Algebraic generation of minimum size orthogonal fractional factorial designs: an approach based on integer linear programming.

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Roberto Fontana

Abstract Generation of orthogonal fractional factorial designs (OFFDs) is an important and extensively studied subject in applied statistics. In this paper we show how searching for an OFFD that satisfies a set of constraints, expressed in terms of orthogonality between simple and interaction effects, is, in many applications, equivalent to solving an integer linear programming problem. We use a recent methodology, based on polynomial counting functions and *strata*, that represents OFFDs as the positive integer solutions of a system of linear equations. We use this system to set up an optimization problem where the cost function to be minimized is the size of the OFFD and the constraints are represented by the system itself. Finally we search for a solution using standard integer programming techniques. Some applications are also presented in the computational results section. It is worth noting that the methodology does not put any restriction either on the number of levels of each factor or on the orthogonality constraints and so it can be applied to a very wide range of designs, including mixed orthogonal arrays.

Keywords Design of experiments · Orthogonal fractional factorial designs · Algebraic statistics · Integer linear programming · Orthogonal arrays

1 Introduction

Orthogonal Fractional Factorial Designs (OFFDs) are frequently used in many fields of application, including medicine, engineering and agriculture. They offer a valuable

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tool for dealing with problems where there are many factors involved and each run is expensive. They also keep the statistical analysis of the data quite simple. The literature on the subject is extremely rich. A non-exhaustive list of references, mainly related to the theory of the design of experiments, includes the fundamental paper of Bose (1947) and the following books: Raktoe et al. (1981), Collombier (1996), Dey and Mukerjee (1999), Wu and Hamada (2000), Mukerjee and Wu (2006) and Bailey (2008).

Orthogonal Arrays (OAs) represent an important class of OFFDs, see, for example, Hedayat et al. (1999) and Schoen et al. (2010). Indeed an Orthogonal Array of appropriate strength can be used to solve the wide range of problems related to the study of the size of the main effects and interactions up to a given order of interest.

It is evident that in many real-life experiments, finding an OFFD with the smallest possible number of runs is of great importance. This is particularly true in the case where the cost of each experiment is high in terms of resources and/or time, such as in the study of the relationship between fuel consumption and the design parameters of a new car engine.

A large number of techniques are known to generate OFFDs and, in particular, OAs. For example:

- the case where all factors have the same number p of levels and p is a prime number or a power of a prime number, is commonly studied using Galois Fields and finite geometries;
- Hadamard Matrices are used for OAs where all factors have 2 levels and where strength is less than or equal to 3;
- difference schemes are a tool for constructing mixed orthogonal arrays of strength 2.

From the above it is clear that there are several different methods covering different situations. When different methods are applied to certain problems the solutions that are found can be significantly different. For example, as we will discuss in Sect. 4, minimum size orthogonal arrays with eleven 2-level factors and strength 2 obtained using Galois field $GF(2) \equiv \mathbb{Z}_2$ have 16 runs while those obtained using Hadamard matrices have 12 runs. Thus the problem of finding minimum size OFFD can be difficult for the non-expert user due to the difficulty of selecting the most appropriate method.

The joint use of polynomial indicator functions and complex coding of levels provides a general theory for mixed level orthogonal fractional factorial designs, see Pistone and Rogantin (2008). This theory does not put any restriction either on the number of levels of each factor or on the orthogonality constraints. It also makes use of commutative algebra, see Pistone and Wynn (1996), and generalizes the approach to two-level designs as discussed in Fontana et al. (2000). The definition of *strata* provided in Sect. 2 makes it possible to transform each OFFD into a solution of a homogeneous system of linear equations where the unknowns are positive integers.

In Sect. 2 we briefly review the algebraic theory of orthogonal fractional facto-rial designs based on polynomial counting functions and *strata*. In Sect. 3 we set up an optimization problem whose solutions are minimum size OFFDs. Some applications of the methodology are presented in Sect. 4. Finally, concluding remarks are in Sect. 5.

2 Algebraic description of fractional factorial designs using *strata*

In this Section, we report some relevant results of the algebraic theory of OFFDs, following the approach of Fontana and Pistone (2010a). The interested reader can find further information, including the proofs of the propositions in Fontana et al. (2000), Pistone and Rogantin (2008) and Fontana and Pistone (2010b).

2.1 Fractions of a full factorial design

Let us consider an experiment which includes m factors $\mathcal{D}_j,\ \ j = 1, \ldots, m$. Let us code the n_j levels of the factor $\mathcal{D}_j$ by the n_j-th roots of the unity

$$\mathcal{D}_j = \{\omega_0^{(n_j)}, \ldots, \omega_{n_j-1}^{(n_j)}\},$$

where $\omega_k^{(n_j)} = \exp\left(\sqrt{-1}\,\frac{2\pi}{n_j}\,k\right), k = 0, \ldots, n_j - 1,\ \ j = 1, \ldots, m.$

The *full factorial design* with *complex coding* is $\mathcal{D} = \mathcal{D}_1 \times \cdots \mathcal{D}_j \cdots \times \mathcal{D}_m$. We denote its cardinality by $\#\mathcal{D}$, $\#\mathcal{D} = \prod_{j=1}^{m} n_j$.

