Algebraic Generation of Orthogonal Fractional Factorial Designs

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[Fontana and Pistone(2010)]

Outline

- Aim of the work
- Full factorial design, fractions and counting functions
- Strata
- Generation of fractions
- Concluding remarks

Aim of the work

To find a general method for fractional factorial design generation, where *general* means without any restriction for the number of factors/level

Full factorial design - complex coding of levels

We refer to [Pistone and Rogantin(2008)]

- m factors, $\mathcal{D}_1, \ldots, \mathcal{D}_m$
- $\mathcal{D}_j$ has n_j levels coded with the n_j-th roots of the unity:

$$\mathcal{D}_j = \{\omega_0, \ldots, \omega_{n_j-1}\} \qquad \omega_k = \exp\left(\sqrt{-1}\,\frac{2\pi}{n_j}\;k\right) \equiv \exp\left(\mathrm{i}\,\frac{2\pi}{n_j}\;k\right)\;;$$

- $\mathcal{D}$ is the *full factorial design* with *complex coding*

$$\mathcal{D} = \mathcal{D}_1 \times \cdots \mathcal{D}_j \cdots \times \mathcal{D}_m\;.$$

- $\zeta = (\zeta_1, \ldots, \zeta_m)$ is a point of $\mathcal{D}$
- $\#\mathcal{D}$ is the cardinality of $\mathcal{D}$, $\#\mathcal{D} = \prod_{i=1}^m n_j$

Fractions and Counting functions

- A fraction $\mathcal{F}$ of $\mathcal{D}$ 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 $\mathcal{F}$.

Definition

The *counting function* R of a fraction $\mathcal{F}$ is a response defined on $\mathcal{D}$ so that for each $\zeta \in \mathcal{D}$, $R(\zeta)$ equals the number of appearances of ζ in the fraction. We denote by c_α the coefficients of the representation of R on $\mathcal{D}$ using the monomial basis $\{X^\alpha, \ \alpha \in L = \mathbb{Z}_{n_1} \times \cdots \times \mathbb{Z}_{n_j} \cdots \times \mathbb{Z}_{n_m}\}$:

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

Full factorial design - complex coding of levels

- L is the *full factorial design* with *integer coding*

$$L = \mathbb{Z}_{n_1} \times \cdots \times \mathbb{Z}_{n_j} \cdots \times \mathbb{Z}_{n_m} \ ,$$

- $\alpha = (\alpha_1, \ldots, \alpha_m) \quad \alpha_j = 0, \ldots, n_j - 1, j = 1, \ldots, m$ is an element of L
- X_j is the j-th component function, which maps a point to its i-th component:

$$X_j : \quad \mathcal{D} \ni (\zeta_1, \ldots, \zeta_m) \longmapsto \zeta_j \in \mathcal{D}_j \ ;$$

  the function X_j is called *simple term* or, by abuse of terminology, *factor*.
- X^α is the *interaction term* $X_1^{\alpha_1} \cdots X_m^{\alpha_m}$, i.e. the function

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

Counting functions

Proposition

Let $\mathcal{F}$ be a fraction of a full factorial design $\mathcal{D}$ and $R = \sum_{\alpha \in L} c_\alpha X^\alpha$ be its counting function.

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

Projectivity and Orthogonal Arrays

Definition

A fraction $\mathcal{F}$ *factorially projects* onto the I-factors, $I \subset \{1, \ldots, m\}$, if the projection is a multiple full factorial design, i.e. a full factorial design where each point appears equally often.

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

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

Proposition (Projectivity)

1. *A fraction factorially projects onto the I-factors if, and only if, all the coefficients of the counting function involving only the I-factors are 0.*
2. *A fraction is an orthogonal array of strength t if, and only if, all the coefficients of the counting function up to the order t are zero:*

$$c_\alpha = 0 \quad \textit{for all } \alpha \textit{ of order up to } t, \; \alpha \neq (0, 0, \ldots, 0) \, .$$

Orthogonal array of strength t and indicator functions

- Let $F = \sum_{\alpha \in L} b_\alpha X^\alpha$ an indicator function of a fraction $\mathcal{F}$ of $\mathcal{D}$
- Let $\mathcal{C} = \{\alpha \in L : 0 < \|\alpha\| \leq t\}$;
- F is an indicator function of an Orthogonal Array of strengt t if it is a solution of the following system

$$\begin{cases} b_\alpha = \sum_{\beta \in L} b_\beta b_{[\alpha - \beta]} \\ b_\alpha = 0, \alpha \in \mathcal{C} \end{cases}$$

Remark

F is an indicator function $\Leftrightarrow F(F-1) = 0 \Leftrightarrow b_\alpha = \sum_{\beta \in L} b_\beta b_{[\alpha - \beta]}$

Level set of X^α

Proposition (level set 1)

Let X_j the simple term with level set $\Omega_{n_j} = \{\omega_0, \ldots, \omega_{n_j-1}\}$. Let's consider the term X_j^r and let's define

$$s_{j,r} = \begin{cases} 1 & r = 0 \\ n_j / \gcd(r, n_j) & r > 0 \end{cases}$$

Over $\mathcal{D}$, the term X_j^r takes all the values of $\Omega_{s_{j,r}}$ equally often.

