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A Description of Experimental Design on the Basis of an Orthonormal System

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1. Introduction

The Fourier series representation of a function is a classic representation which is widely used to approximate real functions (Stein & Shakarchi, 2003). In digital signal processing (Oppenheim & Schaffer, 1975), the sampling theorem states that any real valued function f can be reconstructed from a sequence of values of f that are discretely sampled with a frequency at least twice as high as the maximum frequency of the spectrum of f . This theorem can also be applied to functions over finite domains (Stankovic & Astola, 2007; Takimoto & Maruoka, 1997). Then, the range of frequencies of f can be expressed in more detail by using a bounded set instead of the maximum frequency. A function whose range of frequencies is confined to a bounded set I is referred to as "bandlimited to I ". Ukita et al. obtained a sampling theorem for bandlimited functions over Boolean (Ukita et al., 2003) and $GF(q)^n$ domains (Ukita et al., 2010a), where q is a prime power and $GF(q)$ is Galois field of order q . The sampling theorem can be applied in various fields as well as in digital signal processing, and one of the fields is the experimental design.

In most areas of scientific research, experimentation is a major tool for acquiring new knowledge or a better understanding of the target phenomenon. Experiments usually aim to study how changes in various factors affect the response variable of interest (Cochran & Cox, 1992; Toutenburg & Shalabh, 2009). Since the model used most often at present in experimental design is expressed through the effect of each factor, it is easy to understand how each factor affects the response variable. However, since the model contains redundant parameters and is not expressed in terms of an orthonormal system, a considerable amount of time is often necessary to implement the procedure for estimating the effects.

In this chapter, we propose that the model of experimental design be expressed as an orthonormal system, and show that the model contains no redundant parameters. Then, the model is expressed by using Fourier coefficients instead of the effect of each factor. As there is an abundance of software for calculating the Fourier transform, such a system allows for a straightforward implementation of the procedures for estimating the Fourier coefficients by using Fourier transform. In addition, the effect of each factor can be easily obtained from the Fourier coefficients (Ukita & Matsushima, 2011). Therefore, it is possible to implement easily the estimation procedures as well as to understand how each factor affects the response variable in a model based on an orthonormal system. Moreover, the analysis of variance can also be performed in a model based on an orthonormal system (Ukita et al., 2010b). Hence,

it is clear that two main procedures in the experimental design, that is, the estimation of the effects and the analysis of variance can be executed in a description of experimental design on the basis of an orthonormal system.

This chapter is organized as follows. In Section 2, we give preliminaries that are necessary for this study. In Section 3, we provide an introduction to experimental design and describe the characteristic of the previous model in experimental design. In Section 4, we propose the new model of experimental design on the basis of an orthonormal system and clarify the characteristic of the model. Finally, Section 5 concludes this chapter.

2. Preliminaries

2.1 Fourier analysis on finite Abelian groups

Here, we provide a brief explanation of Fourier analysis on finite Abelian groups. Characters are important in the context of finite Fourier series.

2.1.1 Characters

Let G be a finite Abelian group (with additive notation), and let S^1 be the unit circle in the complex plane. A character on G is a complex-valued function $\chi : G \rightarrow S^1$ that satisfies the condition

$$\chi(x + x') = \chi(x)\chi(x') \quad \forall x, x' \in G. \quad (1)$$

In other words, a character is a homomorphism from G to the circle group.

2.1.2 Fourier transform

Let $G_i, i = 1, 2, \dots, n$, be Abelian groups of respective orders $|G_i| = g_i, i = 1, 2, \dots, n, g_1 \leq g_2 \leq \dots \leq g_n$, and let

$$G = \times_{i=1}^n G_i \quad \text{and} \quad g = \prod_{i=1}^n g_i. \quad (2)$$

Since the character group of G is isomorphic to G , we can index the characters by the elements of G , that is, $\{\chi_a(x) | a \in G\}$ are the characters of G . Note that $\chi_0(x)$ is the principal character and identically equal to 1. The characters $\{\chi_a(x) | a \in G\}$ form an orthonormal system:

$$\frac{1}{g} \sum_{x \in G} \chi_a(x) \chi_b^*(x) = \begin{cases} 1, & a = b, \\ 0, & a \neq b, \end{cases} \quad (3)$$

where $\chi_b^*(x)$ is the complex conjugate of $\chi_b(x)$.