Definition 1 A fraction $\mathcal{F}$ is a multiset $(\mathcal{F}_*, f_*)$ whose underlying set of elements $\mathcal{F}_*$ is contained in $\mathcal{D}$ and f_* is the multiplicity function $f_* : \mathcal{F}_* \to \mathbb{N}$ that for each element in $\mathcal{F}_*$ gives the number of times it belongs to the multiset $\mathcal{F}$.

We recall that the underlying set of elements $\mathcal{F}_*$ is the subset of $\mathcal{D}$ that contains all the elements of $\mathcal{D}$ that appear in $\mathcal{F}$ at least once. We denote the number of elements of a fraction $\mathcal{F}$ by $\#\mathcal{F}$, with $\#\mathcal{F} = \sum_{\zeta \in \mathcal{F}_*} f_*(\zeta)$.

Example 1 Let us consider $m = 1, n_1 = 3$. We get

$$\mathcal{D} = \left\{1, \exp\left(\sqrt{-1}\,\frac{2\pi}{3}\right), \exp\left(\sqrt{-1}\,\frac{4\pi}{3}\right)\right\}.$$

The fraction $\mathcal{F} = \{1, 1, \exp\left(\sqrt{-1}\,\frac{2\pi}{3}\right)\}$ is the multiset $(\mathcal{F}_*, f_*)$ where $\mathcal{F}_* = \{1, \exp\left(\sqrt{-1}\,\frac{2\pi}{3}\right)\}$, $f_*(1) = 2$, and $f_*(\exp\left(\sqrt{-1}\,\frac{2\pi}{3}\right)) = 1$. We get $\#\mathcal{F} = f_*(1) + f_*(\exp\left(\sqrt{-1}\,\frac{2\pi}{3}\right)) = 2 + 1 = 3$.

In order to use polynomials to represent all the functions defined over $\mathcal{D}$, including multiplicity functions, we define

– X_j, the j-th component function, which maps a point $\zeta = (\zeta_1, \ldots, \zeta_m)$ of $\mathcal{D}$ to its j-th component,

$$X_j \colon \mathcal{D} \ni (\zeta_1, \ldots, \zeta_m) \longmapsto \zeta_j \in \mathcal{D}_j.$$

The function X_j is called *simple term* or, by abuse of terminology, *factor*.

– $X^\alpha = X_1^{\alpha_1} \cdot \ldots \cdot X_m^{\alpha_m}$, $\alpha \in L = \mathbb{Z}_{n_1} \times \cdots \times \mathbb{Z}_{n_m}$, i.e. the monomial function

$$X^\alpha : \mathcal{D} \ni (\zeta_1, \ldots, \zeta_m) \mapsto \zeta_1^{\alpha_1} \cdot \ldots \cdot \zeta_m^{\alpha_m}.$$

The function X^α is called *interaction term*

We observe that $\{X^\alpha : \alpha \in L = \mathbb{Z}_{n_1} \times \cdots \times \mathbb{Z}_{n_m}\}$ is a basis of all the complex functions defined over $\mathcal{D}$. We use this basis to represent the counting function of a fraction according to Definition 2.

Definition 2 The *counting function* R of a fraction $\mathcal{F}$ is a complex polynomial defined over $\mathcal{D}$ so that for each $\zeta \in \mathcal{D}$, $R(\zeta)$ equals the number of appearances of ζ in the fraction. A $0 - 1$ valued counting function is called an *indicator function* of a single replicate fraction $\mathcal{F}$. We denote by c_α the coefficients of the representation of R on $\mathcal{D}$ using the monomial basis $\{X^\alpha,\ \alpha \in L\}$:

$$R(\zeta) = \sum_{\alpha \in L} c_\alpha X^\alpha(\zeta),\ \zeta \in \mathcal{D},\ c_\alpha \in \mathbb{C}.$$

Remark 1 Vector orthogonality is defined with respect to the Hermitian product defined as

$$f \cdot g = E_{\mathcal{F}}(f\,\overline{g}) \equiv \frac{1}{\#\mathcal{F}} \sum_{\zeta \in \mathcal{F}} f(\zeta)\overline{g(\zeta)}\,,$$

where $\overline{g}$ is the complex conjugate of g. It should be noted that $\sum_{\zeta \in \mathcal{F}} f(\zeta)$ means $\sum_{\zeta \in \mathcal{F}_*} f_*(\zeta) f(\zeta)$.

