Automatic generation of generalised regular factorial designs

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Abstract The R package *planor* enables the user to search for, and construct, factorial designs satisfying given conditions. The user specifies the factors and their numbers of levels, the factorial terms which are assumed to be non-zero, and the subset of those which are to be estimated. Both block and treatment factors can be allowed for, and they may have either fixed or random effects, as well as hierarchy relationships. The designs are generalised regular designs, which means that each one is constructed by using a design key and that the underlying theory is that of finite abelian groups. We develop and illustrate the main theoretical results and algorithms on which *planor* is based, with emphasis on mathematical rather than programming details. The first sections are dedicated to the elementary case, when the numbers of levels of all factors are powers of the same prime. The ineligible factorial terms associated with users' specifications are defined and it is shown how they can be used to search for a design key by a backtrack algorithm. Then the results are extended to the case when different primes are involved, by making use of the Sylow decomposition of finite abelian groups. The proposed approach provides a unified framework for many types of factorial designs.

Key words backtrack algorithm; design key; estimate specification; factorial design; hierarchy constraint; ineligible factorial term; model specification

1 Introduction

Factorial designs that may include several block and treatment factors date back to the pioneering work of Fisher and Yates at Rothamsted Experimental Station (Yates, 1933, 1937; Fisher, 1942), followed by Finney (1945) and Bose (1947). Since then, the construction of fractional designs has been a constantly active field of research in the theory of design of experiments. It has also been widely applied in many different application areas, including food research, biology, industry, and—more recently—computer experiments.

The designs we are interested in are known today as regular factorial designs. Their construction, which is based on algebra and group theory, gives a large class of orthogonal factorial designs, including as special cases block and row-column designs (Yates, 1937) as well as fractional designs (Finney, 1945). Regular fractional designs became a standard method of construction very early. Their main principles in standard cases have been explained in numerous text books including classics (Kempthorne, 1957; Cochran and Cox, 1957) and more recent ones (Ryan, 2007; Bailey, 2008; Morris, 2011; Cheng, 2014).

The construction of a regular fraction involves two steps: first, finding defining relationships or generators of the fraction ensuring that factorial effects of interest will be estimable; second, generating the actual design. Despite its apparent simplicity in standard cases, the first step still represents a major challenge in general situations. It has been applied and programmed mainly in the case of symmetric designs, which require all factors to have the same number of levels or, at least, numbers of levels that are powers of the same prime.

An important notion in fractional designs is resolution (Box and Hunter, 1961a,b). If R is a positive integer, a fraction of resolution R allows the estimation all factorial effects up to interactions of order strictly smaller than $R/2$, assuming that all interactions of order strictly larger than $R/2$ are zero. More discriminating criteria such as minimum aberration (Fries and Hunter, 1980) or maximum estimation capacity (Cheng and Mukerjee, 1998) have been developed. The construction of optimal designs with respect to these criteria is still an active field of research, which includes analytical as well as algorithmic issues. However resolution and aberration imply that the model of interest be symmetric with respect to all factors.

Most work in this area thus deals with problems which are highly symmetric with respect to the factors and models of interest. However, there is also a need to find generic and user-friendly methods of construction adapted to much more flexible problem specifications, allowing for unconstrained numbers of levels and flexible model assumptions.

Algorithms were developed and studied in the 1970s and 1980s (Patterson, 1965, 1976; Bailey *et al.*, 1977; Franklin and Bailey, 1977; Patterson and Bailey, 1978; Bailey, 1985; Franklin, 1985) and some of them implemented in statistical packages (SAS Institute Inc., 2010; Payne, 2012; Groemping, 2014). Lewis (1982) tabulated generators for asymmetric factorial designs with resolution 3. In this paper, we extend these approaches to a generalised class of regular designs. We follow the theoretical framework detailed in Kobilinsky (1985) and Kobilinsky and Monod (1991, 1995), although we occasionally modify a term or notation for the sake of simplicity. We also make intensive use of pseudofactors (Monod and Bailey, 1992). The generalised class includes symmetric as well as asymmetric designs, and the construction method allows the user to define the model and specify what should be estimated. In addition to the more usual fractional designs, we show that our results apply to the construction of generalised split-plot or criss-cross designs. The approach and results have been implemented in the R package *planor* (Kobilinsky *et al.*, 2012; Monod *et al.*, 2012), based on the initial APL version by Kobilinsky (Kobilinsky, 2005).

2 Overview of the design search issue

In this paper, generating a factorial design means specifying the combination of levels of the factors that must be allocated to each experimental unit. This will be formalised in Section 3.1 as a function from the set of units to the set of treatments. However, before talking about design generation, we explain the design specifications that we want to allow for.

We start with three examples to illustrate the diversity of situations we want to consider. We then introduce some results and notation. We use the notation of Bailey (2008, Chapter 10) for the hierarchy relationships between factors. In particular:

- $B \preccurlyeq A$ means that factor B is or must be nested in factor A, in other words B must be finer than or equivalent to A and, reciprocally, A must be coarser than or equivalent to B, so that each level of B occurs with a single level of A;
- $A \wedge C$ denotes the product or *infimum* of A and C, which is the factor whose levels are the combinations of levels of A and C.

Note that $A \wedge C \preccurlyeq A$ and $A \wedge C \preccurlyeq C$.

Of course, there is a difference between a factor and the effect of that factor, but we follow standard practice in using the same notation A both for a factor and for its main effect. The interaction between factors A and B is denoted $A.B$.

2.1 Examples

Example 1 There are four treatment factors F_1, F_2, F_3, F_4 with 6, 4, 3, 4 levels respectively. A complete factorial design would require 288 experimental units but we assume this is much larger than possible, so that a smaller fractional design is looked for.

The experimenter intends to analyse the data using a model that consists of the four main effects of F_1, F_2, F_3, F_4 and of the interaction $F_1.F_2$, with good reasons to consider the other interactions as negligible. The factorial terms he or she wants to estimate are the four main effects only. The factorial terms in the model and those that must be estimated are listed in the following sets $\underline{\mathcal{M}}$ and $\underline{\mathcal{E}}$:

$$\underline{\mathcal{M}} = \{\emptyset,\, F_1,\, F_2,\, F_3,\, F_4,\, F_1.F_2\}\ , \quad \underline{\mathcal{E}} = \{F_1,\, F_2,\, F_3,\, F_4\} = \underline{\mathcal{M}} \setminus \{\emptyset,\, F_1.\, F_2\}\ ,$$

where $\emptyset$ denotes the general mean.

Example 2 A row-and-column design has to be constructed with two columns (factor C), three rows (factor R) and two units in each of the six blocks defined by a row and a column. There are three treatment factors: two 2-level factors D, E and one 3-level factor A. The experimenter wants to estimate the interactions $D.A$, $E.A$, considering a model that includes the row, column and block effects and all interactions between two treatment factors. The sets $\underline{\mathcal{M}}$ and $\underline{\mathcal{E}}$ now are:

$$\underline{\mathcal{M}} = \{\emptyset,\, C,\, R,\, C.R,\, D,\, E,\, A,\, D.A,\, E.A,\, D.E\}\ , \quad \underline{\mathcal{E}} = \{D.A,\, E.A\}\ .$$

An additional constraint is that, for practical reasons, the factor A must remain constant on each row. We call this a hierarchy constraint, imposing that factor R be nested in factor A and denote it by $R \preccurlyeq A$.

Example 3 The experimental units consist of four blocks, each containing two subblocks of four units. This structure can be described by three factors P, Q, U with four, two and four levels respectively. The levels of P define the blocks, the levels of the infimum $P \wedge Q$ define the subblocks, and the levels of the infimum $P \wedge Q \wedge U$ determine the units. In addition, there are four treatment factors A, B, C, D with two levels. There is again a hierarchy constraint: we assume that the levels of A cannot be varied between the four units of a given subblock, which is denoted by $P \wedge Q \preccurlyeq A$.

The model to be applied contains the main effects and two-factor interactions of A, B, C, D, plus the block and subblock effects. The experimenter wants the main effects and the two-factor interactions of A, B, C, D to be estimable as efficiently as possible. Thus the sets $\underline{\mathcal{M}}$ and $\underline{\mathcal{E}}$ should be, ideally,

$$\begin{aligned} \underline{\mathcal{M}} &= \{\emptyset,\, P,\, Q,\, P.Q,\, A,\, B,\, C,\, D,\, A.B,\, A.C,\, A.D,\, B.C,\, B.D,\, C.D\}\ , \\ \underline{\mathcal{E}} &= \{A,\, B,\, C,\, D,\, A.B,\, A.C,\, A.D,\, B.C,\, B.D,\, C.D\}\ . \end{aligned}$$

However, the hierarchy constraint means that the main effect of A is necessarily confounded with subblock effects so that it cannot be estimated in a model with fixed subblock effects. Instead, provided a proper randomization is performed, subblock effects can be considered as centred random effects and the analysis can be decomposed into two levels of variability, or strata (Bailey, 2008). The objective now is to estimate all effects of interest except the main effect A in the within-subblock stratum, which includes residual variability only, and to estimate the main effect A in the subblock stratum, which includes the variability between subblocks but which is orthogonal to block effects. These requirements can be described by using two pairs of model-estimate lists, where in each case the model is restricted to the fixed-effect factorial terms. The first pair deals with the within-subblock stratum or, equivalently, with the model containing all block factors:

$$\underline{\mathcal{M}}_1 = \underline{\mathcal{M}}\ , \quad \underline{\mathcal{E}}_1 = \underline{\mathcal{E}} \setminus \{A\}.$$

The second pair deals with the between-subblock stratum or, equivalently, with the model containing the block effects but not the subblock effects:

$$\underline{\mathcal{M}}_2 = \underline{\mathcal{M}} \setminus \{Q,\, P.Q\}\ , \quad \underline{\mathcal{E}}_2 = \{A\}.$$

2.2 Factorial terms and model specifications

We let $F_1, \ldots, F_h$ denote all the genuine factors involved in the experiment, that is, those which have a direct meaning for the experimenter and which will be taken into account for the design construction. The set of treatments, denoted by T, includes all n combinations of levels of $F_1, \ldots, F_h$, with $n = n_1 \cdots n_h$ where n_i is the number of levels of F_i. It is convenient at first not to make the usual distinction between block and treatment factors. So, unless explicitly specified, we shall call $F_1, \ldots, F_h$ the *treatment* factors, even if some of them correspond to the block structure of the experiment. Occasionally, we shall call them the *genuine* factors and distinguish between *block* and *treatment* genuine factors in the usual sense.

The vector τ of treatment effects belongs to the treatment vector space $\mathbb{R}^n$, whose elements we consider to be column vectors. In the standard analysis of variance (ANOVA), the treatment vector space is decomposed into mutually orthogonal subspaces $\mathcal{W}_I$ associated with the 2^h subsets of factors $\{F_i : i \in I\}$, for $I \subseteq \{1, \ldots, h\}$. These subspaces are given by the recurrence relation

$$\mathcal{W}_I = \mathcal{V}_I \cap \left(\bigoplus_{J \subset I} \mathcal{W}_J \right)^{\perp},$$

where $\mathcal{V}_\emptyset$ is the subspace spanned by the all-one vector and $\mathcal{V}_I$ is the subspace spanned by the indicator vectors of the level-combinations of all factors in $\{F_i : i \in I\}$ (Bailey, 2008). According to this decomposition, the treatment effects can be decomposed into factorial effects, as given by the equation

$$\tau = \sum_{I \subseteq \{1,\ldots,h\}} \mathbf{S}_I\, \tau,$$

where $\mathbf{S}_I\tau$ is the orthogonal projection of τ onto $\mathcal{W}_I$. By convention, the subsets $\{F_i : i \in I\}$ are called *factorial terms* and denoted by $\prod_{i\in I} F_i$ as in the examples in Section 2.1. The order of a factorial term $\prod_{i\in I} F_i$ is given by the cardinality of I. Factorial terms of order 1 are called main effects, and factorial terms of order 2 or more are called interactions.

When constructing a fractional design it is necessary to consider that some factorial terms $\prod_{i\in I} F_i$ are negligible, that is, to assume that $\mathbf{S}_I\tau$ is zero. In the examples above, the model set $\underline{\mathcal{M}}$ contains the non-negligible effects and its subset $\underline{\mathcal{E}}$ contains the non-negligible effects that the experimenter wants to estimate. In some cases, such as Example 3, it is useful to consider several such pairs of model and estimate sets.

2.3 Ingredients of the search

The design problems that we consider generalise the examples of Section 2.1, using the generic factorial decomposition of Section 2.2. Their specifications consist of

- the list of treatment factors $F_1, \ldots, F_h$, together with their numbers of levels and any hierarchy constraint;
- one or more joint model and estimate specifications $(\underline{\mathcal{M}}, \underline{\mathcal{E}})$, where $\underline{\mathcal{M}}$ contains the factorial terms in the model and $\underline{\mathcal{E}}$ contains the terms to estimate ($\underline{\mathcal{E}} \subseteq \underline{\mathcal{M}}$);
- the size of the experiment, *i.e.* the number N of experimental units.

For the statistician, the elements of $\underline{\mathcal{M}}$ and $\underline{\mathcal{E}}$ are factorial terms $\prod_{i\in I} F_i$ as given in a model formula when performing an analysis of variance. Mathematically, however, it will be more convenient to consider that the elements of $\underline{\mathcal{M}}$ and $\underline{\mathcal{E}}$ are the associated subsets I of $\{1, \ldots, h\}$. Both representations will be used, depending on the context.

Note that we allow for two ways to handle the case when a factor F_j at $n_i \times n_j$ levels is nested in a factor F_i at n_i levels: either F_j is declared as a n_j-level factor and its actual levels are the levels of $F_i \wedge F_j$, or F_j is declared as a $n_i n_j$-level factor and the hierarchy constraint $F_j \preccurlyeq F_i$ must be specified. We advise using the first option when F_j is a natural refinement of F_i and the second option when the hierarchy is due to experimental constraints rather than genuine relationships between factors. Thus, in Example 3, we used the first option for the hierarchy between blocks and subblocks, with factors P and Q in the roles of F_i and F_j respectively. In contrast, we used the second option for the hierarchy between A and the block factors (with factors A and $P \wedge Q$ in the roles of F_i and F_j respectively), because these factors have no relationship except for experimental constraints.

