Indicator polynomial function for multilevel factorial designs

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The description of fractional factorial designs using the polynomial representations of their indicator functions has been introduced for **binary designs** in

Fontana, R., Pistone, G. and Rogantin, M. P. (2000). Classification of two-level factorial fractions, *J. Statist. Plann. Inference* **87**(1), 149–172.

and generalized to replicates by

Ye, K. Q. (2003). Indicator function and its application in two-level factorial designs, *The Annals of Statistics*. In press.

For a similar approach see also:

Tang, B. and Deng, L. Y. (1999). Minimum G_2-aberration for nonregular fractinal factorial designs, *The Annals of Statistics* **27**(6), 1914–1926.

Here we generalize to **multilevel factorial designs**, representing the *levels of a factor* as the elements of the multiplicative group of *complex roots of unity*, generalizing all the properties already known for binary designs to the case where the numbers of levels are prime numbers.

Complex coding for full factorial designs

Notations:

- m the number of factors
- n_j the number of levels of each factor, $j = 1, \ldots, m$, *with* n_j *a prime number*.

We code the n levels of a factor A with the complex solutions of the equation $\zeta^n = 1$:

$$\omega_k = \exp\left(\mathrm{i}\,\frac{2\pi}{n}k\right) \qquad \text{for } k = 0, \ldots, n-1$$

- $[k]_n$ the residue of $k \mod n$; expecially, for integer h, $(\omega_k)^h = \omega_{[hk]_n}$

The mapping $\mathbb{Z}_n \ni k \leftrightarrow \exp\left(\mathrm{i}\,\frac{2\pi}{n}k\right)$ is a group isomorphism on the multiplicative group of $\mathbb{C}$.

The **full factorial design** $\mathcal{D}$, as a subset of $\mathbb{C}^m$ with $N = \prod_{j=1}^m n_j$ points, is defined by the system of equations

$$\zeta_j^{n_j} - 1 = 0 \qquad \text{for } j = 1, \ldots, m$$

A **fraction** is a subset $\mathcal{F} \subseteq \mathcal{D}$; all the fractions are obtained by adding equations (*generating equations*) to restrict the set of solutions.

Example

$$\begin{bmatrix} \omega_0 & \omega_0 & \omega_0 & \omega_0 \\ \omega_0 & \omega_1 & \omega_1 & \omega_1 \\ \omega_0 & \omega_2 & \omega_2 & \omega_2 \\ \omega_1 & \omega_0 & \omega_1 & \omega_2 \\ \omega_1 & \omega_1 & \omega_2 & \omega_0 \\ \omega_1 & \omega_2 & \omega_0 & \omega_1 \\ \omega_2 & \omega_0 & \omega_2 & \omega_1 \\ \omega_2 & \omega_1 & \omega_0 & \omega_2 \\ \omega_2 & \omega_2 & \omega_1 & \omega_0 \end{bmatrix}$$

The classical 3_{III}^{4-2} regular fraction is defined by

$$\zeta_j^3 - 1 = 0 \qquad \text{for } j = 1, \ldots, 4$$

together with the generating equations

$$\zeta_1\zeta_2\zeta_3 - 1 = 0 \qquad \text{and} \qquad \zeta_1\zeta_2^2\zeta_4 - 1 = 0$$

Such a representation is classically termed "multiplicative" notation. In our approach the equations are defined on the complex field $\mathbb{C}$. The recoding maps between the residue class group $\mathbb{Z}_3$ and the field $\mathbb{C}$.

Responses

A *complex* response f on the design $\mathcal{D}$ is a $\mathbb{C}$-valued function defined on $\mathcal{D}$. It is a restriction to $\mathcal{D}$ of a complex polynomial.

- $L = \left\{\alpha = (\alpha_1, \ldots, \alpha_m) : \alpha_j = 0, \ldots, n_j - 1, j = 1, \ldots, m\right\}$

- X_i the i-th component function, mapping a design point $(\zeta_1, \ldots, \zeta_m)$ into its i-th component ζ_i. Frequently called factor.

- Interaction terms or *monomial responses* X^α with $\alpha = (\alpha_1, \ldots, \alpha_m)$, $\alpha \in L$: $\quad X^\alpha := X_1^{\alpha_1} \cdots X_m^{\alpha_m}$

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

- The term X^α has *order* k if in the m-tuple α there are k non-null values: X^α is an interaction of order k
(in the binary case the order is equal to the degree)

Responses on the design

- Each response f is represented as an unique linear combination of constant, effects, interactions: $f = \sum_{\alpha \in L} \theta_\alpha \, X^\alpha, \quad \theta_\alpha \in \mathbb{C}$

- **Mean value of** f on $\mathcal{D}$, $E_{\mathcal{D}}(f)$: $E_{\mathcal{D}}(f) = \frac{1}{N} \sum_{\zeta \in \mathcal{D}} f(\zeta)$

- A **contrast** is a response f such that $E_{\mathcal{D}}(f) = 0$.