With the complex coding, over a generic $\mathcal{F}$, the vector orthogonality of two interaction terms, X^α and X^β corresponds to the combinatorial orthogonality of the corresponding multisets $\{X^\alpha(\zeta) : \zeta \in \mathcal{F}\}$ and $\{X^\beta(\zeta) : \zeta \in \mathcal{F}\}$, i.e. each point of their Cartesian product appears equally often.

With Proposition 1 from Pistone and Rogantin (2008), we link the orthogonality of two interaction terms with the coefficients of the polynomial representation of the counting function.

Proposition 1 *If $\mathcal{F}$ is a fraction of a full factorial design $\mathcal{D}$, $R = \sum_{\alpha \in L} c_\alpha X^\alpha$ is its counting function and $[\alpha - \beta]$ is the m-tuple made by the componentwise difference in the rings $\mathbb{Z}_{n_j}$, $([\alpha_1 - \beta_1]_{n_1}, \ldots, [\alpha_j - \beta_j]_{n_j}, \ldots, [\alpha_m - \beta_m]_{n_m})$, then*

1. *the coefficients c_α are given by $c_\alpha = \frac{1}{\#\mathcal{D}} \sum_{\zeta \in \mathcal{F}} \overline{X^\alpha(\zeta)}$;*
2. *the term X^α is centered on $\mathcal{F}$, i.e. $\frac{1}{\#\mathcal{F}} \sum_{\zeta \in \mathcal{F}} X^\alpha(\zeta) = 0$ if, and only if, $c_\alpha = c_{[-\alpha]} = 0$;*
3. *the terms X^α and X^β are orthogonal on $\mathcal{F}$ if and only if, $c_{[\alpha-\beta]} = 0$.*

Proof Item (1) follows from

$$\sum_{\zeta\in\mathcal{F}} \overline{X^\alpha(\zeta)} = \sum_{\zeta\in\mathcal{D}} R(\zeta)\overline{X^\alpha(\zeta)} = \sum_{\zeta\in\mathcal{D}}\sum_{\beta\in L} c_\beta X^\beta(\zeta)\overline{X^\alpha(\zeta)}$$
$$= \sum_{\beta\in L} c_\beta \sum_{\zeta\in\mathcal{D}} X^\beta(\zeta)\overline{X^\alpha(\zeta)} = \#\mathcal{D} c_\alpha$$

where we use

$$\sum_{\zeta\in\mathcal{D}} X^\beta(\zeta)\overline{X^\alpha(\zeta)} = \begin{cases} 0 & \text{if } \alpha \neq \beta \\ \#\mathcal{D} & \text{if } \alpha = \beta \end{cases}.$$

Items (2) and (3) follow from Item (1). □

We now define projectivity and, in particular, its relation with orthogonal arrays. Given $I = \{i_1, \ldots, i_k\} \subset \{1, \ldots, m\}$, $i_1 < \cdots < i_k$ we define the projection π_I as

$$\pi_I : \mathcal{D} \ni \zeta = (\zeta_1, \ldots, \zeta_m) \mapsto \zeta_I \equiv (\zeta_{i_1}, \ldots, \zeta_{i_k}) \in \mathcal{D}_{i_1} \times \cdots \times \mathcal{D}_{i_k}.$$

Definition 3 A fraction $\mathcal{F}$ *factorially projects* onto the I-factors, $I = \{i_1, \ldots, i_k\} \subset \{1, \ldots, m\}$, $i_1 < \cdots < i_k$, if the projection $\pi_I(\mathcal{F})$ is a multiple full factorial design, i.e. the multiset $(\mathcal{D}_{i_1} \times \cdots \times \mathcal{D}_{i_k}, f_*)$ where the multiplicity function f_* is constantly equal to a positive integer over $\mathcal{D}_{i_1} \times \cdots \times \mathcal{D}_{i_k}$.

Example 2 Let us consider $m = 2, n_1 = n_2 = 2$ and the fraction $\mathcal{F} = \{(-1, 1), (-1, 1), (1, -1), (1, 1)\}$. We obtain $\pi_1(\mathcal{F}) = \{-1, -1, 1, 1\}$ and $\pi_2(\mathcal{F}) = \{-1, 1, 1, 1\}$. It follows that $\mathcal{F}$ projects on the first factor and does not project on the second factor.

Definition 4 A fraction $\mathcal{F}$ is a *mixed orthogonal array* of strength t if it factorially projects onto any I-factors with $\#I = t$.

Proposition 2 *A fraction* factorially projects onto the I-factors, $I = \{i_1, \ldots, i_k\} \subset \{1, \ldots, m\}$, $i_1 < \cdots < i_k$, *if and only if, all the coefficients of the counting function involving the I-factors only are* 0.