In regular factorial designs, the number of units N is constrained by the other specifications. Indeed, for a solution to exist, N must be a multiple of $p_1^{\rho_1} \cdots p_l^{\rho_l}$, where $p_1, \ldots, p_l$ are the prime numbers that divide n and $\rho_1, \ldots, \rho_l$ are lower bounds on the exponents which depend on the factor and model specifications. The algorithm described in this paper assumes that N is given by the user (or by a higher-level algorithm). So it is up to the user to propose for N a value of the form $N = q \cdot p_1^{r_1} \cdots p_l^{r_l}$, where q is coprime to $p_1, \ldots, p_l$ and $\rho_1 \leq r_1, \ldots, \rho_l \leq r_l$. In practice, the user may proceed by trial and error by testing different values of N, provided the computing time is not too long. In Examples 2 and 3, the number of units is imposed by the problem, with $N = 2^2 \cdot 3 = 12$ and $N = 2^5 = 32$, respectively. In Example 1, the complete factorial design has size $2^5 \cdot 3^2 = 288$ but we look for smaller design sizes. We know that $\rho_1 \leq 5$ and $\rho_2 \leq 2$ and so we can proceed by trial and error to find them.

3 Elementary regular factorial designs

In this section and the following two, we consider the case when the number of units and the number of levels of all factors are powers of the same prime p. Thus $N = p^r$ and $n = p^s$ for some scalars r and s. This is the case in Example 3 with $p = 2$, but not in Examples 1 and 2, which both involve primes 2 and 3. For the design construction, we use elementary abelian groups of order p, and so the designs will be called *elementary designs* when they have to be distinguished from those considered in Section 6 and later.

The cyclic group of order p is denoted by C_p and it is identified with the integers modulo p under addition. The experimental units are identified with the elements of a product group $U \cong (C_p)^r$, and the treatments with the elements of a product group $T \cong (C_p)^s$. A design d is a function from U to T, with $d(u)$ the treatment allocated to unit u. From now on, we regard elements of both U and T as column vectors and we use $v^\top$ to denote the transpose of a vector v.

3.1 Pseudofactors

The canonical projections $V_1, \ldots, V_r$ from U onto the cyclic group C_p are called the *unit pseudofactors*. Similarly the canonical projections $A_1, \ldots, A_s$ from T onto the cyclic group C_p are called the *treatment pseudofactors*. If $u = (u_1, \ldots, u_r)^\top$ is a unit in U and $t = (t_1, \ldots, t_s)^\top$ a treatment in T, then $V_i(u) = u_i$ and $A_j(t) = t_j$.

Both kinds of pseudofactors must be considered as technical intermediates in the design construction. The genuine treatment factors considered in Section 2 are the products of one or more treatment pseudofactors. If F_i is the product of a family $(A_j)_{j \in J}$ of pseudofactors, this family is said to be a *decomposition of F into pseudofactors*. For instance, if $F_i = A_1 \wedge A_2$, then F_i is said to be decomposed into two pseudofactors A_1, A_2, which means that $F_i(t) = (A_1(t), A_2(t))^\top$ for every $t \in T$. To represent the mapping from the set of factors to the set of pseudofactors, we shall denote the set of pseudofactors in the decomposition of F_i by $\mathcal{P}(F_i)$. Alternatively, we will use $\mathcal{P}(i)$ to denote the indices of the pseudofactors in $\mathcal{P}(F_i)$.

The decomposition of factors into pseudofactors induces a decomposition of factorial terms into pseudofactorial terms. Thus, the factorial term $\prod_{i \in I} F_i$ is decomposed into the pseudofactorial terms $\prod_{j \in J} A_j$ such that $J \cap \mathcal{P}(i) \neq \emptyset$ if and only if $i \in I$. We shall use the notation $\widetilde{\mathcal{P}}(.)$ to denote the set of pseudofactorial terms that decompose a given factorial term.

Example 3 (continued) There are $32 = 2^5$ units and thus five unit pseudofactors $V_1, \ldots, V_5$ at two levels. The nine treatment pseudofactors $(A_1, \ldots, A_9)$ will rather be denoted by P_1, P_2, Q, U_1, U_2, A, B, C, D to keep the correspondence with the genuine factors more explicit. With this notation, we have $\mathcal{P}(P) = \{P_1, P_2\}$, $\mathcal{P}(Q) = \{Q\}$, $\mathcal{P}(U) = \{U_1, U_2\}$, $\mathcal{P}(A) = \{A\}, \ldots, \mathcal{P}(D) = \{D\}$.

For the decomposition of factorial terms, we give the following examples, which include two main effects and three interactions:

$$
\begin{aligned}
\widetilde{\mathcal{P}}(A) &= \{A\}, \\
\widetilde{\mathcal{P}}(P) &= \{P_1,\ P_2,\ P_1.P_2\}, \\
\widetilde{\mathcal{P}}(A.B) &= \{A.B\}, \\
\widetilde{\mathcal{P}}(P.Q) &= \{P_1.Q,\ P_2.Q,\ P_1.P_2.Q\}, \\
\widetilde{\mathcal{P}}(P.U) &= \{P_1.U_1,\ P_1.U_2,\ P_1.U_1.U_2,\ P_2.U_1, P_2.U_2,\ P_2.U_1.U_2, \\
&\qquad P_1.P_2.U_1,\ P_1.P_2.U_2,\ P_1.P_2.U_1.U_2\}.
\end{aligned}
$$

3.2 Characters

Our methods are based on the theory of duals of abelian groups, which can be found in Ledermann (1977). The group homomorphisms from T into C_p are all the linear combinations $A = a_1A_1 + \cdots + a_sA_s$ of the treatment pseudofactors, with $a_j \in C_p$. These homomorphisms are called the *characters* of T and they make up a group T^* called the dual of T. Each character can be represented by its vector of coefficients $a = (a_1, \ldots, a_s)^\top$ in the product group $(C_p)^s$, and the group T^* can be consequently identified with this product group. The characters and dual of U are defined and represented in the same way. The elements of T^* will be called treatment characters and the elements of U^* unit characters.

Each character A of T^* is associated with a *pseudofactorial effect* $e_\tau(A)$. Here, a pseudofactorial effect means a precise linear combination of treatment effects in $\mathbb{R}^n$ or $\mathbb{C}^n$, either the general mean of τ if $A = 0$ or a contrast if $A \neq 0$ (see Kobilinsky, 1985, or Pistone and Rogantin, 2008, for more details). The important point is that each *pseudofactorial effect* belongs to a unique *pseudofactorial term* in the ANOVA decomposition of the treatment effects, and this term is easy to identify by the non-zero coefficients of A. For example, if there is only one non-zero coefficient a_j, then $A = a_jA_j$ and $e_\tau(A)$ belongs to the main effect of pseudofactor A_j. If $a_j \neq 0$ and $a_k \neq 0$ then the effect $e_\tau(a_jA_j + a_kA_k)$ belongs to the interaction between A_j and A_k, and so on. When $p = 2$, the pseudofactorial terms have one degree of freedom each, so each includes a single character and a single pseudofactorial effect. In the general case, a pseudofactorial term of order q includes $(p-1)^q$ characters and the same number of pseudofactorial effects.

In this paper, this additive notation will be used throughout to represent the characters and associated pseudofactorial effects. However, a more conventional notation is the multiplicative one: $A_1^{a_1} \cdots A_s^{a_s}$ is used instead of $a_1A_1 + \cdots + a_sA_s$. Then $A_j^{a_j}$ belongs to the main effect of pseudofactor A_j, while $A_j^{a_j} A_k^{a_k}$ belongs to the interaction $A_j A_k$, and so on. This has the disadvantage that $A_1 A_2$ might mean an interaction or one of the characters whose effect is part of that interaction.

3.3 Link between factorial terms and characters

Consider now the genuine treatment factors F_i, for $i = 1, \ldots, h$. Let E_i denote the subset of T^* consisting of all characters $\sum a_j A_j$ involving the pseudofactors in $\mathcal{P}(F_i)$ only. Let $\widetilde{E}_i = E_i \setminus \{0\}$, so that $\widetilde{E}_i$ consists of all the non-zero elements of E_i. By extension, put $E_\emptyset = \{0\}$ and, for each main effect or interaction $\prod_{i \in I} F_i$, let us define:

$$E_I = \bigoplus_{i \in I} E_i \ , \qquad \widetilde{E}_I = \bigoplus_{i \in I} \widetilde{E}_i \ ,$$

where $E \oplus E' = \{A + B : A \in E, B \in E'\}$. The first set E_I includes all the characters associated with pseudofactors coming from the decomposition of the factors F_i, for $i \in I$. Those among them which have at least one non-zero coefficient for each factor make up the set $\widetilde{E}_I$, which is therefore the subset of T^* associated with the factorial term $\prod_{i \in I} F_i$.

Example 3 (continued) For brevity, we give only one example based on the interaction $P.Q$. The corresponding set of characters E_I is

$$\{0, P_1, P_2, P_1 + P_2\} \oplus \{0, Q\} = \{0, P_1, P_2, P_1 + P_2, Q, P_1 + Q, P_2 + Q, P_1 + P_2 + Q\},$$

while $\widetilde{E}_I$ is restricted to

$$\{P_1, P_2, P_1 + P_2\} \oplus \{Q\} = \{P_1 + Q, P_2 + Q, P_1 + P_2 + Q\}.$$

3.4 Elementary regular design and its key matrix

In a regular factorial design, the treatment pseudofactors are algebraically derived from the unit ones.

Definition 3.1 (regular design) *A design d with $U \cong (C_p)^r$ and $T \cong (C_p)^s$ is called* C_p-regular *if there are coefficients ϕ_{ij} and α_j in C_p such that, for $j = 1, \ldots, s$,*

$$A_j \circ d = \phi_{1j} V_1 + \cdots + \phi_{ij} V_i + \cdots + \phi_{rj} V_r + \alpha_j \qquad (1)$$

where $V_1, \ldots, V_r$ are the unit pseudofactors and $A_1, \ldots, A_s$ the treatment pseudofactors.

In a C_p-regular factorial design, the treatment t allocated to unit u satisfies $t = \Phi^\top u + t_0$, where

$$\Phi = \begin{pmatrix} \phi_{11} & \ldots & \phi_{1s} \\ \vdots & & \vdots \\ \phi_{r1} & \ldots & \phi_{rs} \end{pmatrix}$$

and $t_0 = (\alpha_1, \ldots, \alpha_s)^\top$. The definition below follows the definition of the *design key K* given by Patterson (1976) and Bailey *et al.* (1977). We have just adapted their definition so that the subscripts on the entries in Φ appear in the usual order. Cheng (2014) also writes the matrix this way but note that Kobilinsky and Monod (1991) use its transpose.

Definition 3.2 (key matrix) *Let d be a regular design as specified in Definition 3.1. The matrix Φ is called the* key matrix *of d.*

Define the mapping $\psi \colon U \to T$ by $\psi(u) = d(u) - t_0 = \Phi^\top u$. Then ψ is a group homomorphism, in the sense that if u and u' are in U then $\psi(u + u') = \psi(u) + \psi(u')$. The dual of the homomorphism ψ, denoted by φ, is the homomorphism from T^* to U^* sending a character A of T to the character $\varphi(A)$ of U defined by

$$(\varphi(A))(u) = A(\psi(u)) = A(\Phi^\top u).$$

It is clear from (1) that if $A = a_1 A_1 + \cdots + a_s A_s$ then $\varphi(A) = B = b_1 V_1 + \cdots + b_r V_r$, where

$$b_i = \sum_j \phi_{ij} a_j \qquad \text{for } i = 1, \ldots, r.$$

If we represent the characters A and B by their column vectors a and b, we have $b = \Phi a$. The jth column $(\phi_{1j}, \ldots, \phi_{rj})^\top$ of Φ is the unit character $\varphi(A_j)$ in U^* which is the image of the treatment character A_j in T^*. It will be denoted by $\tilde{A}_j$ from now on.

3.5 Confounding

The statistical properties of regular designs with key matrix Φ and corresponding homomorphism φ are summarised by the proposition given in this section. For a vector c in $\mathbb{R}^n$ indexed by the treatments, let $c^{(d)}$ denote the vector in $\mathbb{R}^N$ indexed by the units and defined by $(c^{(d)})_u = (c)_{d(u)}$. We say that the two treatment effects $c_1^\top \tau$ and $c_2^\top \tau$ are confounded with each other in design d if there is a constant γ such that $c_1^{(d)} = \gamma\, c_2^{(d)}$. In this case, it is impossible to estimate the effects $c_1^\top \tau$ and $c_2^\top \tau$ separately. We say that the treatment effects $c_1^\top \tau$ and $c_2^\top \tau$ are orthogonal to each other if $c_1^{(d)\top} c_2^{(d)} = 0$.

The basis of the regular factorial designs is given by the following proposition (see *e.g.* Kobilinsky and Monod, 1995). Here $\mathrm{Ker}(\varphi)$ denotes the kernel of φ, which is $\{A \in T^* : \varphi(A) = 0\}$.

Proposition 3.1 *Let A and B denote two characters in T^*. A regular design with key matrix Φ and corresponding homomorphism φ satisfies the following four properties:*

(i) The pseudofactorial effect $e_\tau(A)$ is confounded with the general mean $e_\tau(0)$ if and only if $A \in \mathrm{Ker}(\varphi)$;

(ii) The pseudofactorial effects $e_\tau(A)$ and $e_\tau(B)$ are confounded with each other if and only if $A - B \in \mathrm{Ker}(\varphi)$;

(iii) The sets of mutually confounded pseudofactorial effects are given by the cosets of the subgroup $\mathrm{Ker}(\varphi)$*;*

(iv) The pseudofactorial effects $e_\tau(A)$ *and* $e_\tau(B)$ *are orthogonal if* A *and* B *are in different cosets of* $\mathrm{Ker}(\varphi)$*.*

An effect $e_\tau(A)$, for $A \in T^*$, is estimable if and only if it is not confounded with any other non-zero effect. It follows from Proposition 3.1 that this occurs if all the other characters B in the same coset of $\mathrm{Ker}(\varphi)$ as A are assumed to have no effect on the response to be measured ($e_\tau(B) = 0$).

4 Conditions on the design key matrix

4.1 Ineligible characters and factorial terms

4.1.1 Ineligible characters due to model specifications

For the experimenter, the model and the effects to estimate consist of factorial terms defined on the real factors, as illustrated by the examples in Section 2. As shown in Section 3.3, each such factorial term is associated with a set $\widetilde{E}_I$ of characters in T^*. Thus, for each pair of model-estimate sets $(\underline{\mathcal{M}}, \underline{\mathcal{E}})$ of factorial terms, there is an associated pair $(\mathcal{M}, \mathcal{E})$ of character sets. The model set $\mathcal{M}$ is the union of the sets $\widetilde{E}_I$, for all factorial terms $\prod_{i \in I} F_i$ in $\underline{\mathcal{M}}$, while the estimate set $\mathcal{E}$ is the union of the sets $\widetilde{E}_I$ for all terms $\prod_{i \in I} F_i$ in $\underline{\mathcal{E}}$. If E and E' are any two subsets of T^*, we write $E - E' = \{A - B : A \in E,\ B \in E'\}$.