Any function $f : G \rightarrow \mathbb{C}$, where \mathbb{C} is the field of complex numbers, can be uniquely expressed as a linear combination of the following characters:

$$f(x) = \sum_{a \in G} f_a \chi_a(x), \quad (4)$$

where the complex number

$$f_a = \frac{1}{g} \sum_{x \in G} f(x) \chi_a^*(x) \quad (5)$$

is the a -th Fourier coefficient of f .

2.2 Fourier analysis on $GF(q)^n$

Assume that q is a prime power. Let $GF(q)$ be a Galois field of order q which contains a finite number of elements. We also use $GF(q)^n$ to denote the set of all n -tuples with entries from $GF(q)$. The elements of $GF(q)^n$ are referred to as vectors.

Example 1. Consider $GF(3) = \{0, 1, 2\}$. Addition and multiplication are defined as follows:

+	0	1	2
0	0	1	2
1	1	2	0
2	2	0	1

·	0	1	2
0	0	0	0
1	0	1	2
2	0	2	1

Moreover, consider $n = 5$.

$$GF(3)^5 = \{00000, 10000, \dots, 22222\}, \quad (6)$$

and $|GF(3)^5| = 243$. □

Specifying the group G in Section 2.1.2 to be the support group of $GF(q)^n$ and $g = q^n$, the relations (3), (4) and (5) also hold over the $GF(q)^n$ domain.

3. Experimental design

In this section, we provide a short introduction to experimental design.

3.1 Model in experimental design

Let F_1, F_2, \dots, F_n denote n factors to be included in an experiment. The levels of each factor can be represented by $GF(q)$, and the combinations of levels can be represented by the n -tuples $\mathbf{x} = (x_1, x_2, \dots, x_n) \in GF(q)^n$.

Example 2. Let Machine (F_1) and Worker (F_2) be factors that might influence the total amount of the product. Assume each factor has two levels.

F_1 : new machine (level 0), old machine (level 1).

F_2 : skilled worker (level 0), unskilled worker (level 1).

For example, $\mathbf{x} = 01$ represents a combination of new machine and unskilled worker.

Then, the effect of the machine, averaged over both workers, is referred to as the effect of main factor F_1 . Similarly, the effect of the worker, averaged over both machines, is referred to as the effect of main factor F_2 . The difference between the effect of the machine for an unskilled worker and that for a skilled worker is referred to as the effect of the interaction of F_1 and F_2 . □

Let the set $A \subseteq \{0, 1\}^n$ represent all factors that might influence the response of an experiment. The Hamming weight $w(\mathbf{a})$ of a vector $\mathbf{a} = (a_1, a_2, \dots, a_n) \in A$ is defined as the number of nonzero components. The main factors are represented by $MF = \{l | a_l = 1, \mathbf{a} \in A_1\}$, where $A_1 = \{\mathbf{a} | w(\mathbf{a}) = 1, \mathbf{a} \in A\}$. The interactive factors are represented by $IF = \{l, m | a_l = 1, a_m = 1, \mathbf{a} \in A_2\}$, where $A_2 = \{\mathbf{a} | w(\mathbf{a}) = 2, \mathbf{a} \in A\}$.

Example 3. Consider $A = \{000, 100, 010, 001, 110\}$. Then, $A_1 = \{100, 010, 001\}$ and $MF = \{1, 2, 3\}$, $A_2 = \{110\}$ and $IF = \{1, 2\}$.

For example, $1 \in MF$ indicates the main factor F_1 , and $\{1, 2\} \in IF$ indicates the interactive factors F_1 and F_2 . □

It is usually assumed that the set A satisfies the following monotonicity condition (Okuno & Haga, 1969).

Definition 1. *Monotonicity*

$$a \in A \rightarrow b \in A \quad \forall b (b \sqsubseteq a), \quad (7)$$

where $(b_1, b_2, \dots, b_n) \sqsubseteq (a_1, a_2, \dots, a_n)$ indicates that if $a_i = 0$ then $b_i = 0, i = 1, 2, \dots, n$. \square

Example 4. Consider $A = \{00000, 10000, 01000, 00100, 00010, 00001, 11000, 10100, 10010\}$.

