compared are smaller after reducing to spreads. Appendix C illustrates the usage of our R implementation.

In the plutonium alloy example, $PA_1 = \{\langle A, B, CDE \rangle, \langle C, AD, BE \rangle, \langle D, E, ABC \rangle\}$ is derived from a balanced covering star $St(5, 5, 3, 1)$ of \mathcal{P}_5 , whereas, $PA_2 = \{\langle A, B, DE, ACD \rangle, \langle C, AB, DE, ACD \rangle, \langle D, E, AB, ACD \rangle\}$ represents a covering star $St(5, 3, 4, 3)$ of \mathcal{P}_5 . Since the sizes of the two nuclei are different, the two designs are trivially non-isomorphic.

6 Results on Special Cases

Thus far we have developed theoretical results and algorithms for checking whether or not two RDCSS-based designs are isomorphic. However, we often want to compare all possible admissible designs and find the optimal one as per some ranking criterion. For this purpose, we need to construct all possible different (or non-isomorphic) admissible designs. This is a much bigger challenge for RDCSS-based designs because formal construction methods for all possible spreads or stars are not known yet. In this section, we discuss some results from the Combinatorics literature on the complete classification of spreads that can be used for small RDCSS-based designs in \mathcal{P}_n .

6.1 Complete Classification

A balanced $(t-1)$ -spread of \mathcal{P}_n is referred to as *trivial* for $t = 1$ and $t = n$. Of course, we are more interested in the non-trivial cases. As expected, complete classification of non-isomorphic balanced spreads is known for only small n .

- A1. [$n \leq 3$]: All balanced spreads are trivial, meaning for every given $n \leq 3$ all $(t-1)$ -spreads of \mathcal{P}_n are isomorphic.
- A2. [$n = 4$]: André (1954) ensures the existence of non-trivial spreads for $t = 2$. Soicher (2000) show that all 1-spreads of \mathcal{P}_4 are isomorphic.
- A3. [$n = 5$]: All covering spreads are trivial, as $n = 5$ is prime. However, a complete classification of partial spreads of \mathcal{P}_5 is available in Gordon et al. (2004), indicating that there are 4 isomorphism classes of maximal 1-spreads of \mathcal{P}_5 consisting of 9 RDCSSs.
- A4. [$n = 6$]: There exist non-trivial balanced spreads for $t = 2$ and $t = 3$. Topalova and Zhelezova (2010) showed that all 2-spreads ($t = 3$) of \mathcal{P}_6 are isomorphic, and Mateva and Topalova (2009) used exhaustive search to show that there exist 131044 mutually non-isomorphic 1-spreads ($t = 2$) of \mathcal{P}_6 .
- A5. [$n = 7$]: All covering spreads are trivial, as $n = 7$ is prime. However, Honold et al. (2019) have shown that there exist 715 isomorphism classes of maximal partial 2-spreads of \mathcal{P}_7 consisting of 17 RDCSSs.

For $n \geq 8$, we are unaware of any such results. For an example of two non-isomorphic 1-spreads of \mathcal{P}_6 , consider $d_1 = \{f_1, \dots, f_{21}\}$, shown in Table 3, and $d_2 = \{g_1, \dots, g_{21}\}$, where $g_i = f_i$ for $i = 1, \dots, 18$, and $g_{19} = \{ACE, AF, CEF\}$, $g_{20} = \{BCDF, CF, BD\}$, and $g_{21} = \{ABCD, AEF, BCDEF\}$. Here, the spread for d_2 was obtained via partitioning the RDCSSs f_{19} , f_{20} , and f_{21} in d_1 into 3 new RDCSSs. The non-isomorphism of the spreads was verified using Algorithm 1.