Definition 4.1 (ineligible characters) *Let* $(\underline{\mathcal{M}}, \underline{\mathcal{E}})$ *be model-estimate sets of factorial terms and* $(\mathcal{M}, \mathcal{E})$ *be the associated model-estimate sets of characters. Put*

$$\mathcal{I} = \{A - B\ : A \in \mathcal{E},\ B \in \mathcal{M},\ A \neq B\} = (\mathcal{E} - \mathcal{M}) \setminus \{0\}. \tag{2}$$

Then $\mathcal{I}$ *is called the set of* ineligible characters *with respect to* $(\underline{\mathcal{M}}, \underline{\mathcal{E}})$ *or, equivalently, to* $(\mathcal{M}, \mathcal{E})$*.*

Proposition 4.1 *Consider a regular design with key matrix* Φ *and corresponding homomorphism* φ*. Also consider the model consisting of the factorial terms in* $\underline{\mathcal{M}}$*. Then all factorial terms in* $\underline{\mathcal{E}}$ *are estimable if and only if* $\mathrm{Ker}(\varphi) \cap \mathcal{I} = \emptyset$*, where* $\mathcal{I}$ *is the set of ineligible characters with respect to* $(\underline{\mathcal{M}}, \underline{\mathcal{E}})$*.*

Proof: According to Proposition 3.1, the design must satisfy

$$A - B \notin \mathrm{Ker}(\varphi) \quad \text{for all } A \in \mathcal{E},\ B \in \mathcal{M} \text{ with } A \neq B, \tag{3}$$

in order to satisfy the experimenter's requirement. Condition (3) means that $\mathrm{Ker}(\varphi)$ must not contain any ineligible character. □

4.1.2 Ineligible factorial terms

In general, a set of characters of T may not be a union of the subsets $\tilde{E}_I$ associated with factorial terms $\prod_{i\in I} F_i$. However, Proposition 4.2 below shows that, for any given model-estimate pair $(\underline{\mathcal{M}}, \underline{\mathcal{E}})$, there is a set $\underline{\mathcal{I}}$ of factorial terms such that

$$\mathcal{I} = \bigcup_{K\in\underline{\mathcal{I}}} \tilde{E}_K. \qquad (4)$$

Thus it makes sense to say that $\prod_{i\in K} F_i$ is an *ineligible factorial term* if $K \in \underline{\mathcal{I}}$.

Furthermore, $\underline{\mathcal{I}}$ can be calculated explicitly. In three important special cases,

$$\underline{\mathcal{I}} = \{I \triangle J : I \in \underline{\mathcal{E}},\ J \in \underline{\mathcal{M}},\ I \neq J\}. \qquad (5)$$

Here $I \triangle J$ denotes the symmetric difference between I and J, which is $(I \setminus J) \cup (J \setminus I)$.

Proposition 4.2 *Let I and J be subsets of $\{1, \ldots, h\}$. Then*

$$\tilde{E}_I - \tilde{E}_J = \bigcup_{K\in\underline{\mathcal{I}}(I,J)} \tilde{E}_K,$$

where $\underline{\mathcal{I}}(I, J) = \{K : I \triangle J \subseteq K \subseteq (I \triangle J) \cup L\}$ and $L = \{i \in I \cap J : n_i > 2\}$, so that $\underline{\mathcal{I}}(I, J) = \{K : I \triangle J \subseteq K \subseteq I \cup J\}$ if $p \geq 3$.

Proof: If $A \in \tilde{E}_I$ and $B \in \tilde{E}_J$ then $A - B$ has zero coefficients for all factors F_i with $i \notin I \cup J$ and has at least one non-zero coefficent for factor F_i if $i \in I \triangle J$.

Now let $i \in I \cap J$ and $j \in \mathcal{P}(i)$. If $p \geq 3$ then we can choose A and B to have any non-zero coefficients a_j and a'_j of A_j: thus the coefficient of A_j in $A - B$ may be any value in C_p, including zero.

If $p = 2$ and $n_i = 2$ then $\mathcal{P}(i)$ consists of a single index j. Then $a_j = a'_j = 1$ and so the coefficient of A_j in $A - B$ is zero.

If $p = 2$ and $n_i > 2$ then $\mathcal{P}(i)$ contains at least two different indices j and k. We may choose A with $a_j = 1$ and $a_k = 0$, and B with $a'_j = a'_k = 1$. Then $A - B$ has a non-zero coefficient for A_k.

Because $\tilde{E}_I$ and $\tilde{E}_J$ are complete factorial terms, it is clear that, in each case, if $K \in \underline{\mathcal{I}}(I, J)$ then $\tilde{E}_I - \tilde{E}_J$ contains the whole of $\tilde{E}_K$. □

The model $\underline{\mathcal{M}}$ is usually *complete* in the sense that, when it contains an effect, it also contains all effects marginal to it. For instance, if it contains the interaction $F.G$, it also contains the main effects F and G and the general mean $\emptyset$.

Proposition 4.3 *If the model $\underline{\mathcal{M}}$ is complete, or if the estimate-set $\underline{\mathcal{E}}$ is complete, or if all treatment factors have two levels, then the set $\underline{\mathcal{I}}$ of ineligible factorial terms is given by equation (5).*

Proof: The third case follows directly from Proposition 4.2, because $\underline{\mathcal{I}}(I,J) = I \bigtriangleup J$ and $\emptyset$ is excluded from $\underline{\mathcal{I}}$.

Suppose that $\underline{\mathcal{M}}$ is complete, that $\prod_{i\in I} F_i$ is in $\underline{\mathcal{E}}$ and that $\prod_{i\in J} F_i$ is in $\underline{\mathcal{M}}$. Then Proposition 4.2 shows that $\tilde{E}_I - \tilde{E}_J$ is the union of the sets $\tilde{E}_K$ for various subsets K for which $I \bigtriangleup J \subseteq K \subseteq I \cup J$. For such a subset K, put $J' = J \setminus (I \cap J \cap K)$. Then $K = I \bigtriangleup J'$. Because $\underline{\mathcal{M}}$ is complete, $\underline{\mathcal{M}}$ contains every subset J' of J, and so

$$\{I \bigtriangleup J' : J' \subseteq J\} = \bigcup_{J' \subseteq J} \underline{\mathcal{I}}(I, J').$$

Therefore

$$\underline{\mathcal{I}} = \bigcup_{I\in\underline{\mathcal{E}}} \bigcup_{J\in\underline{\mathcal{M}}} \underline{\mathcal{I}}(I,J) \setminus \{\emptyset\} = \bigcup_{I\in\underline{\mathcal{E}}} \bigcup_{J\in\underline{\mathcal{M}}} \{I \bigtriangleup J\} \setminus \{\emptyset\} = \{I \bigtriangleup J : I \in \underline{\mathcal{E}},\, I \in \underline{\mathcal{M}},\, I \neq J\}.$$

The argument is similar when $\underline{\mathcal{E}}$ is complete. □

Thus the first step to determine the set $\mathcal{I}$ of ineligible characters is to determine the set $\underline{\mathcal{I}}$ of ineligible factorial terms. If the model $\underline{\mathcal{M}}$ is complete, or if all treatment factors have two levels, this is done by identifying the sets $K = I \bigtriangleup J$ for I in $\underline{\mathcal{E}}$ and J in $\underline{\mathcal{M}}$. Otherwise, the sets $\underline{\mathcal{I}}(I,J)$ of ineligible factorial terms in Proposition 4.2 must be used, for I in $\underline{\mathcal{E}}$ and J in $\underline{\mathcal{M}}$. This step can be performed before the decomposition into pseudofactors. In a second step, the ineligible characters can be deduced from equation (4).

When equation (5) holds, the elements of $\underline{\mathcal{I}}$ can be identified by representing each main effect or interaction $\prod_{i\in I} F_i$ by a vector of dimension h over C_p with i-th coordinate equal to 1 if $i \in I$, to 0 otherwise. With this representation, if x represents $\prod_{i\in I} F_i$ and z represents $\prod_{i\in J} F_j$, then the vector representing $\prod_{i\in I\bigtriangleup J} F_i$ is simply $x + z$, whose a-th coordinate is 1 if $x_a \neq z_a$ and is 0 otherwise.

Example 4 For sake of brevity, we give an example simpler than Example 3. Suppose that there are three factors A, B, C and

$$\underline{\mathcal{M}} = \{\emptyset, A, B, C, A.B, B.C\}, \quad \underline{\mathcal{E}} = \{A, B, C, A.B\}\ .$$

Table 1 gives for each model term $\prod_{i\in I} F_i$ and each estimate term $\prod_{i\in J} F_i$ the associated ineligible factorial term $\prod_{i\in I\bigtriangleup J} F_i$. Therefore $\underline{\mathcal{I}}$ includes all non-zero terms in this table, that is $\{A, B, C, A.B, A.C, B.C, A.B.C\}$.

The associated vectors x, z and $x + z$ for $x \neq z$ are

- for $\underline{\mathcal{M}}$ (x) : $\begin{pmatrix}0\\0\\0\end{pmatrix}, \begin{pmatrix}1\\0\\0\end{pmatrix}, \begin{pmatrix}0\\1\\0\end{pmatrix}, \begin{pmatrix}0\\0\\1\end{pmatrix}, \begin{pmatrix}1\\1\\0\end{pmatrix}, \begin{pmatrix}0\\1\\1\end{pmatrix}$;
- for $\underline{\mathcal{E}}$ (z) : $\begin{pmatrix}1\\0\\0\end{pmatrix}, \begin{pmatrix}0\\1\\0\end{pmatrix}, \begin{pmatrix}0\\0\\1\end{pmatrix}, \begin{pmatrix}1\\1\\0\end{pmatrix}$;

Estimate set $\underline{\mathcal{E}}$	Model set $\underline{\mathcal{M}}$ $\emptyset$	A	B	C	$A.B$	$B.C$
A	A	$\emptyset$	$A.B$	$A.C$	B	$A.B.C$
B	B	$A.B$	$\emptyset$	$B.C$	A	C
C	C	$A.C$	$B.C$	$\emptyset$	$A.B.C$	B
$A.B$	$A.B$	B	A	$A.B.C$	$\emptyset$	$A.C$

Table 1: *Construction of the ineligible set $\underline{\mathcal{I}}$ by symmetric differences (Example 4)*

- for $\underline{\mathcal{I}}$ $(x+z)$: $\begin{pmatrix}1\\0\\0\end{pmatrix}, \begin{pmatrix}0\\1\\0\end{pmatrix}, \begin{pmatrix}0\\0\\1\end{pmatrix}, \begin{pmatrix}1\\1\\0\end{pmatrix}, \begin{pmatrix}1\\0\\1\end{pmatrix}, \begin{pmatrix}0\\1\\1\end{pmatrix}, \begin{pmatrix}1\\1\\1\end{pmatrix}.$

Example 5 Suppose that there are two factors A, B and we choose $\underline{\mathcal{M}} = \{\emptyset, B, A.B\}$ and $\underline{\mathcal{E}} = \{B\}$. Because it does not contain A, the model $\underline{\mathcal{M}}$ is not complete, and because it does not contain $\emptyset$, $\underline{\mathcal{E}}$ is not complete. Proposition 4.2 implies that $\underline{\mathcal{I}} = \{A, B\}$ if factor B has two levels, whereas $\underline{\mathcal{I}} = \{A, B, A.B\}$ if factor B has three or more levels. Here are some possibilities.

- If factors A and B have two levels, then $\mathcal{M} = \{0, B, A+B\}$, $\mathcal{E} = \{B\}$ and $\mathcal{I} = \{A, B\}$. So the only ineligible factorial terms are the main effects of A and B. We could construct a design by confounding the character $A+B$.
- If factors A and B have three levels, then $\mathcal{M} = \{0, B, 2B, A+B, A+2B, 2A+B, 2A+2B\}$, $\mathcal{E} = \{B, 2B\}$ and $\mathcal{I} = \{A, 2A, B, 2B, A+B, A+2B, 2A+B, 2A+2B\}$. So the ineligible factorial terms are the main effects of A and B and the interaction $A.B$. If we confound either part of the $A.B$ interaction then B is confounded with the other part and so cannot be estimated.
- If factor A has four levels and factor B has two levels, then $\mathcal{M} = \{0, B, A_1+B, A_2+B, A_1+A_2+B\}$, $\mathcal{E} = \{B\}$ and $\mathcal{I} = \{B, A_1, A_2, A_1+A_2\}$. We could construct a design confounding any one of A_1+B, A_2+B, A_1+A_2+B.
- If factor A has two levels and factor B has four levels, then $\mathcal{M} = \{0, B_1, B_2, B_1+B_2, A+B_1, A+B_2, A+B_1+B_2\}$, $\mathcal{E} = \{B_1, B_2, B_1+B_2\}$ and $\mathcal{I} = \{A, B_1, B_2, B_1+B_2, A+B_1, A+B_2, A+B_1+B_2\}$. Again, no non-zero character is eligible for confounding.

As this example shows, if the model is incomplete, the ineligible factorial terms may depend on the numbers of levels of the factors.

4.1.3 Extension to mixed models

In mixed models, some factorial terms are assumed to be random and centred rather than fixed. An interesting special case for the design of experiments concerns block factors as in Examples 2 and 3. Provided the proper randomization is applied, the block effects can indeed be considered as random and centred.

If the model $\underline{\mathcal{M}}$ includes such random terms, the requirement in equation (3) implies that all the (other) terms in $\underline{\mathcal{E}}$ be orthogonal to them, which may turn out to be impossible. A more flexible constraint is to allow some terms in $\underline{\mathcal{E}}$ to be completely or partially confounded with the random terms. As shown with subblock effects in Example 3, this can be done by partitioning $\underline{\mathcal{E}}$ into two disjoint subsets $\underline{\mathcal{E}}_1$ and $\underline{\mathcal{E}}_2$ and by including the random terms in $\underline{\mathcal{M}}_1$ but not $\underline{\mathcal{M}}_2$. In that case the set of ineligible characters which must not belong to Ker(φ) is

$$\mathcal{I} = (\mathcal{E}_1 - \mathcal{M}_1) \cup (\mathcal{E}_2 - \mathcal{M}_2) \setminus \{0\} \,. \tag{6}$$

More complicated situations may require more than two sets of differences. Now the set $\underline{\mathcal{I}}$ of ineligible factorial terms is given by $\underline{\mathcal{I}} = \underline{\mathcal{I}}_1 \cup \underline{\mathcal{I}}_2 \cup \cdots$, where $\underline{\mathcal{I}}_j$ is derived from $\underline{\mathcal{E}}_j$ and $\underline{\mathcal{M}}_j$ by equation (5) if $\underline{\mathcal{M}}_j$ is complete or if all factors involved in $\underline{\mathcal{M}}_j$ have two levels, and otherwise is derived from $\underline{\mathcal{E}}_j$ and $\underline{\mathcal{M}}_j$ by using Proposition 4.2. Thus again the first step is to determine $\underline{\mathcal{I}}_1$, $\underline{\mathcal{I}}_2$, …, then to deduce their union $\underline{\mathcal{I}}$, and then to deduce the set $\mathcal{I}$ of ineligible characters.