Example

$n_j = 4$, $\mathcal{D}_j = \{\omega_0, \omega_1, \omega_2, \omega_3\} \equiv \{1, \mathrm{i}, -1, -\mathrm{i}\}$

ζ_j	X_j^0	X_j^1	X_j^2	X_j^3
1	1	1	1	1
ω_1	1	ω_1	ω_2	ω_3
ω_2	1	ω_2	1	ω_2
ω_3	1	ω_3	ω_2	ω_1

Level set of X^α

Proposition (level set 2)

Let $X^\alpha = X_1^{\alpha_1} \cdots X_m^{\alpha_m}$ an interaction. $X_i^{\alpha_i}$ takes values in $\Omega_{s_{i,\alpha_i}}$ where s_{i,α_i} is determined according to the previous Proposition "level set 1". Let's define $s_\alpha = \mathrm{lcm}(s_{1,\alpha_1}, \ldots, s_{m,\alpha_m})$. Over $\mathcal{D}$, the term X^α takes all the values of Ω_{s_α} equally often.

Example

$n_j = n_k = 4$, $X_j^2 X_k^2$.

From Proposition "level set 1" we have $s_j = s_k = 2$. We obtain $s = 2$.

Indeed $X_j^2(\zeta_j) \in \{1, -1\}$, $X_k^2(\zeta_k) \in \{1, -1\} \Rightarrow X_j^2 X_k^2(\zeta_j, \zeta_k) \in \{1, -1\}$

Strata

Definition

Given a term $X^\alpha, \alpha \in L = \mathbb{Z}_{n_1} \times \ldots \times \mathbb{Z}_{n_m}$ the full design $\mathcal{D}$ is partitioned into the the following strata

$$D_h^\alpha = \left\{ \zeta \in \mathcal{D} : \overline{X^\alpha(\zeta)} = \omega_h \right\}$$

where $\omega_h \in \Omega_{s_\alpha}$ and s_α is determined according to the previous Propositions "level set 1" and "level set 2".

We use $n_{\alpha,h}$ to denote the number of points of the fraction $\mathcal{F}$ that are in the stratum D_h^α, with $h = 0, \ldots, s_\alpha - 1$,

$$n_{\alpha,h} = \sum_{\zeta \in D_h^\alpha} y_\zeta$$

Counting function as linear combination of indicator functions

Let's consider the indicator functions 1_ζ of all the single points of $\mathcal{D}$

$$1_\zeta : \quad \mathcal{D} \ni (\zeta_1, \ldots, \zeta_m) \mapsto \begin{cases} 1 & \zeta = (\zeta_1, \ldots, \zeta_m) \\ 0 & \zeta \neq (\zeta_1, \ldots, \zeta_m) \end{cases}$$

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 corresponds to $y_\zeta \in \{0, 1\}$.

Proposition

Let $\mathcal{F}$ be a fraction of $\mathcal{D}$. Its counting fraction R can be expressed both as $R = \sum_\alpha c_\alpha X^\alpha$ and $R = \sum_{\zeta \in \mathcal{D}} y_\zeta 1_\zeta$. The relation between the coefficients c_α and y_ζ is

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

c_α and $n_{\alpha,h}$

Proposition

Let $\mathcal{F}$ be a fraction of $\mathcal{D}$ with counting fraction $R = \sum_{\alpha \in L} c_\alpha X^\alpha$. Each $c_\alpha, \alpha \in L$, depends on $n_{\alpha,h}, h = 0, \ldots, s_\alpha - 1$, as

$$c_\alpha = \frac{1}{\#\mathcal{D}} \sum_{h=0}^{s_\alpha - 1} n_{\alpha,h} \omega_h$$

where s_α is determined by X^α (see Proposition "level set 1" and Proposition "level set 2").
Viceversa, each $n_{\alpha,h}, h = 0, \ldots, s_\alpha - 1$, depends on $c_{[-k\alpha]}, k = 0, \ldots, s - 1$ as

$$n_{\alpha,h} = \frac{\#\mathcal{D}}{s_\alpha} \sum_{k=0}^{s_\alpha - 1} c_{[-k\alpha]} \omega_{[hk]}$$

Conditions on $n_{\alpha,h}$ to have X^α centered

Let $\mathcal{F}$ be a fraction of $\mathcal{D}$ with counting fraction
$R = \frac{1}{\#\mathcal{D}} \sum_{\alpha \in L} \sum_{h=0}^{s_\alpha - 1} n_{\alpha,h} \omega_h X^\alpha$.

