

ALGEBRAIC METHOD ON EXPERIMENTAL DESIGN
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HILBERT BASIS IN DESIGN AND LOGLINEAR
MODELS

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1. HILBERT BASES OF ORTHOGONAL DESIGNS

Consider three binary variables X_1, X_2, X_3 with levels $+1, -1$. The table of interactions is

	000	001	010	011	100	101	110	111
+++	1	1	1	1	1	1	1	1
++-	1	-1	1	-1	1	-1	1	-1
+ - +	1	1	-1	-1	1	1	-1	-1
+ - -	1	-1	-1	1	1	-1	-1	1
- + +	1	1	1	1	-1	-1	-1	-1
- + -	1	-1	1	-1	-1	1	-1	1
- - +	1	1	-1	-1	-1	-1	1	1
- - -	1	-1	-1	1	-1	1	1	-1

The matrix K excluding the constant and the 3-way interaction is

$$(1) \quad K = \begin{array}{c} \begin{array}{ccccccc} & & 001 & 010 & 011 & 100 & 101 & 110 \\ +++ & & 1 & 1 & 1 & 1 & 1 & 1 \\ ++- & & -1 & 1 & -1 & 1 & -1 & 1 \\ + - + & & 1 & -1 & -1 & 1 & 1 & -1 \\ + - - & & -1 & -1 & 1 & 1 & -1 & -1 \\ - + + & & 1 & 1 & 1 & -1 & -1 & -1 \\ - + - & & -1 & 1 & -1 & -1 & 1 & -1 \\ - - + & & 1 & -1 & -1 & -1 & -1 & 1 \\ - - - & & -1 & -1 & 1 & -1 & 1 & 1 \end{array} \end{array}$$

Consider the lattice

$$OA_{3,2} = \ker(K^t) \cap \mathbb{Z}_{\geq}^{2^3}$$

Each element of $OA_{3,2}$ is the counting function of an orthogonal array.

The lattice has a basis whose elements are the rows of the matrix

$$H = \begin{bmatrix} 1 & 0 & 0 & 1 & 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 & 1 & 0 & 0 & 1 \end{bmatrix}$$

1

i.e. the two fractions 2^{3-1} which are generated by $x_1x_2x_3 = \pm 1$.

This has been done up to five factors in [2] to provide a full classification of orthogonal designs. Computations with six or more factors were unfeasible on 4ti2 [1].

2. HILBERT BASES IN LATTICE EXPONENTIAL FAMILIES

Consider the exponential family on $\mathcal{X} = \{+1, -1\}^3$ with unnormalized density

$$(2) \quad q(x; \theta) = \exp(\theta x_1 x_2 x_3)$$

The model matrix is given by the 3-way interaction

$$A = [1 - 1 - 1 + 1 - 1 + 1 + 1 - 1]^t$$

The matrix K is the basis of the lattice $\text{span}(A) \cap \mathbb{Z}_{\geq}^{2^3} = OA_{3,2}$. Note that K is boolean.

It follows from [3], [7], [6] that the matrix K describes the limits of the exponential family (2) as $\theta \rightarrow \pm\infty$.

3. COMPUTER EXPERIMENTS

Viceversa, the statement about the border of an exponential family could be re-phrased by saying the the exponential family (2) is a *relaxation* or continuous interpolation of the two fractional designs 2^{3-1} .

The unnormalized densities of the exponential family (2) satisfy all the binomial equations derived from from the matrix K in (1). Moreover, at least on this example,

$$\mathbb{E}_{\theta}(X_i) = 0, \quad i = 1, 2, 3.$$

The (continuous) sampling of the exponential family has properties similar to the sampling on the orthogonal fractions.

This suggest the use of the relaxation form of the orthonormal fractions in computer experiments:

- (1) The sampling with fractional factorial is considered inappropriate in computer experiments and could be replaced by Gibbs sampling of the relaxation family.
- (2) Given any function $f : \mathcal{X} \rightarrow \mathbb{R}$ any algorithm of gradient descent on the function $\theta \mapsto \mathbb{E}_{\theta}(f)$ will approach the border of the relaxation family and eventually sample from an orthogonal array with high probability. Such algorithms are discussed e.g. in [4], [5]

This is a joint project with Henry Wynn.

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