Example 3 (continued) We have

$$\begin{aligned}
\underline{\mathcal{I}}_1 &= \{A, B, C, D,\ A.B, A.C, A.D,\ B.C, B.D, C.D,\\
&\quad A.B.C, A.B.D, A.C.D,\ B.C.D,\ A.B.C.D,\\
&\quad B.P, C.P, D.P,\ A.B.P, A.C.P, A.D.P,\ B.C.P, B.D.P, C.D.P,\\
&\quad B.Q, C.Q, D.Q,\ A.B.Q, A.C.Q, A.D.Q,\ B.C.Q, B.D.Q, C.D.Q,\\
&\quad B.P.Q, C.P.Q, D.P.Q,\ A.B.P.Q, A.C.P.Q, A.D.P.Q,\ B.C.P.Q, B.D.P.Q, C.D.P.Q\};\\
\underline{\mathcal{I}}_2 &= \{A, B, C, D,\ A.B, A.C, A.D,\ A.B.C, A.B.D, A.C.D,\ A.P\}.
\end{aligned}$$

The set of model-based ineligible factorial terms is given by

$$\begin{aligned}
\underline{\mathcal{I}}_{1,2} &= \underline{\mathcal{I}}_1 \cup \underline{\mathcal{I}}_2\\
&= \underline{\mathcal{I}}_1 \cup \{A, A.P\}.
\end{aligned}$$

Note that the interactions $A.Q$ and $A.P.Q$ are absent from $\underline{\mathcal{I}}$.

4.1.4 Ineligibility due to combinatorial requirements

In some situations, it is required that all the combinations of levels of some factors are in the experiment, whatever the model and estimate constraints are. Then all the terms including the corresponding pseudofactors have to be included in the ineligible set. For instance, in a row-and-column design, all combinations of levels of the row and column factors must be present. If the rows are defined by a factor R, the columns by a factor C, then $\underline{\mathcal{I}}$ must include the factorial terms R, C and $R.C$ whatever the model specifications, and $\mathcal{I}$ will include the corresponding characters.

Example 3 (continued) The experimental units consist of all levels combinations of P, Q and U. To ensure that the design is complete with respect to all three factors, the set of ineligible terms must become

$$\underline{\mathcal{I}} \;=\; \underline{\mathcal{I}}_{1,2} \cup \{P,\ Q,\ P.Q,\ U,\ P.U,\ Q.U,\ P.Q.U\}.$$

4.2 Reduced set of ineligible characters

Once the full set $\underline{\mathcal{I}}$ of ineligible factorial terms has been determined, the ineligible characters can be deduced as the union of the sets $\widetilde{E}_I$, for $I \in \underline{\mathcal{I}}$. If $\mathcal{I}$ is the set of ineligible characters, the homomorphism φ must satisfy

$$\varphi(A) \neq 0 \quad \text{for every character } A \in \mathcal{I}. \tag{7}$$

However if A and B in $\mathcal{I}$ are such that A is an integer multiple of B, that is $A = kB$, then the inequality $\varphi(A) \neq 0$ clearly implies $\varphi(B) \neq 0$. In the search for φ, the inequality (7) has therefore to be checked only for an adequately chosen subset $\mathcal{R}$ of $\mathcal{I}$ called a *reduced ineligible set*.

Definition 4.2 (reduced set) *A reduced ineligible set $\mathcal{R} \subseteq \mathcal{I}$ is any subset of ineligible characters such that the condition (7) on φ is equivalent to the apparently weaker condition*

$$\varphi(A) \neq 0 \quad \textit{for every } A \in \mathcal{R}. \tag{8}$$

We now indicate how such a reduced ineligible set can be selected. Let $\langle A \rangle$ be the cyclic subgroup generated by A. The relation

$$\langle A \rangle = \langle B \rangle \iff \exists \delta, \delta' \in \mathbb{N} \text{ such that } A = \delta B \text{ and } B = \delta' A \tag{9}$$

defines an equivalence relation on $\mathcal{I}$. Clearly it is enough to check inequality (7) for only one representative in each equivalence class.

When T^* and U^* are elementary abelian p-groups, all non-zero characters have order p, the non-zero equivalence classes contain $p-1$ characters, and the representatives can be chosen, for example, as the characters whose first non-zero coordinate is 1. In Section 5, the representatives will be chosen as the characters whose last non-zero coordinate is -1 unless there is only one non-zero coordinate, in which case we will take it to be 1.

Example 3 (continued) We have $\mathcal{I} = \bigcup_{I \in \underline{\mathcal{I}}} \widetilde{E}_I$. The result is too long to give *in extenso*, but note that the set $\underline{\mathcal{I}}$ and examples of the sets $\widetilde{E}_I$ have been presented earlier. In this example, $p = 2$ so that each equivalence class has a single element. Thus there is no choice to select a representative and so the set of ineligible characters cannot be reduced.

Example 6 If factors A and B both have three levels and $\underline{\mathcal{I}}$ contains their two-factor interaction then a possible reduced set $\mathcal{R}$ contains the characters $A - B$ $(= A + 2B)$ and $2A - B$ $(= 2A + 2B)$ for this term but neither $A + B$ nor $2A + B$.

4.3 Hierarchy constraints

In practice, besides constraints of ineligibility, it may be necessary to satisfy hierarchy constraints between factors, such as those shown in Examples 2 and 3. It is assumed that all constraints are of the form $F_{i_1} \wedge \cdots \wedge F_{i_k} \preccurlyeq F_{i_0}$. This assumption is satisfied in most practical cases. We recall that $\mathcal{P}(i)$ denotes the pseudofactors A_j that decompose the genuine factor F_i, or more precisely the set of indices of these pseudofactors.

Proposition 4.4 *Let F_{i_0}, F_{i_1}, ..., F_{i_k} be $k+1$ treatment factors and let $J = \mathcal{P}(i_1) \cup \cdots \cup \mathcal{P}(i_k)$ denote the set of pseudofactors that decompose F_{i_1}, ..., F_{i_k}. For a regular design with design key matrix Φ, the following three conditions are equivalent:*

(i) $F_{i_1} \wedge \cdots \wedge F_{i_k} \preccurlyeq F_{i_0}$;

(ii) $\bigwedge_{j \in J} A_j \preccurlyeq A_{j_0}$, *for all* $j_0 \in \mathcal{P}(i_0)$;

(iii) *if* $j_0 \in \mathcal{P}(i_0)$ *then each column* $\tilde{A}_{j_0}$ *of* Φ *is a linear combination of the columns* $\tilde{A}_j$, *for* $j \in J$.

Proof: The equivalence between *(i)* and *(ii)* results from simple partition properties. They state that the level of any given pseudofactor A_{j_0} associated with F_{i_0} must be a function of the levels of the pseudofactors A_j associated with F_{i_1}, ..., F_{i_k}. Equivalently, the column j_0 of Φ must be a linear combination of the columns $j \in J$. □

According to Proposition 4.4, each hierarchy constraint between treatment factors generates one or more hierarchy constraints $\left(A_{j_1} \wedge \cdots \wedge A_{j_l} \preccurlyeq A_{j_0}\right)$ between pseudofactors, each of which must be satisfied during the design search. In the sequel, it will be assumed that the pseudofactors are ordered so that for any such constraint, j_0 is greater than j_1, ..., j_l. The set of all coarser pseudofactors A_{j_0} involved in such constraints will be denoted by $\mathcal{H}_+$. It results from the decomposition of the coarser factors in the original constraints. The set of all pseudofactors in the finer part of the constraint $\left(A_{j_1} \wedge \cdots \wedge A_{j_l} \preccurlyeq A_{j_0}\right)$ will be denoted by $\mathcal{H}_{\prec z}$, where, depending on the context, z may refer to the coarser pseudofactor A_{j_0} or to its index j_0.

Example 3 (continued) Recall that there is a unique hierarchy constraint $P \wedge Q \preccurlyeq A$. It follows that $\mathcal{H}_+ = \{A\}$ and $\mathcal{H}_{\prec A} = \{P, Q\}$.

5 Search for key matrices of elementary designs

5.1 Main steps

According to the results in Section 4, the search for a key matrix solution can be decomposed into the following steps:

1. determine the set $\underline{\mathcal{I}}$ of ineligible factorial terms;

2. deduce from $\underline{\mathcal{I}}$ a reduced set $\mathcal{R}$ of representative ineligible treatment characters;

3. search for one or more key matrices Φ satisfying condition *(iii)* of Proposition 4.4 (hierarchies) and equation (8) of Definition 4.2 (ineligibility).

The first step was described in Section 4.1. The second step was explained in Section 4.2. The remainder of this section is dedicated to the third step.

5.2 Elementary backtrack search

Searching for the key matrix Φ is equivalent to searching for its columns $\tilde{A}_1, \ldots, \tilde{A}_s$ among the set U^* of unit characters. For the homomorphism φ to satisfy (8), these characters must satisfy:

$$\text{for every } a_1A_1 + \cdots + a_sA_s \in \mathcal{R}, \quad a_1\tilde{A}_1 + \cdots + a_s\tilde{A}_s \neq 0. \tag{10}$$

In addition, because of the hierarchy constraints, some columns must be linear combinations of other ones of smaller index, as shown in Proposition 4.4. More precisely, for the indices j in the subset $\mathcal{H}_+$, the columns $\tilde{A}_j$ must satisfy

$$\tilde{A}_j = \sum_{k \in \mathcal{H}_{\prec j}} a_k \tilde{A}_k \tag{11}$$

for some values a_k. Note that all indices k in $\mathcal{H}_{\prec j}$ are strictly smaller than j.

The columns $\tilde{A}_j$ can be found successively by the backtrack search presented in Algorithm 1 below. Once $\tilde{A}_1, \ldots, \tilde{A}_{j-1}$ have been selected among the unit characters, the admissible choices for $\tilde{A}_j$ are determined. If there is no (or no more) admissible choice, the search goes backward to try the next admissible choice for $\tilde{A}_{j-1}$. Otherwise, the first possible choice for $\tilde{A}_j$ is selected and, if $j < s$, the search goes forward to look for $\tilde{A}_{j+1}$. If $j = s$, an admissible $\tilde{A}_s$ has been found and so a solution for the key matrix Φ has also been found. The process may either end by such a success or continue until there is no more admissible $\tilde{A}_1$ to select.

Algorithm 1 involves non-trivial calculations only when determining the set $\texttt{aA}_j$ in Step 1. A unit character is considered to be admissible for column j if it satisfies the inequalities (10) involving it and the previous columns $\tilde{A}_1, \ldots, \tilde{A}_{j-1}$. Let $\mathcal{R}_j$ be the subset of characters $A = a_1A_1 + \cdots + a_jA_j$ in $\mathcal{R}$ having $a_j = -1$ as the last non-zero coordinate. The inequalities in (10) to consider when searching for $\tilde{A}_j$ are all those involving a character A in $\mathcal{R}_j$. They can be written:

$$\text{for every } a_1A_1 + \cdots + a_{j-1}A_{j-1} - A_j \text{ in } \mathcal{R}_j, \quad \tilde{A}_j \neq a_1\tilde{A}_1 + \cdots + a_{j-1}\tilde{A}_{j-1}, \tag{12}$$

which includes $\tilde{A}_j \neq 0$ if $A_j \in \mathcal{R}$. The admissible characters satisfying (12) are looked for among U^* unless j belongs to $\mathcal{H}_+$. In that case, the hierarchy constraints (11) allow the search to be restricted to the subgroup of U^* generated by the columns in $\mathcal{H}_{\prec j}$.

Algorithm 1 Backtrack search

```
jprev ← 0 and j ← 1
while j > 0 do
  {Step 1: update the admissible set}
  if jprev < j then {forward case}
    determine the set aA_j of currently admissible unit characters for column j of Φ
  else {backward case}
    delete the current character in column j from aA_j
  end if
  {Step 2: next move}
  if aA_j is empty then
    j ← j − 1 {move backward}
  else
    set column j to the first element in aA_j
    if j < s then
      j ← j + 1 {move forward}
    else {j = s so that all columns have been found}
      save the current key matrix in the solution set
      either stop or continue to find more solutions
    end if
  end if
  jprev ← j
end while
```

5.3 Accelerating the search

Optimising the backtrack algorithm is a complex task which is not the subject of this paper. In this subsection, however, we describe a few tricks implemented in *planor* (Kobilinsky, 2005) to make the backtrack search run faster.

5.3.1 Fixing some pseudofactors without loss of generality

In many circumstances, it may be possible to identify the first f unit pseudofactors with the first f treatment pseudofactors. If $f = r$ this means that the first f columns of Φ are set to the identity matrix. Then the backtrack search starts at column $f + 1$ and failure possibly occurs when there is no more admissible $\tilde{A}_{f+1}$ to select. This can make the search faster.

Example 3 (continued) The units may be identified with the combinations of the block factors P, Q and U since any design solution must contain all 32 combinations of levels of these factors. Thus the treatment pseudofactors P_1, P_2, Q, U_1 and U_2 can be identified with the unit pseudofactors V_1 to V_5. In that case, we have $f = r = 5$ and

$$\Phi = \begin{array}{c} \\ V_1 \\ V_2 \\ V_3 \\ V_4 \\ V_5 \end{array} \begin{array}{c} \begin{array}{ccccccccc} \tilde{P}_1 & \tilde{P}_2 & \tilde{Q} & \tilde{U}_1 & \tilde{U}_2 & \tilde{A} & \tilde{B} & \tilde{C} & \tilde{D} \end{array} \\ \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & \phi_{1,6} & \phi_{1,7} & \phi_{1,8} & \phi_{1,9} \\ 0 & 1 & 0 & 0 & 0 & \phi_{2,6} & \phi_{2,7} & \phi_{2,8} & \phi_{2,9} \\ 0 & 0 & 1 & 0 & 0 & \phi_{3,6} & \phi_{3,7} & \phi_{3,8} & \phi_{3,9} \\ 0 & 0 & 0 & 1 & 0 & \phi_{4,6} & \phi_{4,7} & \phi_{4,8} & \phi_{4,9} \\ 0 & 0 & 0 & 0 & 1 & \phi_{5,6} & \phi_{5,7} & \phi_{5,8} & \phi_{5,9} \end{pmatrix} \end{array} .$$

The first five columns of Φ are set to the identity matrix. There are four more columns $\tilde{A}$, $\tilde{B}$, $\tilde{C}$, $\tilde{D}$ to search for.