- Two responses f and g are **orthogonal on** $\mathcal{D}$ if $E_{\mathcal{D}}(f \, \overline{g}) = 0$.

The set of all responses is a complex Hilbert space with scalar product

$$< f, g >= E_{\mathcal{D}}(f \ \overline{g})$$

Basic properties connecting the algebra with the Hilbert structure:

1. $X^{\alpha}\overline{X^{\beta}} = X^{[\alpha-\beta]}$, where $[\cdot]$ denotes the modulo operation extended to L;

2. $E_{\mathcal{D}}(X^0) = 1$, and $E_{\mathcal{D}}(X^{\alpha}) = 0$ for $\alpha \neq 0$;

3. $E_{\mathcal{D}}(X^{\alpha}\overline{X^{\beta}}) = E_{\mathcal{D}}(X^{[\alpha-\beta]}) = \begin{cases} 1 & \text{if } \alpha = \beta \\ 0 & \text{if } \alpha \neq \beta \end{cases}$

Responses on the fraction

Algebraic methods allow to find bases of the vectorial space of responses on $\mathcal{F}$.

We denote such bases by $\text{Est}_\tau(\mathcal{F})$, where τ is an ordering on the terms, and by $C(\mathcal{F})$ the set of all (complex) functions identified on $\mathcal{F}$:

$$\text{Est}_\tau(\mathcal{F}) = \left\{X^\beta : \beta \in M\right\} \quad \text{and} \quad \mathbb{C}(\mathcal{F}) = \left\{\sum_{\beta \in M} \theta_\beta X^\beta,\ \theta_\beta \in \mathbb{C}\right\}$$

The vector space $\mathbb{C}(\mathcal{D})$ of the responses on $\mathcal{D}$ can be decomposed into two orthogonal sub-spaces: the space $\mathbb{C}(\mathcal{F})$ of the identifiable responses on $\mathcal{F}$ and the space of the null responses on $\mathcal{F}$, see

Galetto F., Pistone G. and Rogantin M. P. (2003). Confounding revisited with commutative computational algebra, *J. Statist. Plann. Inference* In press.

Indicator function

The *indicator function* F of $\mathcal{F}$ is a particular response such that

$$F(\zeta) = \begin{cases} 1 & \text{if } \zeta \in \mathcal{F} \\ 0 & \text{if } \zeta \in \mathcal{D} \setminus \mathcal{F} \end{cases}$$

A polynomial F is an indicator function of some fraction $\mathcal{F}$ if and only if $F^2 - F = 0$ on $\mathcal{D}$. It is represented as

$$F = \sum_{\alpha \in L} b_\alpha X^\alpha$$

Note that $\bar{b}_\alpha = b_{[-\alpha]}$ because F is real valued.

Mean value of a response f on $\mathcal{F}$

$$E_{\mathcal{F}}(f) = \frac{1}{\#\mathcal{F}} \sum_{\zeta \in \mathcal{F}} f(\zeta) = \frac{1}{\#\mathcal{F}} \sum_{\zeta \in \mathcal{D}} F(\zeta) f(\zeta) = \frac{N}{\#\mathcal{F}} \, E_{\mathcal{D}}(Ff) \quad .$$

If X^α and X^β are simple or interaction terms then:

1. $E_{\mathcal{F}}(\overline{X^\alpha}) = \frac{N}{\#\mathcal{F}} b_\alpha$

2. $E_{\mathcal{F}}(X^\alpha \overline{X^\beta}) = E_{\mathcal{F}}(\overline{X^{[\beta-\alpha]}}) = \frac{N}{\#\mathcal{F}} b_{[\beta-\alpha]}$

Contrasts and orhogonalities on $\mathcal{F}$

- A **contrast on** $\mathcal{F}$ is a response f such that $E_{\mathcal{F}}(f) = 0$.

- Two responses f and g are **orthogonal on** $\mathcal{F}$ if $E_{\mathcal{F}}(f \, \overline{g}) = 0$.

Main results: Orthogonalities

Generalization of Fontana, Pistone, Rogantin (2000) to the case of mixed fractional factorial designs.

Important statistical features of the fraction can be read out from the form of the polynomial representation of the indicator function.

1. *A simple term or an interaction term X^α is a contrast on $\mathcal{F}$ if and only if $b_\alpha = b_{[-\alpha]} = 0$.*

2. *Two simple or interaction terms X^α and X^β are orthogonal on $\mathcal{F}$ if and only if $b_{[\alpha-\beta]} = b_{[\beta-\alpha]} = 0$;*

3. *If X^α is a contrast then, for any β and γ such that $\alpha = [\beta - \gamma]$ or $\alpha = [\gamma - \beta]$, X^β is orthogonal to X^γ.*

Main results: Types of fractions

1. *If $\mathcal{F}$ and $\mathcal{F}'$ are complementary fractions and b_α and b'_α are the coefficients of the respective indicator functions, then $b_\emptyset = 1 - b'_\emptyset$ and $b_\alpha = -b'_\alpha$*

2. *Let $\mathcal{L}$ be the set of indices $\alpha \in L$ such that $b_\alpha \neq 0$ and let $l = \#\mathcal{L}$. Then $\mathcal{F}$ is regular if and only if the non-zero coefficients are of the form: $b_\alpha = \frac{\omega_k}{l}$.*

Regular fractions (proof)

Let $\mathcal{H}$ be a sub-group of L and $\#\mathcal{H} = h$.