Admittedly, multi-stage factorial experiments with a small number of basic factors have been typically more common in industrial experiments. However some of the modern experiments, for instance using computer simulation models, involve a large number of factors. We

Table 3 A 1-spread of $\mathcal{P}_6 = PG(5, 2)$

f_1	f_2	f_3	f_4	f_5	f_6	f_7	f_8
F	E	D	C	B	A	EF	DE
ABCEF	ABDF	ACF	BF	AE	DEF	CDE	BCD
ABCE	ABDEF	ACDF	BCF	ABE	ADEF	CDF	BCE
f_9	f_{10}	f_{11}	f_{12}	f_{13}	f_{14}	f_{15}	f_{16}
CD	BC	AB	DF	CE	AC	BEF	ADE
ABC	ABEF	ADF	BE	AD	BDE	ACD	BCEF
ABD	ACEF	BDF	BDEF	ACDE	ABCDE	ABCDEF	ABCDF
f_{17}	f_{18}	f_{19}	f_{20}	f_{21}			
CDEF	BCDE	ABCD	AEF	BD			
ABDE	ACDEF	BCDF	CF	CEF			
ABCF	ABF	AF	ACE	BCDEF			

now argue that the classification of balanced spreads presented above generates a rich class of star-based designs.

One may not find 0-spreads to be useful for a spread-based design, but such spreads can play a crucial role in constructing useful star-based designs, e.g., via Lemma 2. For instance, in the plutonium alloy example, a 0-spread of \mathcal{P}_2 is used to construct the balanced covering star $St(5, 3, 4, 3)$ of \mathcal{P}_5 which generates PA_2 – a 3-stage 2^5 split-lot design with four randomization factors at each stage. This design is desirable as the significance of all effects can be assessed using four half-normal plots (see Ranjan et al. (2010) for details). Similarly, 1-spreads and 2-spreads can also be augmented with different sized nuclei to form a variety of stars, providing flexibility for constructing small to large star-based designs.

We now use the results from A1 – A5 and the theoretical results presented in Sections 3 and 5 to classify the non-isomorphic balanced covering stars $St(n, \mu, t, t_0)$ of \mathcal{P}_n . For convenience we follow the same notation, $u = n - t_0$ and $h = t - t_0$, as in Lemma 2.

- B1. For any given $0 \leq u \leq 5$, $t_0 \geq 0$ and h that divides u , all balanced covering stars $St(u + t_0, \mu, h + t_0, t_0)$ of \mathcal{P}_{u+t_0} are isomorphic to each other. The proof follows from Lemma 1 and A1 – A3.
- B2. For $t_0 \geq 0$, all balanced covering stars $St(6 + t_0, \mu, 2 + t_0, t_0)$ of \mathcal{P}_{6+t_0} are isomorphic to each other. The result follows from A4.
- B3. For every $t_0 \geq 0$, there exist 131044 mutually non-isomorphic balanced stars $St(6 + t_0, \mu, 3 + t_0, t_0)$ of \mathcal{P}_{6+t_0} . The result follows from A4.

The categories defined by B1 and B2 contain most of the popular stars used to obtain RDCSS-based designs. For cases falling outside of these categories, it may be necessary to search over representatives from all isomorphism classes when searching for designs. This is a difficult problem because other than the exhaustive search methods used by Topalova and Zhelezova (2010) and Mateva and Topalova (2009), there is no known strategy for obtaining representatives of all isomorphism classes.

6.2 Cyclic-spread based Designs

In this section we provide results demonstrating that the most popular approach of constructing a balanced spread – the cyclic approach of Hirschfeld (1998) – only accesses a single isomorphism class, even if many exist. The algebraic results used in the proofs (presented in Appendix B) are mostly based on Lidl and Niederreiter (1994).

Although the spreads obtained via the cyclic construction method (outlined in Section 2.2) may vary with the choice of the primitive element and primitive polynomial of $GF(2^u)$, the next two results establish that such spreads are equivalent or isomorphic.

Theorem 1 *Let $\psi_1 = \{f_1, \dots, f_\mu\}$ and $\psi_2 = \{g_1, \dots, g_\mu\}$ be two $(h - 1)$ -spreads of \mathcal{P}_u constructed using the cyclic method with two different roots α and β of the same primitive polynomial $P(\omega)$. Then ψ_1 is equivalent to ψ_2 .*

Theorem 2 *Let $\psi_1 = \{f_1, \dots, f_\mu\}$ and $\psi_2 = \{g_1, \dots, g_\mu\}$ be two $(h - 1)$ -spreads of \mathcal{P}_u constructed using the cyclic method with two different primitive polynomials $P_1(\omega)$ and $P_2(\omega)$ respectively. Then ψ_1 is isomorphic to ψ_2 .*

See Appendix B for the proofs of Theorems 1 and 2. Although the cyclic construction method for $(h - 1)$ -spreads of \mathcal{P}_u is widely-used, it accesses only a fraction of all possible spread/star-based designs. For example, only one of the 131044 isomorphism classes of 1-spreads of \mathcal{P}_6 is obtained using the cyclic method. As per our knowledge, one may have to rely on exhaustive search to find non-isomorphic spread/star-based designs.