Since the set A satisfies (7), A is monotonic. \square

Let $y(x)$ denote the response of the experiment with level combination x . Assume the model

$$y(x) = \mu + \sum_{l \in MF} \alpha_l(x_l) + \sum_{\{l,m\} \in IF} \beta_{l,m}(x_l, x_m) + \epsilon_x, \quad (8)$$

where μ is the general mean, $\alpha_l(x_l)$ is the effect of the x_l -th level of Factor F_l , $\beta_{l,m}(x_l, x_m)$ is the effect of the interaction of the x_l -th level of Factor F_l and the x_m -th level of Factor F_m and ϵ_x is a random error with a zero mean and a constant variance σ^2 .

Since the model is expressed through the effect of each factor, it is easy to understand how each factor affects the response variable. However, because the constraints

$$\sum_{\varphi=0}^{q-1} \alpha_l(\varphi) = 0, \quad (9)$$

$$\sum_{\varphi=0}^{q-1} \beta_{l,m}(\varphi, \psi) = 0, \quad (10)$$

$$\sum_{\psi=0}^{q-1} \beta_{l,m}(\varphi, \psi) = 0, \quad (11)$$

are assumed, the model contains redundant parameters.

Example 5. Consider $q = 3, n = 5$ and $A = \{00000, 10000, 01000, 00100, 00010, 00001, 11000, 10100, 10010\}$. Then,

$\mu, \alpha_1(0), \alpha_1(1), \alpha_1(2), \alpha_2(0), \alpha_2(1), \alpha_2(2), \alpha_3(0), \alpha_3(1), \alpha_3(2), \alpha_4(0), \alpha_4(1), \alpha_4(2), \alpha_5(0), \alpha_5(1), \alpha_5(2), \beta_{1,2}(0,0), \beta_{1,2}(0,1), \beta_{1,2}(0,2), \beta_{1,2}(1,0), \beta_{1,2}(1,1), \beta_{1,2}(1,2), \beta_{1,2}(2,0), \beta_{1,2}(2,1), \beta_{1,2}(2,2), \beta_{1,3}(0,0), \beta_{1,3}(0,1), \beta_{1,3}(0,2), \beta_{1,3}(1,0), \beta_{1,3}(1,1), \beta_{1,3}(1,2), \beta_{1,3}(2,0), \beta_{1,3}(2,1), \beta_{1,3}(2,2), \beta_{1,4}(0,0), \beta_{1,4}(0,1), \beta_{1,4}(0,2), \beta_{1,4}(1,0), \beta_{1,4}(1,1), \beta_{1,4}(1,2), \beta_{1,4}(2,0), \beta_{1,4}(2,1), \beta_{1,4}(2,2)$

are parameters. The number of parameters is 43, but the number of the independent parameters is 23 by the constraints. \square

In experimental design, we are presented with a model of an experiment, which consists of a set $A \subseteq \{0, 1\}^n$. First, we determine a set of level combinations $x \in X, X \subseteq GF(q)^n$. The set X is referred to as a design. Then, we perform a set of experiments in accordance to the design X and estimate the effects from the obtained results $\{(x, y(x)) | x \in X\}$.

An important standard for evaluating experimental design is the maximum of the variances of the unbiased estimators of effects, as calculated from the results of the conducted experiments. It is known that, for a given number of experiments, this criterion is minimized when using orthogonal design (Takahashi, 1979). Hence, there has been extensive research focusing on orthogonal design (Hedayat et al., 1999; Takahashi, 1979; Ukita et al., 2003; 2010a,b; Ukita & Matsushima, 2011).

3.2 Orthogonal design

Definition 2. (*Orthogonal design*)

Define $v(\mathbf{a}) = \{i | a_i \neq 0, 1 \leq i \leq n\}$. For $A \subseteq \{0, 1\}^n$, let H_A be the $k \times n$ matrix

$$H_A = \begin{bmatrix} h_{11} & h_{12} & \dots & h_{1n} \\ h_{21} & h_{22} & \dots & h_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ h_{k1} & h_{k2} & \dots & h_{kn} \end{bmatrix}. \quad (12)$$

The components of this matrix, $h_{ij} \in GF(q)$ ($1 \leq i \leq k, 1 \leq j \leq n$), satisfy the following conditions.