Proof We give a sketch of the proof available in full in Pistone and Rogantin (2008). It can be shown that the number of times that a point $\zeta_I \in \mathcal{D}_I \equiv \mathcal{D}_{i_1} \times \cdots \times \mathcal{D}_{i_k}$ appears in the projection of $\mathcal{F}$ onto the I-factors is equal to $\frac{\#\mathcal{D}}{\#\mathcal{D}^I} \sum_{\alpha_I \in L_I} c_{\alpha_I} X^{\alpha_I}(\zeta_I)$ where $L_I = \pi_I(L)$. It follows that it will be constant if and only if all the coefficients c_{α_I}, with $\alpha_I \neq (0, \ldots, 0)$ are zero. □

Proposition 2 can be immediately stated for mixed orthogonal arrays.

Proposition 3 *A fraction is an* orthogonal array of strength t *if and only if, all the coefficients c_α of the counting function up to the order t are* 0.

2.2 Counting functions and strata

It follows from Propositions 1, 2 and 3 that the problem of finding orthogonal fractional factorial designs can be written as a polynomial system in which the indeterminates are the complex coefficients c_α of the counting polynomial fraction.

Let us now introduce a different way to describe the full factorial design $\mathcal{D}$ and all its subsets. We consider the indicator functions 1_ζ of all the single points of $\mathcal{D}$. The counting function R of a fraction $\mathcal{F}$ can be written as $\sum_{\zeta \in \mathcal{D}} y_\zeta 1_\zeta$ with $y_\zeta \equiv R(\zeta) \in \{0, 1, \ldots, n, \ldots\}$. The particular case in which R is an indicator function cor-responds to $y_\zeta \in \{0, 1\}$. From Proposition 1 we obtain that the values of the counting function over $\mathcal{D}$, y_ζ, are related to the coefficients c_α by $c_\alpha = \frac{1}{\#\mathcal{D}} \sum_{\zeta \in \mathcal{D}} y_\zeta \overline{X^\alpha(\zeta)}$. As described in Section 2.1, we consider m factors, $\mathcal{D}_1, \ldots, \mathcal{D}_m$ where $\mathcal{D}_j \equiv \Omega_{n_j} = \{\omega_0^{(n_j)}, \ldots, \omega_{n_j-1}^{(n_j)}\}$, for $j = 1, \ldots, m$. From Pistone and Rogantin (2008), we recall two basic properties which hold true for the full design $\mathcal{D}$.

Proposition 4 *Let X_j be the simple term with level set $\mathcal{D}_j = \Omega_{n_j} = \{\omega_0^{(n_j)}, \ldots, \omega_{n_j-1}^{(n_j)}\}$, $j = 1, \ldots, m$. Let $X^\alpha = X_1^{\alpha_1} \cdots X_m^{\alpha_m}$ be an interaction.*

1. *Over $\mathcal{D}$, the term X_j^r takes all the values of Ω_{s_j} equally often, where $s_j = 1$ if $r = 0$ and $s_j = n_j / \gcd(r, n_j)$ if $r > 0$.*
2. *Over $\mathcal{D}$, the term X^α takes all the values of Ω_s equally often, where $s = \operatorname{lcm}(s_1, \ldots, s_m)$ and s_i, that is determined according to the previous Item 4, corresponds to $X_i^{\alpha_i}$, $i = 1, \ldots, m$.*

Let us now define the *strata* that are associated with simple and interaction terms.

Definition 5 Given a term $X^\alpha, \alpha \in L = \mathbb{Z}_{n_1} \times \cdots \times \mathbb{Z}_{n_m}$, the full design $\mathcal{D}$ is partitioned into the strata $D_h^\alpha = \{\zeta \in \mathcal{D} : \overline{X^\alpha(\zeta)} = \omega_h^{(s)}\}$, where $\omega_h^{(s)} \in \Omega_s$ and s is determined according to the previous Proposition 4.

We use $n_{\alpha,h}$ to denote the number of points of the fraction $\mathcal{F}$ that are in the stratum D_h^α, $n_{\alpha,h} = \sum_{\zeta \in D_h^\alpha} y_\zeta$, $h = 0, \ldots, s-1$. Proposition 5 links the coefficients c_α with $n_{\alpha,h}$.

Proposition 5 *Let $\mathcal{F}$ be a fraction of $\mathcal{D}$ with counting function $R = \sum_{\alpha \in L} c_\alpha X^\alpha$. Each c_α, $\alpha \in L$, depends on $n_{\alpha,h}$, $h = 0, \ldots, s-1$, as $c_\alpha = \frac{1}{\#\mathcal{D}} \sum_{h=0}^{s-1} n_{\alpha,h} \omega_h^{(s)}$, where s is determined by X^α according to Proposition 4.*

Proof From Proposition 1 we know that $c_\alpha = \frac{1}{\#\mathcal{D}} \sum_{\zeta \in \mathcal{F}} \overline{X^\alpha(\zeta)}$. It follows

$$c_\alpha = \frac{1}{\#\mathcal{D}} \sum_{\zeta \in \mathcal{D}} y_\zeta \overline{X^\alpha(\zeta)} = \frac{1}{\#\mathcal{D}} \sum_{h=0}^{s-1} \sum_{\zeta \in D_h^\alpha} y_\zeta \overline{X^\alpha(\zeta)}$$

$$= \frac{1}{\#\mathcal{D}} \sum_{h=0}^{s-1} \omega_h^{(s)} \sum_{\zeta \in D_h^\alpha} y_\zeta = \frac{1}{\#\mathcal{D}} \sum_{h=0}^{s-1} n_{\alpha,h} \omega_h^{(s)}.$$

We now use a part of Proposition 3 from Pistone and Rogantin (2008) to obtain conditions on $n_{\alpha,h}$ that make X^α centered on the fraction $\mathcal{F}$.