7 Concluding Remarks

In this paper, we formalize the definition of isomorphism of multi-stage factorial designs under the unified framework based on randomization defining contrast subspace (RDCSS), developed by Ranjan (2007). Focussing on the RDCSS-based designs that are derived from balanced spreads and balanced covering stars, we have developed isomorphism check algorithms that are more efficient than the naive approach of iterating through all possible relabelings and reorderings. We have also provided a complete classification of small designs that are typically assumed to be important from practical standpoint. Furthermore, the proposed algorithms and relevant functions are implemented in R for easy access.

A few remarks are as follows. Both the theoretical results and the algorithms can easily be generalized for unbalanced spreads and stars, however, the construction and complete classification of such designs require more work. Some of the theoretical results will also hold when generalized to q -level multi-stage factorial designs with randomization restrictions. The proposed relabeling approach can also be used to find a design that meet the pre-specified randomization restrictions.

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Conflict of interest

The authors declare that they have no conflict of interest.

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Appendix A: Proofs of Results in Section 4

Proof of Proposition 1. Without loss of generality, suppose that f_1, \dots, f_ℓ are the RDCSSs for d_1 that contain at least one of x_1, \dots, x_n . Then, by the partial RDCSS mapping property, the elements of distinct f_1, \dots, f_ℓ must be mapped to distinct RDCSSs in d_2 . There are $\mu!/(\mu-\ell)!$ different ways to choose a correspondences between these ℓ RDCSSs in d_1 and ℓ of the μ RDCSSs which comprise d_2 . Subsequently, there are $\prod_{j=1}^{m_i} (2^t - 2^{j-1})$ distinct choices of linearly independent points in each RDCSS of d_2 to which we can map the m_i points f_i . Combining these counts as a product yields the result.

Comment on Proposition 1. The upper bound given in Proposition 1 is not necessarily tight—it is possible that some RDCSS correspondences do not yield full rank solutions. For example, if $n = 6$, $m_1 = m_2 = m_3 = 2$ and $g_1 = \langle A, B \rangle$, $g_2 = \langle C, D \rangle$, $g_3 = \langle AC, BD \rangle$, then no collineations exist for the RDCSS correspondence $(f_1, f_2, f_3) \rightarrow (g_1, g_2, g_3)$ because $\langle g_1 \cup g_2 \cup g_3 \rangle$ is not full rank. Therefore, this entire correspondence can be discarded from the search, providing an even greater reduction.

Proof of Proposition 2. When $t = 1$, the result is trivial, so we limit our consideration to $t > 1$. Suppose that within ψ there exists k $(t-1)$ -flats f_{u_1}, \dots, f_{u_k} of \mathcal{P}_n such that $|\langle \cup_{i=1}^k f_{u_i} \rangle| = 2^{kt} - 1$ for some integer $k \leq n/t$. This is guaranteed to at least hold for $k = 1$ by definition of a spread. If $k = n/t$, then the result is immediate. Otherwise, $k \leq n/t - 1$, and of the $2^n - k2^t$ points not contained within $\cup_{i=1}^k f_{u_i}$, $2^n - 2^k$ are not contained by $\langle \cup_{i=1}^k f_{u_i} \rangle$ leaving $2^k - k2^t$ that do fall within that span. Recall that all $(t-1)$ -spreads of \mathcal{P}_n contain $\mu = (2^n - 1)/(2^t - 1)$ $(t-1)$ -flats. Then, $|\psi| - k$ is given by

$$\mu - k = \frac{2^n - 1}{2^t - 1} - k = \sum_{i=1}^{n/t} 2^{(i-1)t} - k \geq 2^k - k.$$

The pigeonhole principle guarantees that at least one $(t-1)$ -flat $f_{u_{k+1}}$ shares no elements with $\langle \cup_{i=1}^k f_{u_i} \rangle$. This flat can be appended to the list f_{u_1}, \dots, f_{u_k} without introducing any linear dependence. Proceeding inductively, additional flats can be included until $k = n/t$. \square

Appendix B: Proofs of Results in Section 6.2

First we give a technical lemma and then the proofs of the two theorems.