Proposition (*)

Let X^α be a term with level set Ω_{s_α} on full design $\mathcal{D}$.
s_α is prime The term X^α is centered on the fraction $\mathcal{F}$ if, and only if, its s_α levels appear equally often:

$$n_{\alpha,0} = n_{\alpha,1} = \ldots = n_{\alpha,s-1} = \lambda_\alpha$$

s_α is not prime Let $P_\alpha(\zeta) = \sum_{h=0}^{s_\alpha - 1} n_{\alpha,h} \zeta^h$ and let's denote by Φ_{s_α} the cyclotomic polynomial of the s_α-roots of the unity. The term X^α is centered on the fraction $\mathcal{F}$ if, and only if, the remainder

$$H_\alpha(\zeta) = P_\alpha(\zeta) mod \Phi_{s_\alpha}(\zeta)$$

whose coefficients are integer linear combinations of $n_{\alpha,h}, h = 0, \ldots, s_\alpha - 1$, is identically zero.

Conditions on $R(\zeta)$ to have X^α centered

$n_{\alpha,h}$ are related to the values of the counting function R of a fraction $\mathcal{F}$ by the following relation

$$n_{\alpha,h} = \sum_{\zeta \in D_h^\alpha} y_\zeta ,$$

Proposition "*" allows to express the condition X^α *is centered on* $\mathcal{F}$ ($\Leftrightarrow c_\alpha = 0$) as integer linear combinations of the values y_ζ of the counting function over the full design $\mathcal{D}$.

Orthogonal Arrays

For Orthogonal Arrays, using Proposition "projectivity" we have

$$c_\alpha = 0 \ \forall \alpha \in \mathcal{C}$$

where $\mathcal{C} = \{\alpha \in L : 0 < \|\alpha\| \leq t\}$ and $\|\alpha\|$ is the number of non null elements of α.

$OA(n, s^m, t)$, s prime, as a system of linear equations

Let's consider $OA(n, s^m, t)$, s prime. We consider $\alpha \in \mathcal{C}$ and, using Proposition "*", we write the condition $c_\alpha = 0$ using strata as

$$\begin{cases} \sum_{\zeta \in D_0^\alpha} y_\zeta = \lambda \\ \sum_{\zeta \in D_1^\alpha} y_\zeta = \lambda \\ \ldots \\ \sum_{\zeta \in D_{s-1}^\alpha} y_\zeta = \lambda \end{cases}$$

Varying $\alpha \in \mathcal{C}$ we get

$$AY = \lambda \underline{1}$$

Considering λ as a variable,

$$\tilde{A}\tilde{Y} = 0$$

where $\tilde{A} = [A, -\underline{1}]$ and $\tilde{Y} = (Y, \lambda)$.

Computation of generators for $OA(n, s^m, t)$, s prime

- The sum of two Orthogonal Arrays, $Y_1 \in OA(n_1, s^m, t)$ and $Y_2 \in OA(n_2, s^m, t)$, is an Orthogonal Array $Y_1 + Y_2 \in OA(n_1 + n_2, s^m, t)$.
- The Hilbert Basis [Schrijver(1986)] is a minimal set of generators such that any $OA(n, s^m, t)$ becomes a linear combination of the generators with positive or null integer coefficients.
  - This approach extends that of [Carlini and Pistone(2007)] where homogeneous 2-level fractions were considered and the conditions $c_\alpha = \frac{1}{\#\mathcal{D}} \sum_{\zeta \in \mathcal{F}} \overline{X^\alpha(\zeta)} = 0$ were used.
  - The advantage of using strata is that we avoid computations with complex numbers $(\overline{X^\alpha(\zeta)})$.
  - We give some examples. For the computation we use 4ti2 [4ti2 team(2008)].

Some examples of $OA(n, s^m, t)$, s prime

- Some classes of OA's:

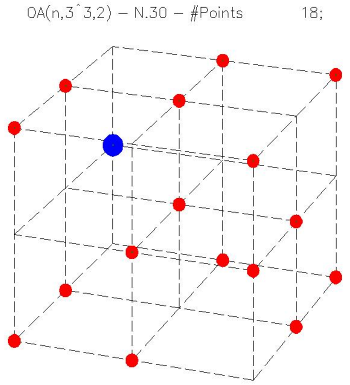
$OA(n, 2^5, 2)$ The matrix $\tilde{A}$ has 30 rows and 33 columns. We find 26, 142 solutions

$OA(n, 3^3, 2)$ The matrix $\tilde{A}$ has has 54 rows and 28 columns. We find 66 solutions:

  - 12 have 9 points, all different
  - 54 have 18 points, 17 different.