5.3.2 Initially admissible elements

An element V of U^* is called *initially admissible* for $\tilde{A}_j$ if it is admissible with respect to the predetermined columns $\tilde{A}_1, \ldots, \tilde{A}_f$, that is if it satisfies the inequalities (10) and the hierarchy constraints (11) involving it and the predetermined columns. The set of initially admissible elements for a column $\tilde{A}_j$ is denoted by $\mathtt{iaA}_j$. It can be determined once and for all when this column is first reached.

During the search, the admissible elements for column $\tilde{A}_j$ are determined as a subset of the initially admissible ones, conditional on the current previous columns of Φ. Then they are successively tried by going forwards and searching for the next columns. A counter $\mathtt{niaA}_j$ gives the index of the last choice in $\mathtt{iaA}_j$. This counter is increased each time the search comes back to $\tilde{A}_j$. Whenever column $\tilde{A}_j$ is reached in the forwards direction, the status of the initially admissible elements has to be checked again (see Section 5.3.3) and the counter is reset to the first admissible element.

To avoid trying the possible choices for column $\tilde{A}_j$ always in the same order, the set of initially admissible elements for column $\tilde{A}_j$ can be randomly permuted. The solution of the process, if any, then depends on the realised randomisation. This gives a way to get several very different solutions, which could take a very long time in a single backtrack search of the whole set of solutions.

Example 3 (continued) Consider the set $\mathtt{iaA}_6$ of initially admissible elements for column $\tilde{A}$. Because of the hierarchy constraints $P \wedge Q \preccurlyeq A$, it may include only linear combinations of $\tilde{P}_1$, $\tilde{P}_2$, $\tilde{Q}$ so that $\phi_{4,6} = \phi_{5,6} = 0$. Because of the inequalities (10) involving the first five columns, the coefficient $\phi_{3,6}$ must be different from 0, otherwise the main effect A would be confounded with block effects. So we have

$$\mathtt{iaA}_6 = \left\{ \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 1 \\ 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \\ 1 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 1 \\ 1 \\ 1 \\ 0 \\ 0 \end{pmatrix} \right\}$$

For column $\tilde{B}$, there is no hierarchy constraint to take into account. For the inequalities to be respected, it is necessary and sufficient that at least one coefficient $\phi_{4,7}$ or $\phi_{5,7}$ be different from zero. So $\texttt{iaA}_7$ contains the 3×2^3 vectors satifying this condition. By symmetry, $\texttt{iaA}_8$ and $\texttt{iaA}_9$ contain the same vectors. Note that such symmetries between factors can be used to reduce the backtrack search, but this possibility is currently not implemented in *planor*.

5.3.3 Reducing the number of admissibility evaluations

Assume that column $\tilde{A}_j$ has been reached and the corresponding set of admissible columns determined. If the search goes back to some index smaller than j and then reaches column $\tilde{A}_j$ again, some work can be spared in the new determination of admissible elements.

For simplicity, we first consider the case with no hierarchy constraint. Thus, we focus on a column j such that $j \notin \mathcal{H}_+$. Consider the element A in (12) and assume that its last non-zero coordinate of index strictly less than j is a_k, that is

$$A = a_1 A_1 + \cdots + a_k A_k - A_j \quad \text{with } a_k \neq 0. \tag{13}$$

Any choice $\tilde{A}_j$ rendered inadmissible by condition (12), that is such that

$$a_1 \tilde{A}_1 + \cdots + a_k \tilde{A}_k = \tilde{A}_j, \tag{14}$$

remains inadmissible so long as column k is not reached backwards. Consequently, no calculus is needed to re-evaluate whether this $\tilde{A}_j$ is admissible or not.

To benefit from these properties, the following measures are taken for each column index j with $j > f + 1$.

- The elements of $\mathcal{R}_j$ are classified in subsets $\mathcal{R}_{jk}$ according to the value of k:

$$\mathcal{R}_{jk} = \{A \in \mathcal{R} : A = a_1 A_1 + \cdots + a_k A_k - A_j \quad \text{with } j > k \text{ and } a_k \neq 0\}. \tag{15}$$

- An indicator $\texttt{ktr}_j$ is set to keep track of the smallest column revisited since the previous visit forwards to column j. It is set to 0 initially and to $f + 1$ after the first visit to column j. Its value later varies between $f + 1$ and $j - 1$.
- Indicators $\texttt{siaA}_{j,V}$ are set to store information on the initially admissible elements V in $\texttt{iaA}_j$. After each visit forwards to column j, the status $\texttt{siaA}_{j,V}$ of V is set to s if V remains admissible. If not, it is set to the index of the first column k, with $f < k < j$, which makes V currently inadmissible.

Algorithm 2 shows how this scheme can be implemented in Step 1 of Algorithm 1. In addition, each time Step 2 of Algorithm 1 results in a backward move, the indicators $\texttt{ktr}_{k'}$, for $k' \geq j$, must be set to $j - 1$.

Algorithm 2 Acceleration of the search

{takes place to determine $\mathtt{aA}_j$ in Algorithm 1, for $\mathtt{j} > f+1$}
if $\mathtt{ktr}_j = 0$ **then** {*First visit to column* j}
  determine the set $\mathtt{iaA}_j$ of initially admissible elements for column j
  for V in $\mathtt{iaA}_j$ **do**
    $\mathtt{siaA}_{j,V} \longleftarrow s$ {so each V is first presumed to be admissible}
  end for
  $\mathtt{ktr}_j \longleftarrow f+1$ {since admissibility has been checked for the first f columns}
end if
{*On any forward visit to column* j}
for $\mathtt{k}$ from $\mathtt{ktr}_j$ to $\mathtt{j}-1$ **do**
  update $\mathcal{R}_{jk}$
  for V in $\mathtt{iaA}_j$ such that $\mathtt{k} \leq \mathtt{siaA}_{j,V}$ **do**
    if V satisfies equation (14) for a character A in $\mathcal{R}_{jk}$ **then**
      $\mathtt{siaA}_{j,V} \longleftarrow \mathtt{k}$
    else
      $\mathtt{siaA}_{j,V} \longleftarrow s$
    end if
  end for
end for
define $\mathtt{aA}_j$ as the subset of elements V in $\mathtt{iaA}_j$ such that $\mathtt{siaA}_{j,V} = s$

A simple modification in the definition of initially admissible elements is sufficient for Algorithm 2 to account for hierarchies. For $j \in \mathcal{H}_+$, let $h_{\max}(j) = \max(\mathcal{H}_{\prec j})$ and let an element V of U^* now be called *initially admissible* for $\tilde{A}_j$ if it is admissible with respect to the predetermined columns $\tilde{A}_1, \ldots, \tilde{A}_{h_{\max}(j)}$. The set of linear combinations $\tilde{A}_j$ of the form (11) remains unchanged so long as column $h_{\max}(j)$ remains unchanged, that is, so long as the process does not reach it backwards. It follows that, if $f < h_{\max}(j)$, the set $\mathtt{iaA}_j$ of initially admissible elements for column j must now be determined either when this column is first reached or when $\mathtt{ktr}_j \leq h_{\max}(j)$. The rest of Algorithm 2 can stay the same.

5.3.4 End of the search

It is sometimes necessary to go beyond a success to find other solutions, for instance if the whole set of solutions is searched for, or if the backtrack column search is part of a backtrack process among Sylow components as will be described in Section 7.

When the number of factors involved increases, the time taken by the search may become very long, especially if there is no solution or only a small number of solutions. So it can be necessary to stop a search which takes too much time. In that case, which must clearly be distinguished from a true failure, it is useful to know the index of the last column reached as this indicates the kind of experimental design obtainable in a reasonable time.

Example 3 (continued) For completeness, we give the first solution for Φ found by the *planor* algorithm:

$$\Phi = \begin{array}{c} V_1 \\ V_2 \\ V_3 \\ V_4 \\ V_5 \end{array} \begin{array}{c} \begin{array}{ccccccccc} \tilde{P}_1 & \tilde{P}_2 & \tilde{Q} & \tilde{U}_1 & \tilde{U}_2 & \tilde{A} & \tilde{B} & \tilde{C} & \tilde{D} \end{array} \\ \left(\begin{array}{ccccccccc} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 1 \end{array} \right) \end{array} .$$

In its current implementation, *planor* finds 9216 solutions. Note that these include solutions obtained from others by permutation of B, C, D, or P_1 and P_2, or U_1 and U_2.

6 Generalised regular factorial designs

In this section, we extend the previous methods to deal with designs where more than one prime is involved. The underlying theory is given by Bailey (1977, 1985), Kobilinsky (1985), Kobilinsky and Monod (1995) and Pistone and Rogantin (2008).

6.1 Pseudofactors

The experimental units are now identified with the elements of a product group

$$U = (C_{p_1})^{r_1} \times \cdots \times (C_{p_l})^{r_l}$$

and the treatments with the elements of a product group

$$T = (C_{p_1})^{s_1} \times \cdots \times (C_{p_l})^{s_l},$$

where $p_1, \ldots, p_l$ denote distinct prime numbers. Note that the theory extends to prime powers but, for simplicity, we avoid this level of generality. The number N of units and the number n of treatments factorise into $N = N_1 \times \cdots \times N_l$ and $n = n_1 \times \cdots \times n_l$, with

$$N_k = p_k^{r_k}, \quad n_k = p_k^{s_k}.$$

As in Section 3, the treatment pseudofactors associated with this decomposition of T are a finer decomposition of the genuine factors F_i.

Let $r = \sum_k r_k$ and $s = \sum_k s_k$. In what follows, we denote the r unit pseudofactors by V_i, for $i = 1, \ldots, r$. Similarly we denote the s treatment pseudofactors by A_j, for $j = 1, \ldots, s$. We denote by $\pi(V_i)$ and $\pi(A_j)$ the numbers of levels of pseudofactors V_i and A_j. Occasionally, to stress the structure introduced by the different primes, we shall denote the unit pseudofactors at p_k levels by $V_{[k,i]}$ and the treatment pseudofactors at p_k levels by $A_{[k,j]}$, for $k = 1, \ldots, l$, for $i = 1, \ldots, r_k$ and for $j = 1, \ldots, s_k$. In the examples, though, we shall use p_k rather than k as the first index between square brackets, because we found that it improves clarity. Unless specified otherwise, the pseudofactors are ordered in the natural lexicographic order induced by their double index, which puts together all the pseudofactors associated with the same prime.

To define the pseudofactors properly, all levels are embedded into the same cyclic group C_M where $M = \prod_{k=1}^{l} p_k$. Unit and treatment pseudofactors are considered as mappings into that cyclic group C_M. That is, if $u = (u_1, \dots, u_r)^\top$ is a unit in U and $t = (t_1, \dots, t_s)^\top$ a treatment in T, then

$$V_i(u) = \frac{M}{\pi(V_i)} u_i, \qquad A_j(t) = \frac{M}{\pi(A_j)} t_j \ . \tag{16}$$

Example 1 (continued) The two primes involved in this example are 2 and 3, so that all treatment factors are decomposed into pseudofactors at two or three levels. We have $M = 6$, $s_2 = 5$ and $s_3 = 2$, and the pseudofactors are $A_{[2,1]}$, $A_{[2,2]}$, $A_{[2,3]}$, $A_{[2,4]}$, $A_{[2,5]}$, $A_{[3,1]}$, $A_{[3,2]}$, where the first index denotes the prime and the second index runs from 1 to s_2 or s_3. The association between factors and pseudofactors is given by

$$F_1 = A_{[2,1]} \wedge A_{[3,1]};\ F_2 = A_{[2,2]} \wedge A_{[2,3]};\ F_3 = A_{[3,2]};\ F_4 = A_{[2,4]} \wedge A_{[2,5]}.$$

In an equivalent notation, we keep the lexicographic order on the pseudofactors but use a single index to identify them, and we use the $\mathcal{P}(.)$ notation. The association reads

$$\mathcal{P}(F_1) = \{A_1, A_6\};\ \mathcal{P}(F_2) = \{A_2, A_3\};\ \mathcal{P}(F_3) = \{A_7\};\ \mathcal{P}(F_4) = \{A_4, A_5\}.$$

Consider, for example, the treatment identified with $t = (1, 0, 1, 1, 0, 2, 1)^\top \in (C_2)^5 \times (C_3)^2$. Following equation (16), we have $A_{[2,1]}(t) = 3$, $A_{[2,2]}(t) = 0$, $A_{[2,3]}(t) = 3$, $A_{[2,4]}(t) = 3$, $A_{[2,5]}(t) = 0$, $A_{[3,1]}(t) = 4$, $A_{[3,2]}(t) = 2$.

An option involving prime powers would be to decompose the factors as little as possible. Then, the pseudofactors would be $A'_{[2,1]}$, $A'_{[2,2]}$, $A'_{[2,3]}$, $A'_{[3,1]}$, $A'_{[3,2]}$, at respectively 2, 4, 4, 3, 3 levels, with $M = 12$ and

$$F_1 = A'_{[2,1]} \wedge A'_{[3,1]};\ F_2 = A'_{[2,2]};\ F_3 = A'_{[3,2]};\ F_4 = A'_{[2,3]}.$$

As mentioned before, we shall not consider this option any further in this paper.

Example 2 (continued) The two primes involved are 2 and 3 once again. Using the double index notation, we have:

$$C = A_{[2,1]};\ R = A_{[3,1]};\ D = A_{[2,2]};\ E = A_{[2,3]};\ A = A_{[3,2]}.$$

However, we will rather use C, D, E, R, A to denote the pseudofactors, which are confounded with factors in this example.

6.2 Characters

The *characters* from T into C_M are all the linear combinations $A = a_1A_1 + \cdots + a_sA_s$ of the treatment pseudofactors, with $a_j \in C_{\pi(A_j)}$. They belong to the group T^* which is the dual of T, so that $T^* \cong (C_{p_1})^{s_1} \times \cdots \times (C_{p_l})^{s_l}$. The characters and dual of U are defined and represented in the same way.

As in Section 3, each character A of T^* is associated with a pseudofactorial effect, denoted by $e_\tau(A)$, which belongs to a unique pseudofactorial term in the ANOVA decomposition of the treatment effects. This term is identified by the non-zero coefficients of the character A. We use the same definitions and interpretations as before for the character subsets E_i, $\widetilde{E}_i$, E_I, $\widetilde{E}_I$.