Lemma 3 *Let $\psi = \{f_1, \dots, f_\mu\}$ be an $(h-1)$ -spread of \mathcal{P}_u constructed with the cyclic method using a primitive polynomial $P(\omega)$ and root ω . Then,*

- (a) $x_1 = \omega^a$ and $x_2 = \omega^b$ are in the same $(t-1)$ -flat $f \in \psi$ if and only if $a \equiv b \pmod{\mu}$;
- (b) the set of all nonzero roots of $\omega^{2^h} - \omega$ is equal to the set of all elements of the form ω^a where $a \equiv 0 \pmod{\mu}$. Thus the first $(h-1)$ -flat, $f_1 \in \psi$, corresponds to the set of all nonzero elements of $GF(2^h)$;
- (c) f_2, \dots, f_μ are multiplicative cosets of f_1 in the group $GF(2^u)^*$ of nonzero elements of $GF(2^u)$.

Proof. (a) follows trivially from the cyclic structure in Table 1. For part (b), since $\mu(2^h - 1) = 2^u - 1$, or $\mu 2^h \equiv \mu \pmod{2^u - 1}$,

$$(\omega^{\ell\mu})^{2^h} = (\omega^{\mu 2^h})^\ell = (\omega^\mu)^\ell = \omega^{\ell\mu},$$

and hence, $\omega^{\ell\mu}$ is a root of $\omega^{2^h} - \omega$. Part (c) follows from noting that the elements of f_i are of the form $\omega^{k\mu+i} = \omega^i \omega^{k\mu}$, where $0 \leq i < \mu$. \square

Proof of Theorem 1. We need to show that for every $g_j \in \psi_2$, there exists a unique $f_i \in \psi_1$ such that the elements in g_j are in f_i . Let e_1 and e_2 be two distinct effects in g_j , then from Lemma 3(a), $e_1 = \beta^a$, $e_2 = \beta^b$ and $a \equiv b \pmod{\mu}$. From Theorem 2.14 of Lidl and Niederreiter (1994), there exists $0 \leq k \leq u$ such that $\beta = \alpha^{2^k}$. Thus, $e_1 = \beta^a = (\alpha^{2^k})^a = \alpha^{2^k a}$ and $e_2 = \beta^b = \alpha^{2^k b}$. Note that $a \equiv b \pmod{\mu}$ implies $2^k a \equiv 2^k b \pmod{\mu}$, as $\gcd(2^k, \mu) = 1$. Consequently, e_1 and e_2 must belong to the same flat in ψ_1 (from Lemma 3(a)). \square

Proof of Theorem 2. We establish the existence of an IEC by constructing one. Our isomorphism will be a field isomorphism, which makes it easier to show that it is an IEC.

Let α be the primitive root of $P_1(\omega)$ which is used to construct ψ_1 and let β be the primitive root of $P_2(\omega)$ which is used to construct ψ_2 . By Lidl and Niederreiter (1994, Thm 2.40), there is a primitive polynomial $Q(x)$ of degree u whose roots form a basis for $GF(2^u)$ over \mathbb{Z}_2 . Note that if ω is one of these roots then the other $u-1$ roots are all of the form ω^{2^i} for $i = 1, \dots, u-1$. There are $a, b \in \{1, \dots, 2^u - 2\}$ with both α^a and β^b roots of $Q(x)$. We define our IEC Φ by first setting

$$\Phi((\alpha^a)^{2^i}) = (\beta^b)^{2^i} \quad \text{for } i = 0, 1, \dots, u-1,$$

and then extending Φ to all of $GF(2^u)$ by linearity. Since the roots of $Q(x)$ form a basis, this uniquely defines Φ .