$OA(n, 3^4, 3)$ The matrix $\tilde{A}$ has has 192 rows and 82 columns. We find 131, 892 solutions

One example of $OA(18, 3^3, 2)$



Classification of $OA(n, 3^4, 3)$

# support	# of points	max rep	N
27	27	1	24
49	54	2	972
51	54	2	648
52	54	2	648
58	81	3	3,888
59	81	3	8,424
60	108	3	648
60	108	4	5,184
61	81	2	9,072
62	108	3	7,776
62	108	4	5,184
62	135	5	1,296
63	81	2	5,184
63	108	3	15,552
63	135	4	12,960
63	162	5	1,296
64	108	3	15,552
65	135	4	31,104
66	81	2	1,296
66	135	4	5,184
Total			131,892

$OA(n, s_1^{n_1} \cdot \ldots \cdot s_k^{n_k}, t)$ as a system of linear equations

- Let's consider mixed level orthogonal arrays.
  - $OA(n, s^m, t)$, without the condition s prime, become a particular case.
- Using Proposition "*", we express the condition $c_\alpha = 0, \alpha \in \mathcal{C}$ using strata.
- Let's consider, as an example, $OA(n, 2 \cdot 3^3, 3)$.
  - Let's take
    $\alpha \equiv (1,1,0,0) \in \mathcal{C} = \{\alpha \in \mathbb{Z}_2 \times \mathbb{Z}_3 \times \mathbb{Z}_3 \times \mathbb{Z}_3 : 1 \leq \|\alpha\| \leq 3\}$.
  - We get $s_\alpha = 6$. The condition $c_{1,1,0,0} = 0$ is equivalent to $X^{1,1,0,0}$ is centered that is equivalent to $H_\alpha(\zeta) \equiv P_\alpha(\zeta) mod \Phi_6(\zeta)$ is identically zero.
  - We have

$$\begin{aligned} P_\alpha(\zeta) &= n_{(1,1,0,0),0} + n_{(1,1,0,0),1}\zeta + \ldots + n_{(1,1,0,0),5}\zeta^5 \\ \Phi_6(\zeta) &= 1 - \zeta + \zeta^2 \end{aligned}$$

    and therefore

$$\begin{aligned} H_\alpha(\zeta) &\equiv P_\alpha(\zeta) mod \Phi_6(\zeta) \\ &= n_{(1,1,0,0),0} - n_{(1,1,0,0),2} - n_{(1,1,0,0),3} + n_{(1,1,0,0),6} + \\ &\quad (n_{(1,1,0,0),1} + n_{(1,1,0,0),2} - n_{(1,1,0,0),5} - n_{(1,1,0,0),6})\zeta \end{aligned}$$

$OA(n, s_1^{n_1} \cdot \ldots \cdot s_k^{n_k}, t)$ as a system of linear equations

Varying $\alpha \in \mathcal{C}$ and reminding that $n_{\alpha,h} = \sum_{\zeta \in D_h^\alpha} y_\zeta$ we get $\tilde{A}\tilde{Y} = 0$.

- Some classes of OA's:

$OA(n, 2 \cdot 3^3, 3)$ The matrix $\tilde{A}$ has 89 rows and 54 columns. We find 403 solutions

$OA(n, 4^2, 2)$ The matrix $\tilde{A}$ has 10 rows and 16 columns. We find 24 solutions corresponding to all the LHD.

$OA(n, 6^2, 2)$ The matrix $\tilde{A}$ has 18 rows and 36 columns. We find 620 solutions corresponding to all the LHD.

- Classification of $OA(n, 2 \cdot 3^3, 3)$

# support	# of points	max rep	N
36	54	2	24
40	54	2	216
42	54	2	108
46	54	2	54
54	54	1	1
Total			403

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- we have also experimented the algorithm on
  - $OA(9, 3^4; 3)$; we found one solution in $2,895$ iterations;
  - 4×4 sudoku; we found one solution in $2,852$ iterations;
  - 9×9 sudoku; we did not find any solution in $100,000$ iterations;

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- we used $4ti2$ to generate $\mathcal{M}$, the Markov Basis corresponding to the homogeneous system $AX = 0$.
- $\mathcal{M}$ contains 81 different moves;
- as an initial fraction we considered the nine-run regular fraction $\mathcal{F}_0$ whose indicator function R_0 is $R_0 = \frac{1}{3}(1 + X_1X_2X_3 + X_1^2X_2^2X_3^2)$. We run 1.000 simulations generating R_i as $R_i = R_{i-1} + \epsilon_{M_{R_{i-1}}} M_{R_{i-1}}$ (and moving to $\mathcal{F}_i$ if $R_i \geq 0$);

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- we obtained all the 12 different 9-run fractions, each one with 9 different points as known in the literature and as shown previously.

Concluding remarks

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− computational effort

Some references

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Thanks for your attention!

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