Proposition 6 *Let X^α be a term with level set Ω_s on full design $\mathcal{D}$ and let $P(\zeta)$ be the complex polynomial associated with the sequence $(n_{\alpha,h})_{h=0,\ldots,s-1}$ so that $P(\zeta) = \sum_{h=0}^{s-1} n_{\alpha,h}\zeta^h$ and Φ_s the cyclotomic polynomial of the s-roots of the unity.*

1. *Let s be prime. The term X^α is centered on the fraction $\mathcal{F}$ if, and only if, its s levels appear equally often $n_{\alpha,0} = n_{\alpha,1} = \ldots = n_{\alpha,s-1} = \lambda_\alpha$;*
2. *Let $s = p_1^{h_1} \ldots p_d^{h_d}$, p_i prime, $i = 1, \ldots, d$. The term X^α is centered on the fraction $\mathcal{F}$ if, and only if, the remainder $H(\zeta) = P(\zeta) \bmod \Phi_s(\zeta)$, whose coefficients are integer linear combinations of $n_{\alpha,h}$, $h = 0, \ldots, s-1$, is identically zero.*

We observe that, since D_h^α is a partition of $\mathcal{D}$, if s is prime, we get $\lambda_\alpha = \frac{\#\mathcal{F}}{s}$. If we recall that $n_{\alpha,h}$ are related to the values of the counting function R of a fraction $\mathcal{F}$ by $n_{\alpha,h} = \sum_{\zeta \in D_h^\alpha} y_\zeta$ Proposition 6 allows us to express the condition X^α *is centered on* $\mathcal{F}$ as integer linear combinations of the values $R(\zeta)$ of the counting function over the full design $\mathcal{D}$. In Sect. 2.3, we will show the use of this property to generate fractional factorial designs.

2.3 Generation of fractions

We use strata to generate fractions that satisfy a given set of constraints on the coefficients of their counting functions. Formally, we give the following definition:

Definition 6 Given $\mathcal{C} \subseteq \mathbb{Z}_{n_1} \times \cdots \times \mathbb{Z}_{n_m}$, a counting function $R = \sum_\alpha c_\alpha X^\alpha$ associated with $\mathcal{F}$ is a $\mathcal{C}$-compatible counting function if $c_\alpha = 0, \quad \forall \alpha \in \mathcal{C}$.

The set of all the fractions of $\mathcal{D}$ whose counting functions are $\mathcal{C}$-compatible is denoted by $OF(n_1 \ldots n_m, \mathcal{C})$.

For example let us consider $OA(n, s^m, t)$, i.e. orthogonal arrays with n rows and m columns where each column has s symbols, s prime and with strength t. Using Proposition 3 the coefficients of the corresponding counting functions must satisfy the conditions $c_\alpha = 0$ for all $\alpha \in \mathcal{C}$ where $\mathcal{C} = \{\alpha \in L \equiv (\mathbb{Z}_s)^m : 0 < \|\alpha\| \leq t\}$ and $\|\alpha\|$ is the number of non-null elements of α. It follows that $OF(s^m, \mathcal{C}) = \bigcup_n OA(n, s^m, t)$. Now using Proposition 6, we can express these conditions using strata. If we consider $\alpha \in \mathcal{C}$, we can write the condition $c_\alpha = 0$ as $\sum^{\zeta \in D_h^\alpha} y_\zeta \equiv n_{\alpha,h} = \lambda, h = 0, \ldots, s-1$ or, equivalently, as

$$\begin{cases} n_{\alpha,0} - n_{\alpha,1} = 0 \\ n_{\alpha,1} - n_{\alpha,2} = 0 \\ \ldots \\ n_{\alpha,s-2} - n_{\alpha,s-1} = 0 \end{cases}.$$

To obtain all the conditions it is enough to vary $\alpha \in \mathcal{C}$. We therefore obtain the homogeneous system of linear equations $AY = \underline{0}$ where A is the $(\#\mathcal{C} \cdot (s-1) \times s^m)$

matrix whose rows contain the values, over $\mathcal{D}$, of the difference between two indicator functions of strata, $1_{D_h^\alpha} - 1_{D_{h+1}^\alpha}$ $h = 0, \ldots, s-2$; Y is the s^m column vector whose entries are the values of the counting function over $\mathcal{D}$; $\underline{0}$ is the $(\#\mathcal{C} \cdot (s-1))$ column vector whose entries are all equal to 0.