6.3 Generalised regular factorial designs and key matrices

The definition 3.1 of a regular factorial design can be generalised to the more general setting of the present section (Kobilinsky and Monod, 1995; Pistone and Rogantin, 2008). The design d should satisfy an appropriate generalisation of equation (1). If $u \in U$ then $\pi(A_j)A_j(d(u)) = 0 \pmod M$, by (16), for $j = 1, \ldots, s$. When $u = 0$ then $A_j(d(u)) = \alpha_j$, and so M must divide $\pi(A_j)\alpha_j$. Now consider the unit u defined by $u_i = 1$ and $u_k = 0$ if $k \neq i$. Then $A_j(d(u)) = \phi_{ij}M/\pi(V_i) + \alpha_j$, from (16). Hence $\pi(A_j)\phi_{ij}M/\pi(V_i) = 0 \pmod M$ and so $\pi(V_i)$ divides $\pi(A_j)\phi_{ij}$. If $\pi(V_i) \neq \pi(A_j)$ then $\pi(V_i)$ divides ϕ_{ij} and so $\phi_{ij}M/\pi(V_i) = 0 \pmod M$.

Definition 6.1 (regular design) *A factorial design d with U and T as respective sets of units and treatments is called* regular *if there are coefficients ϕ_{ij} and α_j in C_M such that, for $j = 1, \ldots, s$,*

$$A_j \circ d = \phi_{1j}V_1 + \cdots + \phi_{ij}V_i + \cdots + \phi_{rj}V_r + \alpha_j\,, \tag{17}$$

where $V_1, \ldots, V_r$ are the unit pseudofactors, $A_1, \ldots, A_s$ are the treatment pseudofactors, and the following two conditions are satisfied:

$$M \text{ divides } \pi(A_j)\alpha_j \text{ for all } j = 1, \ldots, s\,, \tag{18}$$

$$\pi(V_i) \text{ divides } \pi(A_j)\phi_{ij} \text{ for all } i = 1, \ldots, r \text{ and } j = 1, \cdots, s\,. \tag{19}$$

Fix j, and put $p = \pi(A_j)$. If $t = d(u)$ and (17)–(19) hold then

$$\begin{aligned} t_j &= \frac{p}{M}A_j(t) = \sum_{i=1}^{r} \frac{p}{M}\phi_{ij}\frac{M}{\pi(V_i)} + \frac{p}{M}\alpha_j \pmod p \\ &= \sum_i{}' \phi_{ij} + \beta_j \pmod p, \end{aligned}$$

where $\beta_j = p\alpha_j/M \pmod p$ and the summation in $\sum'$ is restricted to those i for which $\pi(V_i) = p$, and ϕ_{ij} is interpreted modulo p if $\pi(V_i) = p$.

Proposition 6.1 *A factorial design d is regular if and only if the treatment* $t = (t_1, \ldots, t_s)^\top$ *allocated to unit* $u = (u_1, \ldots, u_r)^\top$ *satisfies*

$$t = \Phi^\top u + t_0 \tag{20}$$

where the calculation of t_j *is performed modulo* $\pi(A_j)$*,*

$$\Phi = \begin{pmatrix} \phi_{11} & \cdots & \phi_{1s} \\ \vdots & \ddots & \vdots \\ \phi_{r1} & \cdots & \phi_{rs} \end{pmatrix},$$

$t_0 = (\beta_1, \ldots, \beta_s)^\top$*,* $\phi_{ij} = 0$ *if* $\pi(V_i) \neq \pi(A_j)$*, and, for* $j = 1, \ldots, s$*,* $\beta_j \in C_{\pi(A_j)}$ *and* $\phi_{ij} \in C_{\pi(A_j)}$*. In particular,* Φ *is block diagonal:*

$$\Phi = \operatorname{diag}(\breve{\Phi}_1, \ldots, \breve{\Phi}_l), \tag{21}$$

where the block $\breve{\Phi}_k$ *corresponds to the prime* p_k*.*

Definition 6.2 (key matrix) *The matrix* Φ *is called the* key matrix *of d.*

Concerning the characters, we have the same relationships as in Section 3.4. The mapping $\psi\colon U \to T$ defined by $u \mapsto t = \Phi^\top u$ is a group homomorphism from U into T. If the dual of the homomorphism ψ is denoted by φ and if $\varphi(A) = B$ (with $A \in T^\star$ and $B \in U^\star$), then we have $b = \Phi a$, where a and b are the vectors of coefficients of A and B.

6.4 Decomposition into Sylow subgroups

For $k = 1, \ldots, l$, the elements of U of order p_k or 1 form a subgroup $\breve{U}_k$ isomorphic to $(C_{p_k})^{r_k}$. These subgroups are called the Sylow subgroups of U. By the fundamental theorem of abelian groups, U is the direct sum $\breve{U}_1 \oplus \cdots \oplus \breve{U}_l$. If $r_k = 0$ then $\breve{U}_k = \{0\}$. Similarly, T has Sylow subgroups $\breve{T}_k$ isomorphic to $(C_{p_k})^{s_k}$ for $k = 1, \ldots, l$, and $T = \breve{T}_1 \oplus \cdots \oplus \breve{T}_l$.

Likewise, the duals are direct sums of their Sylow subgroups, which are the duals of those of U and T: that is, $U^* = \breve{U}_1^* \oplus \cdots \oplus \breve{U}_l^*$ and $T = \breve{T}_1^* \oplus \cdots \oplus \breve{T}_l^*$. For instance, the character A in T^* associated with the element $(\breve{A}_1, \ldots, \breve{A}_l)$ of $\breve{T}_1 \oplus \cdots \oplus \breve{T}_l$ is the mapping $(\breve{t}_1, \ldots, \breve{t}_l) \mapsto \breve{A}_1(\breve{t}_1) + \cdots + \breve{A}_l(\breve{t}_l)$, provided all the characters take their values in the common cyclic group C_M. We can write $A = (\breve{A}_1, \ldots, \breve{A}_l)$ or $A = \breve{A}_1 + \cdots + \breve{A}_l$.

The decomposition into Sylow subgroups corresponds to the block diagonal decomposition of Φ in equation (21), because $\breve{\Phi}_k$ is the restriction of Φ to $\breve{U}_k$ and $\breve{T}_k$.

Definition 6.3 (primary components) *The character* $\breve{A}_k$ *is called the* p_k-primary component *of the character A.*

Definition 6.4 (Sylow components) *The diagonal blocks* $\breve{\Phi}_1, \ldots, \breve{\Phi}_l$ *of the matrix* Φ *associated with the distinct primes* $p_1, \ldots, p_l$*, are called the* Sylow components *of* Φ.

For the homomorphism φ, we have $\varphi(A) = \varphi(\breve{A}_1) + \cdots + \varphi(\breve{A}_l)$, and Proposition 6.1 implies that

$$\varphi(A) = \breve{\varphi}_1(\breve{A}_1) + \cdots + \breve{\varphi}_l(\breve{A}_l), \tag{22}$$

where each $\breve{\varphi}_k$ is the homomorphism from $\breve{T}_k^*$ to $\breve{U}_k^*$ associated with the matrix $\breve{\Phi}_k$. The search for a matrix Φ meeting the requirements can thus be decomposed into the search for its Sylow components. Note that, if there is no treatment pseudofactor with p_k levels ($r_k \neq 0$ and $s_k = 0$), the Sylow component $\breve{\Phi}_k$ does not appear explicitly in Φ. It also does not appear if no unit pseudofactor has p_k levels ($r_k = 0$ and $s_k \neq 0$). In the latter case, the regular designs associated with Φ give a constant value to treatment factors having p_k levels, and this is usually prohibited unless the design is part of a larger one.

Section 7.5.1 shows that the Sylow components can in many cases be searched for independently. Section 7.5.3 provides a backtrack method of search for them in the other cases.

7 Search for key matrices of generalised regular designs

7.1 Main steps

The search for a key matrix follows the same main steps as those in Section 5.1. The first step is to determine the set $\underline{\mathcal{I}}$ of ineligible factorial terms. Let I and J be different subsets of $\{1, \ldots, h\}$. If $i \in I \cap J$ and n_i is not prime then $\mathcal{P}(i)$ contains at least two indices, and so $\tilde{E}_I - \tilde{E}_J$ contains some characters with at least one non-zero coefficient a_j for some j in $\mathcal{P}(i)$, and also some characters for which $a_j = 0$ for all j in $\mathcal{P}(i)$. As in Proposition 4.2,

$$\tilde{E}_I - \tilde{E}_J = \bigcup_{K \in \underline{\mathcal{I}}(I,J)} \tilde{E}_K,$$

where $\underline{\mathcal{I}}(I, J) = \{K : I \triangle J \subseteq K \subseteq (I \triangle J) \cup L\}$ and $L = \{i \in I \cap J : n_i > 2\}$. Hence Proposition 4.3 remains true in this more general setting, and so $\underline{\mathcal{I}}$ can be determined as in Section 4.1.

Concerning the second step, a *reduced ineligible set* of characters $\mathcal{R}$ can be deduced from $\underline{\mathcal{I}}$ by the following steps.

1. Deduce from $\underline{\mathcal{I}}$ a set $\underline{\mathcal{I}}_P$ of ineligible pseudofactorial terms when decomposing the factors into pseudofactors. This set can be reduced as explained in Section 7.3.

2. Deduce from $\underline{\mathcal{I}}_P$ the equivalence classes to be considered for $\mathcal{R}$.

3. Select one representative character in each class and eliminate representatives having a proper multiple in $\mathcal{I}$.

In Examples 1 and 2, the models are complete and so the first main step is based on Proposition 4.3.

Example 1 (continued) Proceeding as in Example 4 (Section 4.1.2), we find the ineligible set

$$\underline{\mathcal{I}} = \{F_1,\ F_2,\ F_3,\ F_4,\ F_1.F_2,\ F_1.F_3,\ F_1.F_4,\ F_2.F_3,\ F_2.F_4,\ F_3.F_4,\ F_1.F_2.F_3,\ F_1.F_2.F_4\}.$$

Example 2 (continued) The set $\underline{\mathcal{M}}$ is complete, so Proposition 4.3 shows that the terms in the ineligible set specified by $\underline{\mathcal{M}}$ and $\underline{\mathcal{E}}$ are those given in Table 2. Furthermore, the design must contain all the level combinations of factors C (columns) and R (rows), so the factorial terms C, R and $C.R$ are also ineligible (see Section 4.1.4). Therefore

$$\begin{aligned} \underline{\mathcal{I}} \; = \; & \{C,\ D,\ E,\ R,\ A,\ C.R,\ D.E,\ D.A,\ E.A, \\ & D.E.A,\ C.D.A,\ C.E.A,\ D.R.A,\ E.R.A,\ C.D.R.A,\ C.E.R.A\}. \end{aligned} \tag{23}$$

	Model $\underline{\mathcal{M}}$									
Set $\underline{\mathcal{E}}$	0	C	R	$C.R$	A	D	E	$D.A$	$E.A$	$D.E$
$D.A$	$D.A$	$C.D.A$	$D.R.A$	$C.D.R.A$	D	A	$D.E.A$	~~0~~	$D.E$	$E.A$
$E.A$	~~$E.A$~~	$C.E.A$	$E.R.A$	$C.E.R.A$	E	~~$D.E.A$~~	~~A~~	~~$D.E$~~	~~0~~	~~$D.A$~~

Table 2: *Terms in the ineligible set (Example 2), obtained by Proposition 4.3 (redundant terms and zeros are crossed out)*

7.2 Main principle of the reduction

In Section 4.2, it was explained how the set $\mathcal{I}$ of ineligible characters can be reduced for elementary regular designs. The basic principle is that, if characters A and B are ineligible and there is a $\delta \in \mathbb{N}$ such that $A = \delta B$, then it is sufficient to check that $\varphi(A) \neq 0$. In other words, the character B can be omitted from the set of ineligible characters. As explained in Section 4.2, it follows that, to be parsimonious, a reduced ineligible set $\mathcal{R}$ must include only one representative per equivalence class defined by (9).

The same principle applies to generalised regular designs, but it is possible to go further. Indeed the relation

$$\langle A \rangle \subseteq \langle B \rangle \iff \exists \delta \in \mathbb{N} \text{ such that } A = \delta B \tag{24}$$

defines a partial order on equivalence classes and it is clear that (7) has to be checked only for representatives of minimal classes. The class of A is minimal if and only if $\langle A \rangle$ does not contain a proper subgroup $\langle B \rangle$, with $B \in \mathcal{I}$. A *reduced ineligible set* $\mathcal{R}$ can thus be obtained by picking one representative in each equivalence class and avoiding representatives having a proper multiple in $\mathcal{I}$.

7.3 Reduction of the set of ineligible pseudofactorial terms

Suppose that the interaction $F_1.F_2$ is ineligible and that $F_1 = A_1 \wedge A_2$, $F_2 = B_1 \wedge B_2$. The character set $\widetilde{E}_{\{1,2\}}$ of the interaction $F_1.F_2$ is the union of the character sets of the nine pseudofactor interactions in $\widetilde{\mathcal{P}}(F_1.F_2)$, where

$$\begin{aligned}\widetilde{\mathcal{P}}(F_1.F_2) \;=\; & \{A_1.B_1,\, A_2.B_1,\, A_1.A_2.B_1,\, A_1.B_2,\, A_2.B_2,\, A_1.A_2.B_2, \\ & A_1.B_1.B_2,\, A_2.B_1.B_2,\, A_1.A_2.B_1.B_2.\}.\end{aligned}$$

We call a term such as A_1 or $A_1.B_1$ a *pseudofactorial term*. Note that a pseudofactorial term is ineligible if and only if it is part of an ineligible factorial term.

In some cases, only a few of the pseudofactor interactions such as the nine above need to be considered when determining $\mathcal{R}$. This property is related to the Sylow decomposition of T and was not relevant for the elementary regular designs. It motivates the construction of a reduced set $\underline{\mathcal{I}}_P$ of ineligible *pseudofactorial* terms, intermediate between the set $\underline{\mathcal{I}}$ of ineligible *factorial* terms and the reduced set $\mathcal{R}$ of ineligible characters.

We use the pseudofactor notation $A_{[k,j]}$ introduced in Section 6.1. Then each pseudofactorial term can be expressed as a product $\prod_{k\in K}\prod_{j\in J_k} A_{[k,j]}$, where the index k varies over a subset K of $\{1,\ldots,l\}$ and, for each k, J_k is a non-empty subset of $\{1,\ldots,s_k\}$. The associated characters in T^* are the linear combinations $\sum_{k\in K}\sum_{j\in J_k} a_{[k,j]}A_{[k,j]}$ for which every coefficient $a_{[k,j]}$ is non-zero. The set E of these characters is the sum $\bigoplus_{k\in K} E_k$ of the pseudofactorial sets E_k of characters associated with the pseudofactorial terms $\prod_{j\in J_k} A_{[k,j]}$.