Let Ω_n be the set of the roots of the unit: $\Omega_n = \{\omega_1, \ldots, \omega_{n-1}\}$.

Let $e : \mathcal{H} \to \Omega_n$ be a homomorphism: $\quad e([\alpha + \beta]) = e(\alpha)\ e(\beta)$

Let $X^\alpha - e(\alpha),\ \alpha \in \mathcal{H}$, be the system of defining equations of a regular fraction $\mathcal{F}$.

Then $X^\alpha(A) = e(\alpha)$ for all $\alpha \in \mathcal{H}$ if and only if $A \in \mathcal{F}$. That is:

$$\sum_{\alpha \in \mathcal{H}} (X^\alpha(A) - e(\alpha))\, \overline{(X^\alpha(A) - e(\alpha))} = 2\left(h - \sum_{\alpha \in \mathcal{H}} \overline{e(\alpha)}\ X^\alpha(A)\right) = 0 \quad ,$$

$$\frac{1}{h} \sum_{\alpha \in \mathcal{H}} \overline{e(\alpha)}\ X^\alpha(A) - 1 = 0 \quad \text{if and only if} \quad A \in \mathcal{F}$$

The function $G = \frac{1}{h} \sum_{\alpha \in \mathcal{H}} e(\alpha)\ X^\alpha$ is an indicator function, because $G = G^2$ on $\mathcal{D}$.

In fact e is a homomorphism and:

$$G^2 = \frac{1}{h^2} \sum_{\alpha \in \mathcal{H}} \sum_{\beta \in \mathcal{H}} \overline{e(\alpha)\ e(\beta)}\, X^{[\alpha+\beta]} = \frac{1}{h^2} \sum_{\alpha \in \mathcal{H}} \sum_{\beta \in \mathcal{H}} \overline{e([\alpha + \beta])}\, X^{[\alpha+\beta]} = \frac{1}{h^2} \sum_{\gamma \in \mathcal{H}} h\, \overline{e(\gamma)}\, X^\gamma = G.$$

Then G is the indicator function of $\mathcal{F}$, $\mathcal{H}$ equals to $\mathcal{L}$ and $b_\alpha = \frac{\overline{e(\alpha)}}{l}$, for all $\alpha \in \mathcal{H}$.

Viceversa, let

$$F = \frac{1}{l} \sum_{\alpha \in \mathcal{L}} \overline{e(\alpha)}\ X^{\alpha}$$

be the indicator function of $\mathcal{F}$. We have

$$\sum_{\alpha \in \mathcal{L}} (X^{\alpha} - e(\alpha))\, \overline{(X^{\alpha} - e(\alpha))} = 2l \left(1 - \frac{1}{l} \sum_{\alpha \in \mathcal{L}} \overline{e(\alpha)} X^{\alpha} \right) = \begin{cases} 0 & \text{on } \mathcal{F} \\ 2\ l & \text{on } \mathcal{D} \setminus \mathcal{F} \end{cases} .$$

In conclusion $X^{\alpha} = e(\alpha)$, $\alpha \in \mathcal{L}$, is the set of the defining equations of $\mathcal{F}$.

The set $\mathcal{L}$ is closed for $[.]_n$; in fact if $\alpha, \beta \in \mathcal{L}$, then $X^{[\alpha+\beta]} = e(\alpha)e(\beta) = e([\alpha+\beta])$ and the correspondent coefficient $b_{[\alpha+\beta]}$ must be equal to $\frac{1}{l}\ e([\alpha+\beta])$.

Example

We consider as example the classical 3_{III}^{4-2} fraction, considered before. Its indicator function is:

$$F = \frac{1}{9}\Big(1 + X_2X_3X_4 + X_2^2X_3^2X_4^2 + X_1X_2X_3^2 + X^2X_2^2X_3 + X_1X_2^2X_4 + X^2X_2X_4^2 + X_1X_3X_4^2 + X^2X_3^2X_4\Big)$$

We check that it is a regular fraction.

Generation of fractions

The following result shows how to derive algebraic equations describing the indicator function of a fraction with a given statistical properties.

The coefficients b_α of the indicator function of $\mathcal{F}$ are related according to:

$$b_\alpha = \sum_{[\beta+\gamma]=\alpha} b_\beta \; b_\gamma$$

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