We can also write an equivalent homogeneous system if we consider λ as a new variable.

It is now straightforward to verify a well-known result, which is the union of two Orthogonal Arrays, $\mathcal{F}_1 \in OA(n_1, s^m, t)$ with counting function represented by Y_1 and $\mathcal{F}_2 \in OA(n_2, s^m, t)$ with counting function represented by Y_2, is another Orthogonal Array $\mathcal{F}_1 \bigcup \mathcal{F}_2 \in OA(n_1+n_2, s^m, t)$ with counting function represented by $Y_1 + Y_2$.

Let us now consider the general case in which there are no restrictions on the number of levels and show our method for $OA\ (n,\ 4^2,\ 1)$. In this case the number of levels is a power of a prime, $4 = 2^2$. Using Proposition 3 the coefficients of the corresponding counting functions must satisfy the conditions $c_\alpha = 0$ for all $\alpha \in \mathcal{C}$ where $\mathcal{C} = \{\alpha \in L \equiv \mathbb{Z}_4 \times \mathbb{Z}_4 : \|\alpha\| = 1\}$. Let us consider $c_{1,0}$. From Item (4) of Proposition 4, X_1 takes the values in Ω_s where $s = 4$. From Proposition 6, X_1 will be centered on $\mathcal{F}$ if and only if, the remainder $H(\zeta) = P(\zeta) \bmod \Phi_4(\zeta)$ is identically zero. We have $\Phi_4(\zeta) = 1 + \zeta^2$ (see Lang 1965) and so we can compute the remainder $H(\zeta) = n_{(1,0),0} - n_{(1,0),2} + (n_{(1,0),1} - n_{(1,0),3})\zeta$. The condition that $H(\zeta)$ must be identically zero translates into

$$\begin{cases} n_{(1,0),0} - n_{(1,0),2} = 0 \\ n_{(1,0),1} - n_{(1,0),3} = 0 \end{cases} .$$

Let us now consider $c_{2,0}$. From Item (4) of Proposition 4, X_1^2 takes the values in Ω_s where $s = 2$. From Proposition 6, X_1^2 will be centered on $\mathcal{F}$ if and only if

$$n_{(2,0),0} - n_{(2,0),1} = 0.$$

If we repeat the same procedure for all the α such that $\|\alpha\| = 1$ we obtain

$$\begin{cases} n_{(1,0),0} - n_{(1,0),2} = 0 \\ n_{(1,0),1} - n_{(1,0),3} = 0 \\ n_{(2,0),0} - n_{(2,0),1} = 0 \\ n_{(3,0),0} - n_{(3,0),2} = 0 \\ n_{(3,0),1} - n_{(3,0),3} = 0 \\ n_{(0,1),0} - n_{(0,1),2} = 0 \\ n_{(0,1),1} - n_{(0,1),3} = 0 \\ n_{(0,2),0} - n_{(0,2),1} = 0 \\ n_{(0,3),0} - n_{(0,3),2} = 0 \\ n_{(0,3),1} - n_{(0,3),3} = 0 \end{cases} .$$

If we recall that $n_{\alpha,h} = \sum_{\zeta \in D_h^\alpha} y_\zeta$, and so, for example, $n_{(1,0),0} = y_{1,1} + y_{1,\mathrm{i}} + y_{1,-1} + y_{1,-\mathrm{i}}$ with $\mathrm{i} = \sqrt{-1}$, the orthogonal arrays $OA(n, 4^2, 1)$ become the positive integer solutions of the following integer linear homogeneous system:

$$AY = \begin{bmatrix} 1 & 0 & -1 & 0 & 1 & 0 & -1 & 0 & 1 & 0 & -1 & 0 & 1 & 0 & -1 & 0 \\ 0 & 1 & 0 & -1 & 0 & 1 & 0 & -1 & 0 & 1 & 0 & -1 & 0 & 1 & 0 & -1 \\ 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 \\ 1 & 0 & -1 & 0 & 1 & 0 & -1 & 0 & 1 & 0 & -1 & 0 & 1 & 0 & -1 & 0 \\ 0 & -1 & 0 & 1 & 0 & -1 & 0 & 1 & 0 & -1 & 0 & 1 & 0 & -1 & 0 & 1 \\ 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & -1 & -1 & -1 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & -1 & -1 & -1 & -1 \\ 1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 \\ 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & -1 & -1 & -1 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & -1 & -1 & -1 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 \end{bmatrix} \begin{bmatrix} y_{1,1} \\ y_{\mathrm{i},1} \\ y_{-1,1} \\ y_{-\mathrm{i},1} \\ y_{1,\mathrm{i}} \\ y_{\mathrm{i},\mathrm{i}} \\ y_{-1,\mathrm{i}} \\ y_{-\mathrm{i},\mathrm{i}} \\ y_{1,-1} \\ y_{\mathrm{i},-1} \\ y_{-1,-1} \\ y_{-\mathrm{i},-1} \\ y_{1.-\mathrm{i}} \\ y_{\mathrm{i},-\mathrm{i}} \\ y_{-1,-\mathrm{i}} \\ y_{-\mathrm{i},-\mathrm{i}} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}.$$

It should be noted that the matrix A of the coefficients is not full rank, e.g. the first and the fourth rows are equal. This aspect is discussed in Fontana and Pistone (2010b). In any case the solution method used here does not require a reduction to a full rank matrix.