Definition 7.1 (support) *The* support *of the character $(\breve{A}_1,\ldots,\breve{A}_l)$ is the set $\{k : 1 \le k \le l \text{ and } \breve{A}_k \neq 0\}$. The support of the pseudofactorial term $\prod_{k\in K}\prod_{j\in J_k} A_{[k,j]}$ is the set K.*

Proposition 7.1 *Let $\prod_{k\in K}\prod_{j\in J_k} A_{[k,j]}$ be an ineligible pseudofactorial term. If L is any proper subset of K then the pseudofactorial term $\prod_{k\in L}\prod_{j\in J_k} A_{[k,j]}$ is different from $\emptyset$ and different from $\prod_{k\in K}\prod_{j\in J_k} A_{[k,j]}$. If there is any such subset L such that $\prod_{k\in L}\prod_{j\in J_k} A_{[k,j]}$ is ineligible, then the ineligible set of characters can be reduced by removing all characters associated with $\prod_{k\in K}\prod_{j\in J_k} A_{[k,j]}$.*

Proof: Let E be the set of characters associated with $\prod_{k\in K}\prod_{j\in J_k} A_{[k,j]}$. If $\emptyset \subsetneq L \subsetneq K$, let E_L be the set of characters associated with $\prod_{k\in L}\prod_{j\in J_k} A_{[k,j]}$, and let $\delta = \prod_{k\in K\setminus L} p_k$. If A is any character in E, then δA belongs to E_L, because multiplication by δ makes the coefficient of index $[k,j]$ equal to zero if and only if $k \notin L$. Moreover, $\langle \delta A\rangle$ is a proper subgroup of $\langle A\rangle$. If $\prod_{k\in L}\prod_{j\in J_k} A_{[k,j]}$ is ineligible then $\langle A\rangle$ is not minimal, and so A can be removed from $\underline{\mathcal{I}}_P$. $\square$

Corollary 7.1 *Consider any two pseudofactors that decompose the same factor F_i and have different prime numbers of levels. Any pseudofactorial term that includes both pseudofactors can be omitted from $\underline{\mathcal{I}}_P$.*

A more thorough elimination can proceed according to the following Algorithm 3, where `iptI` is the initial set $\underline{\mathcal{I}}_P$ deduced directly from $\underline{\mathcal{I}}$, `iptR` denotes the reduced set under construction, and `iptq`, `iptK` are temporary subsets of `iptI`.

Algorithm 3 Reduction of ineligible pseudofactorial terms

```
iptI ⟵ complete set of ineligible pseudofactorial terms
iptR ⟵ ∅
for q = 1, ..., l − 1 do
  iptq ⟵ subset of elements in iptI with support of size q
  iptR ⟵ iptR ∪ iptq
  iptI ⟵ iptI \ iptq
  for each pseudofactorial term pft in iptq do
    determine the support L of pft
    iptK ⟵ subset of elements in iptI whose restriction to the support L equals pft
    iptI ⟵ iptI \ iptK
  end for
end for
return iptR
```

Example 1 (continued) The factorial terms in $\underline{\mathcal{I}}$ are expanded as functions of the pseudofactors. In this process,

- F_1 gives $A_{[2,1]}$, $A_{[3,1]}$, $(A_{[2,1]}.A_{[3,1]})$,
- F_2 gives $A_{[2,2]}$, $A_{[2,3]}$, $A_{[2,2]}.A_{[2,3]}$,
- $F_1.F_2$ gives $A_{[2,1]}.A_{[2,2]}$, $A_{[3,1]}.A_{[2,2]}$, $(A_{[2,1]}.A_{[3,1]}.A_{[2,2]})$, $A_{[2,1]}.A_{[2,3]}$, $A_{[3,1]}.A_{[2,3]}$, $(A_{[2,1]}.A_{[3,1]}.A_{[2,3]})$, $A_{[2,1]}.A_{[2,2]}.A_{[2,3]}$, $A_{[3,1]}.A_{[2,2]}.A_{[2,3]}$, $(A_{[2,1]}.A_{[3,1]}.A_{[2,2]}.A_{[2,3]})$,
- *etc.*,

where the terms between parentheses involve different primes for the same treatment factor and so may be omitted immediately.

Then the algorithm starts with the ineligible pseudofactorial terms with only one non-zero primary component (support size $q = 1$). It can be verified that, in this example, they include all the 31 pseudofactorial terms with support $L = \{2\}$:

$$A_{[2,1]},\ A_{[2,2]},\ A_{[2,3]},\ A_{[2,4]},\ A_{[2,5]},\ A_{[2,1]}.A_{[2,2]},\ A_{[2,1]}.A_{[2,3]},\ A_{[2,1]}.A_{[2,4]},\ A_{[2,1]}.A_{[2,5]},$$
$$A_{[2,2]}.A_{[2,3]},\ A_{[2,2]}.A_{[2,4]},\ A_{[2,2]}.A_{[2,5]},\ A_{[2,3]}.A_{[2,4]},\ A_{[2,3]}.A_{[2,5]},\ A_{[2,4]}.A_{[2,5]},$$
$$A_{[2,1]}.A_{[2,2]}.A_{[2,3]},\ A_{[2,1]}.A_{[2,2]}.A_{[2,4]},\ A_{[2,1]}.A_{[2,2]}.A_{[2,5]},\ A_{[2,1]}.A_{[2,3]}.A_{[2,4]},\ A_{[2,1]}.A_{[2,3]}.A_{[2,5]}$$
$$A_{[2,1]}.A_{[2,4]}.A_{[2,5]},\ A_{[2,2]}.A_{[2,3]}.A_{[2,4]},\ A_{[2,2]}.A_{[2,3]}.A_{[2,5]},\ A_{[2,2]}.A_{[2,4]}.A_{[2,5]}$$
$$A_{[2,3]}.A_{[2,4]}.A_{[2,5]},\ A_{[2,2]}.A_{[2,3]}.A_{[2,4]}.A_{[2,5]},\ A_{[2,1]}.A_{[2,3]}.A_{[2,4]}.A_{[2,5]},\ A_{[2,1]}.A_{[2,2]}.A_{[2,4]}.A_{[2,5]},$$
$$A_{[2,1]}.A_{[2,2]}.A_{[2,3]}.A_{[2,4]},\ A_{[2,1]}.A_{[2,2]}.A_{[2,3]}.A_{[2,5]},\ A_{[2,1]}.A_{[2,2]}.A_{[2,3]}.A_{[2,4]}.A_{[2,5]},$$

and the 3 pseudofactorial terms with support $\{3\}$:

$$A_{[3,1]},\ A_{[3,2]},\ A_{[3,1]}.A_{[3,2]}.$$

It follows that, when considered as subsets of pseudofactors, all pseudofactorial terms with support $\{2, 3\}$ include one or more of the pseudofactorial terms above. Therefore they can be eliminated.

Since this first reduced set of ineligible elements includes only elements with one non-zero primary component, the same will be true of any reduced ineligible set deduced from it. We shall see in Section 7.5.1 that this very often occurs in practice and that it allows us to make the search separately for each prime. But it is not always true as shown by Example 2.

Example 2 (continued) The pseudofactorial terms are confounded with the factorial ones in this example so they are given in (23). Those with support of size one may include C, D, E for $p_1 = 2$ or R, A for $p_2 = 3$, which yields D, E, C, $D.E$, R and A. Among the other pseudofactorial terms, we can eliminate $D.A$, $D.R.A$, $D.E.A$, $E.A$, $E.R.A$ and $C.R$, which have D, E, C or $D.E$ as 2-primary component, and $C.D.A$, $C.E.A$, which have A as 3-primary component. The remaining terms are $C.D.R.A$, $C.E.R.A$. So the reduction of pseudofactorial terms leads to the set

$$\underline{\mathcal{I}}_P = \{C,\ D,\ E,\ D.E,\ R,\ A,\ C.D.R.A,\ C.E.R.A\}.$$

Section 3.3 shows that the subsets of characters associated with the factorial terms $C.D.R.A$ and $C.E.R.A$ are

$$\begin{aligned} &\{C+D+R+A,\ C+D+2R+A,\ C+D+R+2A,\ C+D+2R+2A\} \\ \text{and}\quad &\{C+E+R+A,\ C+E+2R+A,\ C+E+R+2A,\ C+E+2R+2A\} \end{aligned}$$

respectively. After picking one representative in each equivalence class, we get the ten elements in Table 7.3, four of which have two non-zero primary components. Note that the equivalence classes have either one element if the coefficients of the three-level factors R and A are both 0, or two otherwise. In the latter case, the representatives are selected as the linear combinations having $-1 = 2 \pmod 3$ as the last non-zero coefficient of factors A and R, if both are involved.

Support	Representative characters
$\{2\}$	C, D, E, $D+E$
$\{3\}$	R, A
$\{2,3\}$	$C+D+R+2A$, $C+D+2R+2A$,
	$C+E+R+2A$, $C+E+2R+2A$

Table 3: *Representatives of equivalence classes in the ineligible set* $\underline{\mathcal{I}}$

7.4 Reduction of the set of ineligible characters

The first step in getting the reduced ineligible set is to select one representative in each equivalence class for the relation (9). This is easy if there is some *canonical* way of selecting unambiguously the representative in each class. In the general case the following proposition shows that a canonical representative can be formed by picking the canonical representative of each primary component.

Proposition 7.2 *If $A = (\breve{A}_1, \ldots, \breve{A}_l)$ then the equivalence class $\mathcal{A}$ of A is the product of the equivalence classes $\mathcal{A}_1$, …, $\mathcal{A}_l$ of its primary components $\breve{A}_1$, …, $\breve{A}_l$: that is, $\mathcal{A} = \mathcal{A}_1 \times \cdots \times \mathcal{A}_l$.*

In the additive notation of Section 3.2, if $A = \breve{A}_1 + \cdots + \breve{A}_l$ then $\mathcal{A} = \mathcal{A}_1 \oplus \cdots \oplus \mathcal{A}_l$. The proof is an immediate consequence of the fact that $\langle A \rangle$ is the direct sum of $\langle \breve{A}_1 \rangle$, …, $\langle \breve{A}_l \rangle$.

When looking for representatives of minimal classes, the following proposition is useful. We omit the proof.

Proposition 7.3 *Let $A = (\breve{A}_1, \ldots, \breve{A}_l)$, $B = (\breve{B}_1, \ldots, \breve{B}_l)$ be the Sylow decompositions of elements A and B of T^*. Then $\langle A \rangle \subseteq \langle B \rangle$ if and only if $\langle \breve{A}_k \rangle \subseteq \langle \breve{B}_k \rangle$ for $k = 1, \ldots, l$.*

In other words, the class of A is contained in the class of B in the sense defined by (24) if and only if, for each $k \leq l$, the class of $\breve{A}_k$ is contained in that of $\breve{B}_k$; that is, there exists an integer δ_k such that $\breve{A}_k = \delta_k \breve{B}_k$.

Given an ineligible pseudofactorial term $\prod_{k \in K} \prod_{j \in J_k} A_{[k,j]}$, we seek a set of representatives of the equivalence classes in the corresponding set E of characters, by which we mean a set containing exactly one element in each eqiuvalence class. As in Section 7.3, $E = \bigoplus_{k \in K} E_k$, where E_k is the set of characters associated with $\prod_{j \in J_k} A_{[k,j]}$.

The following proposition follows directly from Propositions 7.2 and 7.3.

Proposition 7.4 *For each k in K, let $\mathcal{C}_k$ be a set of representatives of the equivalence classes in E_k. Put $\mathcal{C} = \bigoplus_{k \in K} \mathcal{C}_k$. Then $\mathcal{C}$ is a set of representatives of the equivalence classes in E.*

Thus the search for φ is reduced to the search for the primary homomorphisms $\breve{\varphi}_k$ for each prime p_k. Denote by $\mathcal{I}_k$ the set of ineligible characters A whose support is $\{k\}$. Then $\breve{\varphi}_k$ must satisfy

$$\breve{\varphi}_k(A) \neq 0 \qquad \text{for all } A \text{ in } \mathcal{I}_k,$$

for $k = 1$, …, l. Sometimes this necessary condition is also sufficient for condition (7) to be satisfied; sometimes it is not. We discuss the two cases in Section 7.5.

7.5 Dependencies between Sylow components of the key matrix

7.5.1 A condition leading to independent searches for each Sylow component

For $k = 1, \ldots, l$, we denote by $\breve{\mathcal{R}}_k$ the set of all non-zero p_k-primary components $\breve{A}_k$ of the characters in $\mathcal{R}$.

Proposition 7.5 *Assume that every element in $\mathcal{R}$ has a support of size one. Then the condition* (8) *on φ is equivalent to the conjunction of the l conditions*

$$\breve{\varphi}_k(\breve{A}_k) \neq 0 \quad \text{for every } \breve{A}_k \in \breve{\mathcal{R}}_k, \tag{25}$$

for $k = 1, \ldots, l$.

Proof: If the assumption holds, then

$$\breve{\mathcal{R}}_k = \{\breve{A}_k : (0, \ldots, 0, \breve{A}_k, 0, \ldots, 0) \in \mathcal{R}\}.$$

Thus the result follows immediately from (22). □

Hence under the assumption in Proposition 7.5, it is equivalent to search for φ satisfying (8) or to search separately (and independently) for the primary homomorphisms $\breve{\varphi}_k$ satisfying (25). In practice it is easy to check this assumption directly on the reduced ineligible set $\mathcal{R}$. But a question naturally arises: is this assumption often satisfied in practice? Proposition 7.6 and Corollary 7.2 below give a positive answer by giving a mild condition under which the assumption is true. On the contrary, Example 7 illustrates a practical situation in which the assumption is not satisfied.

Proposition 7.6 *If, for every character A in the ineligible set $\mathcal{I}$, all non-zero integer multiples of A also belong to $\mathcal{I}$, then there exists a reduced ineligible set $\mathcal{R}$ such that the assumption in Proposition 7.5 is satisfied.*

Proof: We have $p_k\breve{A}_k = 0$ for each $\breve{A}_k$ in $\breve{T}_k^*$. Now let A be an element of $\mathcal{I}$ and $A = (\breve{A}_1, \ldots, \breve{A}_l)$ be its Sylow decomposition. Since A is not zero, it has a coordinate, say $\breve{A}_1$, different from 0. Multiplying it by δ, where $\delta = p_2 \cdots p_l$, we get the element $\delta A = (\delta\breve{A}_1, 0, \ldots, 0)$ having only one non-zero primary component (δA_1 is not zero since δ and p_1 are coprime). If A has a second non-zero primary component, then $\langle \delta A \rangle$ is strictly included in $\langle A \rangle$ and A can consequently be excluded from $\mathcal{R}$. □

A subset $\mathcal{S}$ of a group is said to be *closed under integer multiplication* if

$$A \in \mathcal{S} \Longrightarrow \delta A \in \mathcal{S} \quad \text{for every integer } \delta.$$

It is easy to show that the subsets closed under integer multiplication are unions of subgroups. If $\mathcal{I} \cup \{0\}$ is a union of subgroups, then Proposition 7.6 shows that the assumption in Proposition 7.5 is satisfied.