Our next task is to show that Φ is a field isomorphism. By our definition, Φ is linear; we need only show that Φ preserves multiplication. Since $Q(x)$ is primitive and α^a, β^b are both roots of $Q(x)$, it is enough to show $\Phi((\alpha^a)^k) = (\beta^b)^k$ for all $k = 1, \dots, 2^u - 1$. Fix k . Since $\alpha^a, \alpha^{2a}, \dots, \alpha^{2^{u-1}a}$ are the distinct roots of $Q(x)$ and are a basis, there are constants $c_i \in \mathbb{Z}_2$ so that

$$\alpha^{ak} = \sum_i c_i \alpha^{a2^i}.$$

Consider the polynomial $H(x) = x^k - \sum_i c_i x^{2^i}$. Then $H(\alpha^a) = 0$ by definition of c_i . However, since $x \mapsto x^{2^j}$ is a field automorphism for any j , this means that $H(\alpha^{a2^j}) = 0$ as well. Thus all the roots of $Q(x)$ are also roots of $H(x)$. Since β^b is a root of $Q(x)$, then $H(\beta^b) = 0$ or $\beta^{bk} = \sum_i c_i \beta^{b2^i}$. However, then

$$\begin{aligned} \Phi(\alpha^{ak}) &= \Phi\left(\sum_i c_i \alpha^{a2^i}\right) = \sum_i c_i \Phi(\alpha^{a2^i}) \\ &= \sum_i c_i (\beta^b)^{2^i} = \beta^{bk} \end{aligned}$$

and so Φ is also a field isomorphism. We claim that Φ is an IEC. To see this, we first note that by Lidl and Niederreiter (1994, Thm 2.21), Φ maps the roots of $x^{2^h} - x$ to roots of $x^{2^h} - x$. That is, it maps $GF(2^h) \subset GF(2^u)$ to itself. This indicates, by Lemma 3(b), that $\Phi(f_1) = g_1$. Additionally, since Φ is a field isomorphism, it maps any multiplicative coset of $GF(2^h)^*$ in $GF(2^u)^*$ to some multiplicative coset of $GF(2^h)^*$. By Lemma 3(c), each $(h-1)$ -flat f_i of ψ is mapped to a unique $(h-1)$ -flat g_j in ψ_2 . Thus Φ is an IEC for ψ_1 and ψ_2 . \square

Appendix C: R Codes for Easy Implementation

In this section, we discuss various functions that are used to implement Algorithm 1 and Algorithm 2 for checking the isomorphism of balanced spread- and star- based designs. These functions are implemented in R and have been uploaded to GitHub for easy access (see <https://github.com/neilspencer/IsoCheck/>). The usage and brief description of the key functions are as follows:

The isomorphism of two $(t - 1)$ -spreads of $PG(n - 1, 2)$, `spread1` and `spread2`, can be checked using the following R code:

```
R> checkSpreadIsomorphism(spread1, spread2, returnfirstIEC = T).
```

The third argument "`returnfirstIEC = T`" specifies whether the algorithm searches until it finds the first IEC (might only take a few second) or if it continues to search for and returns all IECs (which can take a long time). For non-isomorphic spreads or stars, the run times are the same (none are found). However, for isomorphic spreads, stopping once we have found one IEC (which means they are isomorphic) is much faster.

Similar to spread-isomorphism, two stars `star1` and `star2` can be checked for isomorphism using the following R code

```
R> checkStarIsomorphism(star1, star2, returnfirstIEC = T).
```

It is assumed that both spreads are $(t - 1)$ -spreads, and both stars are $St(n, \mu, t, t_0)$ of $PG(n - 1, 2)$. The isomorphism check for stars is slightly different than for spread — it exploits the spread to star correspondence to reduce the dimension of the search space (as described by Algorithm 2). Both `checkSpreadIsomorphism` and `checkStarIsomorphism` call several important functions such as finding the bitstring representation of flats for checking equivalence, and applying collineations for relabeling of spreads and stars. The usage of these functions are illustrated as follows:

```
R> getBitstrings(spread1)
R> applyCollineation(C, spread1)
R> checkspreadEquivalence(spread1, spread2)
R> checkstarEquivalence(star1, star2)
```

Though the user can input the spreads of their choice in a specified format as discussed in the "`readme`" file and "`exampleScript.R`", we have coded several spreads and stars that are used in this paper (see the help manual of the R package "`IsoCheck`").