3 The optimization problem

In many practical situations, experimenters are interested in finding minimum size orthogonal fractional designs, i.e. fractional factorial designs that satisfy some orthogonality requirements *and* have the minimum number of points.

According to our formalization, the problem is equivalent to extracting one fraction $\mathcal{F}_*$ from $OF(n_1 \dots n_m, \mathcal{C})$, such that the size of the fraction $\#\mathcal{F}_*$ is minimum.

The problem can be written as

$$\begin{cases} \min \underline{1}^T Y \\ \text{subject to} \\ AY = \underline{0} \end{cases},$$

where A is the matrix built as explained in Sect. 2.3, $\underline{0}$ is the column vector that has the same numer of rows of A and whose entries are all equal to 0, $\underline{1}$ is the $\#\mathcal{D}$ column vector whose entries are all equal to 1, $\underline{1}^T$ is its transpose and Y is a vector of positive integer numbers that contains the unknown counting function values, $Y \neq [0, \dots, 0]$.

4 Computational results

We experimented with our approach in the following cases

1. pure orthogonal arrays: $OA(n, 2^{11}, 2)$;
2. mixed level orthogonal arrays: $OA(n, 2 \cdot 3^7, 2)$;
3. sudoku designs: 9 rows, 9 columns and 9 symbols.

The fractions that are the results of the first two items are mainly used in screening analysis for the identification of significant main effects and cover both the homogeneous and mixed level cases. Sudoku can also be considered as a special design of experiment.

We use lp_solve (Berkelaar et al. 2004), a widely-used and well-known open source (Mixed-Integer) linear programming system. It is based on the revised simplex method and the branch-and-bound method for integers. Solutions provided by the software are of course guaranteed to be global optima. We use a common laptop (Intel Pentium(R) Dual-Core CPU E6500 2.93GHz, RAM 4Gb).

We use the Proc Factex of SAS/QC, see SAS (2010), as a term of comparison. We recall that Proc Factex constructs fractional factorial designs by using Galois fields and has a specific option that allows us to search for minimum size design. The SAS code is in the Appendix. We use SAS On Demand for Academics, by connecting to a SAS-hosted server over the web through an interface (see http://www.sas.com/govedu/edu/programs/od_academics.html for more details). In all three cases the computational time is negligible (<1 s).

4.1 $OA(n, 2^{11}, 2)$

Using Proposition 3 the coefficients of the corresponding counting functions must satisfy the conditions $c_\alpha = 0$ for all $\alpha \in \mathcal{C}$ where $\mathcal{C} = \{\alpha \in L \equiv \mathbb{Z}_2^{11} : 0 < \|\alpha\| \leq 2\}$. The corresponding matrix A has $\left(11 + \binom{11}{2}\right) = 66$ rows and $2^{11} = 2{,}048$ columns. We found a solution that has 12 points and belongs to the class of Plackett Burman designs, (Plackett and Burman 1946). The computational time is around 1 min.

Using Proc Factex we obtain a solution that has 16 runs. The reason for this difference is that Proc Factex searches only for fractions that can be expressed as solutions of a system of *confounding rules*. Given m factors, $A_1, \ldots, A_m$, each with q levels that run from 0 to $q - 1$, a *confounding rule* is

$$r_1 A_1 + \cdots + r_m A_m = 0 ,$$

where $r_i, A_i \in \{0, \ldots, q-1\}$ and the computations are made in $(GF(q))^m$. Further details can be found in SAS (2010).

4.2 $OA(n, 2 \cdot 3^7, 2)$

Using Proposition 3 the coefficients of the corresponding counting functions must satisfy the conditions $c_\alpha = 0$ for all $\alpha \in \mathcal{C}$ where $\mathcal{C} = \{\alpha \in L \equiv \mathbb{Z}_2 \times \mathbb{Z}_3^7 : 0 < \|\alpha\| \leq 2\}$. The corresponding matrix A has 225 rows and $2 \cdot 3^7 = 4,374$ columns. We found a solution that has 18 points and belongs to the well-known class of L_{18} designs, Wu and Hamada (2000). The computational time is around 8 minutes.