In practice, a set like $\mathcal{M}$ defining the model is often a union of subgroups of T^* and is thus closed under integer multiplication. This is always true when $\underline{\mathcal{M}}$ is complete. As to the set $\mathcal{E}$ of effects to estimate, it is usual that if it contains an interaction, it also contains all effects marginal to it except for the mean. For instance, if it contains $A.B.C$, it also contains the main effects A, B, C and the two-factor interactions $A.B$, $A.C$, $B.C$. Under these assumptions, $\mathcal{E} \cup \{0\}$ and $\mathcal{M}$ are both closed under integer multiplication, and so is the difference $\mathcal{E} - \mathcal{M}$. Then the following corollary applies, whether or not $\mathcal{E}$ contains 0:

Corollary 7.2 *If $\mathcal{E} \cup \{0\}$, $\mathcal{M}$ are subsets of T^* closed under integer multiplication, and $\mathcal{I} = (\mathcal{E} - \mathcal{M}) \setminus \{0\}$, then there exists a reduced ineligible set $\mathcal{R}$ deduced from $\mathcal{I}$ that satisfies the assumption in Proposition 7.5.*

Proof: Each element of $\mathcal{I}$ can be written $A - B$, with A in $\mathcal{E}$, B in $\mathcal{M}$ and $A \neq B$. The Sylow decomposition of $A - B$ is $(\breve{A}_1 - \breve{B}_1, \ldots, \breve{A}_l - \breve{B}_l)$. Suppose that $A - B$ has two or more non-zero primary components, including $\breve{A}_k - \breve{B}_k$. Multiplying $A - B$ by δ, where $\delta = (p_1 \cdots p_l)/p_k$, we get $\delta \breve{A}_k - \delta \breve{B}_k$ as the only non-zero component. Since δ is prime to p_k, the assumptions imply that $\delta \breve{A}_k$ belongs to $\mathcal{E}$ and $\delta \breve{B}_k$ belongs to $\mathcal{M}$. It follows that $\breve{A}_k - \breve{B}_k$ belongs to $\mathcal{I}$. If it is included in $\mathcal{R}$, then $A - B$ can be discarded from $\mathcal{R}$. □

This result can be generalised easily to ineligible sets of the form (6): if all the sets $\mathcal{E}_1 \cup \{0\}$, $\mathcal{M}_1$, $\mathcal{E}_2 \cup \{0\}$, $\mathcal{M}_2$ are closed under integer multiplication, then the assumption in Proposition 7.5 is satisfied.

Corallary 7.2 gives as a particular case the following classical result (Bailey, 1985): the design is of resolution R if all its Sylow components are.

7.5.2 Counter cases

There are however situations, like in criss-cross experiments, when $\underline{\mathcal{E}}$ includes an interaction but not the main effects of the corresponding factors and when the assumption in Proposition 7.5 is not satisfied. Example 2 and Example 7 below were constructed to illustrate this situation and its different consequences.

Example 2 (continued) As shown in Section 7.3, the reduced set contains characters of support size 2 and so this example does not satisfy the conditions of Propositions 7.5 and 7.6. However, it still allows for separate solutions of the Sylow components of Φ, as we now explain.

The unit pseudofactors are $V_{[2,1]}$, $V_{[2,2]}$, and $V_{[3,1]}$. There is no loss of generality in putting $\breve{\varphi}_2(C) = V_{[2,1]}$ and $\breve{\varphi}_3(R) = V_{[3,1]}$. For example, one possibility for Φ is

$$\begin{array}{c} \\ V_{[2,1]} \\ V_{[2,2]} \\ V_{[3,1]} \end{array} \begin{array}{c} \begin{array}{ccccc} \tilde{C} & \tilde{D} & \tilde{E} & \tilde{R} & \tilde{A} \end{array} \\ \begin{pmatrix} 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 \end{pmatrix} \end{array}$$

It is clear that $\breve{\varphi}_2(D)$ and $\breve{\varphi}_2(E)$ must be two of $V_{[2,1]}$, $V_{[2,2]}$ and $V_{[2,1]} + V_{[2,2]}$. Since the character A is in $\mathcal{R}$, $\breve{\varphi}_3(A)$ must be $V_{[3,1]}$ or $2V_{[3,1]}$ whatever $\breve{\varphi}_2$. If $\breve{\varphi}_3(A)$ is $V_{[3,1]}$ then $\varphi(C + D + R + 2A) = \varphi(C + D)$ and $\varphi(C + E + R + 2A) = \varphi(C + E)$, so $\breve{\varphi}_2(D)$ and $\breve{\varphi}_2(E)$ must both be different from $\breve{\varphi}_2(C)$. If $\breve{\varphi}_3(A)$ is $2V_{[3,1]}$ then exactly the same is true due to $\varphi(C + D + R + A)$ and $\varphi(C + E + R + A)$.

In that example, the solutions for $\breve{\varphi}_2$ do not depend on the solution for $\breve{\varphi}_3$ nor vice-versa. But it is possible to find a similar example with 36 units where the choice for the two-level factors depends on the choice previously made for the three-level ones.

Example 7 This is a small modification of Example 2. Now there are six units in each of the six blocks, and the factor A is no longer constrained to be coarser than R. The sets $\underline{\mathcal{M}}$, $\underline{\mathcal{E}}$ and $\underline{\mathcal{I}}$ are unchanged, and $\underline{\mathcal{M}}$ is complete.

The unit pseudofactors are $V_{[2,1]}$, $V_{[2,2]}$, $V_{[3,1]}$ and $V_{[3,2]}$. There is no loss of generality in putting $\breve{\varphi}_2(C) = V_{[2,1]}$ and $\breve{\varphi}_3(R) = V_{[3,1]}$. Then $\breve{\varphi}_2(D)$ and $\breve{\varphi}_2(E)$ must be two of $V_{[2,1]}$, $V_{[2,2]}$ and $V_{[2,1]} + V_{[2,2]}$, while $\breve{\varphi}_3(A)$ can be any non-zero combination of $V_{[3,1]}$ and $V_{[3,2]}$. If $\breve{\varphi}_3(A)$ is $V_{[3,1]}$ then $\varphi(C+D+R+2A) = \varphi(C+D)$ and $\varphi(C+E+R+2A) = \varphi(C+E)$, so $\breve{\varphi}_2(D)$ and $\breve{\varphi}_2(E)$ must both be different from $\breve{\varphi}_2(C)$. If $\breve{\varphi}_3(A)$ is not a multiple of $V_{[3,1]}$ then there is no such constraint on $\breve{\varphi}_2(D)$ and $\breve{\varphi}_2(E)$.

In this case, the search cannot be made independently in the Sylow components. There are the following three fundamentally different possibilities for Φ.

$$
\begin{array}{c} \\ V_{[2,1]} \\ V_{[2,2]} \\ V_{[3,1]} \\ V_{[3,2]} \end{array}
\begin{array}{c} \begin{array}{ccccc} \tilde{C} & \tilde{D} & \tilde{E} & \tilde{R} & \tilde{A} \end{array} \\ \begin{pmatrix} 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix} \end{array}
\qquad
\begin{array}{c} \\ V_{[2,1]} \\ V_{[2,2]} \\ V_{[3,1]} \\ V_{[3,2]} \end{array}
\begin{array}{c} \begin{array}{ccccc} \tilde{C} & \tilde{D} & \tilde{E} & \tilde{R} & \tilde{A} \end{array} \\ \begin{pmatrix} 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix} \end{array}
\qquad
\begin{array}{c} \\ V_{[2,1]} \\ V_{[2,2]} \\ V_{[3,1]} \\ V_{[3,2]} \end{array}
\begin{array}{c} \begin{array}{ccccc} \tilde{C} & \tilde{D} & \tilde{E} & \tilde{R} & \tilde{A} \end{array} \\ \begin{pmatrix} 1 & 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix} \end{array}
$$

More generally, counter-cases arise when, say, $A = \breve{A}_1 + \breve{A}_2$ belongs to $\mathcal{R}$ but neither $\breve{A}_1$ nor $\breve{A}_2$ do. This case may happen if an interaction has to be estimated but not the associated main effects. In that case, it may well be necessary and sufficient that either $\breve{\varphi}_1(\breve{A}_1) \neq 0$ or $\breve{\varphi}_2(\breve{A}_2) \neq 0$. So there may be solutions with $\breve{\varphi}_1(\breve{A}_1) \neq 0$ and solutions with $\breve{\varphi}_1(\breve{A}_1) = 0$. Thus the equivalence of Proposition 7.5 is not satisfied.

7.5.3 Backtrack search in the non-independent case

When, as in Example 7, the assumption in Proposition 7.5 is not satisfied, the Sylow components of φ and Φ can be found by backtrack search. Assume that $\breve{\varphi}_j$ has already been defined for $j = 1, \ldots, k-1$. Let $\mathcal{R}_{[k]}$ be the subset of elements $A = (\breve{A}_1, \ldots, \breve{A}_k, 0, \ldots, 0)$ in $\mathcal{R}$ having $\breve{A}_k$ as last non-zero primary component. Then, for every A in $\mathcal{R}_{[k]}$,

$$\varphi(A) = \Big(\breve{\varphi}_1(\breve{A}_1), \ldots, \breve{\varphi}_k(\breve{A}_k), 0, \ldots, 0\Big) \ .$$

The choice of $\breve{\varphi}_k$ must ensure that $\varphi(A) \neq 0$ for each such A. If A in $\mathcal{R}_{[k]}$ is such that $\breve{\varphi}_j(\breve{A}_j) \neq 0$ for at least one index j between 1 and $k-1$, then $\varphi(A) \neq 0$ whatever the choice of $\breve{\varphi}_k$. These elements therefore need not be taken into account in the search for $\breve{\varphi}_k$. On the other hand, the inequality $\breve{\varphi}_k(\breve{A}_k) \neq 0$ has to be satisfied for every $A \in \mathcal{R}_{[k]}$ such that

$$\breve{\varphi}_j(\breve{A}_j) = 0 \quad \text{for } j = 1, \ldots, k-1. \tag{26}$$

Let $\mathcal{R}_{[[k]]}$ be the set of elements A in $\mathcal{R}_{[k]}$ satisfying (26). The search for $\breve{\varphi}_k$ can proceed with $\mathcal{R}_{[[k]]}$ as reduced ineligible set. If it succeeds and $k < l$, it goes on to find $\breve{\varphi}_{k+1}$. If it fails and $1 < k$, it goes back and tries to find another choice for $\breve{\varphi}_{k-1}$. The search finally fails if it goes back to $k = 1$ and fails to find another $\breve{\varphi}_1$. It finally succeeds if it reaches $k = l$ and finds an admissible $\breve{\varphi}_l$.

In any case, the elementary step in the search for φ is the search for the primary homomorphisms $\breve{\varphi}_k$ for each prime p_k.

8 Discussion

Quite apart from the computational aspects, this paper shows great unity between different types of factorial design: fractional or not; one prime or many; blocked, split-plot, row-column, criss-cross, and so on. The approach using one or more model-estimate pairs $(\underline{\mathcal{M}}, \underline{\mathcal{E}})$ gives a unified framework. The set of ineligible factorial terms is at the centre of this framework, since it synthesizes all the constraints associated with the users' specifications. The other key component is the design key, which determines the combinatorial and statistical properties of the design. Indeed the design problem essentially consists of finding a design key adapted to the set of ineligible factorial terms.

A few remarks must be made from a statistical point of view. Of course, once an initial design has been generated, it then needs to be randomized. Since the two steps are quite independent, we only focused on the first one in this paper. Another point is that we made no distinction between the key matrices, provided they are solutions to the design specifications of Section 2. To cope with finer criteria such as minimum aberration or maximum estimation capacity (see e.g. Mukerjee and Wu, 2006), the approach developed here gives the possibility (up to computational constraints) to get all solutions and then select the best ones according to such a criterion. An efficient alternative for a user of R is to use the FrF2 R package (Grömping, 2014), which makes better use of such considerations but is restricted to factors at two levels.

The framework could be even more general. For example, if a factor has four levels, it is possible to associate it with the cyclic group C_4 rather than using two pseudofactors with two levels each; similarly for other primes and other powers. Bailey (1977, 1985), Dean and John (1975), John and Dean (1975), Kobilinsky (1985), Kobilinsky and Monod (1991) have shown that the theory presented in Sections 3 and 6 extends to this more general setting with no difficulty, using abelian groups which are not elementary abelian. However, the algorithms underlying *planor* become much more complicated when nontrivial powers of primes are allowed. Such powers can lead to designs which are not obtainable by permutations from designs where no such powers are used. Bailey (1977), Giovagnoli (1977) and Voss and Dean (1987) showed that, in some circumstances, there is a homomorphism φ satisfying condition (7) when all pseudofactors have prime number of levels but not otherwise. Voss (1988) conjectured that if there is a solution using nontrivial prime powers then there is also a solution using only primes; Voss (1993) proved this in some special cases. This suggests that it is not worth the trouble of extending the algorithm to deal with groups that are abelian but not elementary abelian.

The algorithmic approach presented here to generate designs is based on backtracking, which aims at a complete exploration of the possible solutions. The drawback is that the computational burden becomes too hard when the number of factors or the degree of fractionating becomes too high. So there is clearly a need to improve the speed of the algorithm. There are many directions to do so, but we want to stress two of them.

Cheng and Tsai (2013) have shown how templates may be used for the design key in certain situations. Such a template enables us to fix more columns in the matrix Φ. For instance, in the matrix given for Example 3 in Section 5.3.1, we lose nothing by making the column for A the same as the column for Q, and the columns for B and C the same as those for U_1 and U_2 respectively.

Another direction to accelerate the search is to take account of symmetries between factors or pseudofactors, with respect to the design specifications. To do so efficiently, it might be better to implement the search in a language like GAP (2014), which is expressly designed to cut down searches by allowing for symmetries.

The R package *planor* is available on the CRAN (Monod *et al.*, 2012). It deals with the whole class of generalised regular factorial designs presented in this paper. In addition to generating such designs, it can randomise them according to many types of orthogonal block structures. A detailed presentation will be the subject of an other paper.

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