Proc Factex does not directly manage mixed level designs. We use the collapsing factors technique, that is, we replace the factor with 2 levels with a factor with 3 levels. We obtain a fraction with 27 run. This fraction does not project onto the $\{1, j\}$-factors, with $j = 2, \ldots, 8$ while orthogonality is retained in the sense that estimates of different effects are uncorrelated, although not all estimates have equal variance, Chakravarti (1956).

4.3 Sudoku designs

In recent years, sudoku has become a very popular game. In its most common form, the objective of the game is to complete a 9×9 grid with the digits from 1 to 9. Each digit must appear once only in each column, each row and each of the nine 3×3 boxes. It is known that sudoku grids are special cases of Latin squares in the class of *gerechte designs*, see Bailey et al. (2008). In Fontana and Rogantin (2010) the connections between sudoku grids and experimental designs are extensively studied in the framework of Algebraic Statistics.

Formally, the sudoku design is a fraction $\mathcal{F}$ of the full factorial design $\mathcal{D}$:

$$\mathcal{D} = R_1 \times R_2 \times C_1 \times C_2 \times S_1 \times S_2 \ ,$$

where each factor is coded with the p-th roots of the unity.

To be a sudoku, $\mathcal{F}$ must meet the game rules:

1. the fraction has p^4 points, i.e. the number of the cells of the grid;
2. (a) all the cells appear exactly once: the projection of $\mathcal{F}$ over the factors R_1, R_2, C_1, C_2 is a full factorial design;
   (b) each symbol appears exactly once in each row: the projection of $\mathcal{F}$ over the factors R_1, R_2, S_1, S_2 is a full factorial design,
   (c) each symbol appears exactly once in each column: the projection of $\mathcal{F}$ over the factors C_1, C_2, S_1, S_2 is a full factorial design,
   (d) each symbol appears exactly once in each box: the projection of $\mathcal{F}$ over the factors R_1, C_1, S_1, S_2 is a full factorial design.

We translate the previous statements into conditions on the coefficients b_α of the indicator polynomial function $F = \sum_{\alpha \in L} b_\alpha X^\alpha, \ L \equiv (\mathbb{Z}_p)^6$ of $\mathcal{F}$ as in the Proposition 12.5 of Fontana and Rogantin (2010).

Proposition 7 (Sudoku fractions) *Let us consider* 6 *factors, each with p levels, p prime. A fraction $\mathcal{F}$ corresponds to a* sudoku fraction *if and only if the coefficients c_α of its counting function satisfy the following conditions:*

1. $b_{000000} = 1/p^2$;
2. *for all* $i_j \in \{0, 1, \ldots, p-1\}$:
   (a) $b_{i_1 i_2 i_3 i_4 00} = 0$ *for* $(i_1, i_2, i_3, i_4) \neq (0, 0, 0, 0)$,
   (b) $b_{i_1 i_2 00 i_5 i_6} = 0$ *for* $(i_1, i_2, i_5, i_6) \neq (0, 0, 0, 0)$,
   (c) $b_{00 i_3 i_4 i_5 i_6} = 0$ *for* $(i_3, i_4, i_5, i_6) \neq (0, 0, 0, 0)$,
   (d) $b_{i_1 0 i_3 0 i_5 i_6} = 0$ *for* $(i_1, i_3, i_5, i_6) \neq (0, 0, 0, 0)$.

As expected, for the special case $p = 3$, we found a solution that has 81 points and that can be arranged in a 9×9 table as seen in newspaper puzzles. This is further evidence that the method does not put any restriction on the type of orthogonality constraints. The computational time is around 1 min.

The use of Proc Factex provides a fraction that has 81 points.

5 Conclusion

The joint use of polynomial counting functions and *strata* makes it possible to write all the orthogonal fractional factorial designs as solutions of a certain system of linear equations. The search for a minimal size OFFD becomes equivalent to an integer linear programming problem where the cost function is the total number of experiments.

It is worth noting that the methodology does not put any restriction either on the number of levels of each factor or on the orthogonality constraints and so it can be applied to a very wide range of designs. The range of applications is limited only by the amount of computational effort required. Finally we observe that the generalisation to any linear cost function is straightforward.

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Appendix

$OA(n, 2^{11}, 2)$

```
proc factex;
factors x1 x2 x3 x4 x5 x6 x7 x8 x9 x10 x11;
size design= minimum ;
model resolution= 3 ;
examine design;
run;
```

$OA(n, 2 \cdot 3^7, 2)$

```
proc factex;
factors x1-x8 / nlev = 3;
size design= minimum;
model resolution=3;
output out=fraction x1 nvals=(-1 1 -1);
run;
proc print data=fraction;
run;
```

Sudoku designs

```
proc factex;
factors x1-x6 / nlev = 3;
size design= minimum;
model estimate =(
x1|x2 x3|x4 x5|x6 x1|x3);
output out=sudoku;
run;
proc print data=sudoku;
run;
```

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