1. The set $\{\mathbf{h}_{\cdot j} | j \in v(\mathbf{a}' + \mathbf{a}'')\}^1$, where $\mathbf{h}_{\cdot j}$ is the j -th column of H_A , is linearly independent over $GF(q)$ for any given $\mathbf{a}', \mathbf{a}'' \in A$.
2. The set $\{\mathbf{h}_i | 1 \leq i \leq k\}$, where \mathbf{h}_i is the i -th row of H_A , is linearly independent over $GF(q)$.

An orthogonal design C^\perp for main and interactive factors $A \subseteq \{0, 1\}^n$ is defined as

$$C^\perp = \{\mathbf{x} | \mathbf{x} = \mathbf{r}H_A, \mathbf{r} \in GF(q)^k\}, \quad (13)$$

and $|C^\perp| = q^k$. □

Example 6. We consider the case $q = 3, n = 5$ and

$$A = \{00000, 10000, 01000, 00100, 00010, 00001, 11000, 10100, 10010\}. \quad (14)$$

In this case,

$$H_A = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 & 2 \end{bmatrix}, \quad (15)$$

satisfies the conditions in Definition 2. Therefore,

$$C^\perp = \{00000, 00112, 00221, 01011, 01120, 01202, 02022, 02101, 02210, 10000, 10112, \\ 10221, 11011, 11120, 11202, 12022, 12101, 12210, 20000, 20111, 20221, 21011, \\ 21120, 21202, 22022, 22101, 22210\},$$

is an orthogonal design for A . □

Many algorithms for constructing H_A have been proposed (Hedayat et al., 1999; MacWilliams & Sloane, 1977; Takahashi, 1979; Ukita et al., 2003). However, it is still an extremely difficult problem to construct H_A when the number of factors n is large and a large number of interactions are included in the model. In this regard, algorithms for the construction of orthogonal design are not presented here since this falls outside the scope of this chapter.

¹ For $\mathbf{a}_1 = (a_{11}, a_{12}, \dots, a_{1n}), \mathbf{a}_2 = (a_{21}, a_{22}, \dots, a_{2n}) \in \{0, 1\}^n$, the addition of vectors \mathbf{a}_1 and \mathbf{a}_2 is defined as $\mathbf{a}_1 + \mathbf{a}_2 = (a_{11} \oplus a_{21}, a_{12} \oplus a_{22}, \dots, a_{1n} \oplus a_{2n})$, where \oplus is the exclusive OR operator.

3.3 Estimation of effects in experimental design

First, we adopt the following definitions.

$$Y = \sum_{x \in C^\perp} y(x), \tag{16}$$

where $|C^\perp| = q^k$.

$$Y_l(\varphi) = \sum_{x \in C_l^\perp(\varphi)} y(x), \tag{17}$$

where $C_l^\perp(\varphi) = \{x|x_l = \varphi, x \in C^\perp\}$ and $|C_l^\perp(\varphi)| = q^{k-1}$.

$$Y_{l,m}(\varphi, \psi) = \sum_{x \in C_{l,m}^\perp(\varphi, \psi)} y(x), \tag{18}$$

where $C_{l,m}^\perp(\varphi, \psi) = \{x|x_l = \varphi, x_m = \psi, x \in C^\perp\}$ and $|C_{l,m}^\perp(\varphi, \psi)| = q^{k-2}$.

Let $\bar{y} = \frac{1}{q^k} Y, \bar{y}_l(\varphi) = \frac{1}{q^{k-1}} Y_l(\varphi), \bar{y}_{l,m}(\varphi, \psi) = \frac{1}{q^{k-2}} Y_{l,m}(\varphi, \psi)$. Then, the unbiased estimators of the parameters in (8) are given as

$$\hat{\mu} = \bar{y}, \tag{19}$$

$$\hat{\alpha}_l(\varphi) = \bar{y}_l(\varphi) - \hat{\mu}, \tag{20}$$

$$\hat{\beta}_{l,m}(\varphi, \psi) = \bar{y}_{l,m}(\varphi, \psi) - \hat{\alpha}_l(\varphi) - \hat{\alpha}_m(\psi) - \hat{\mu}. \tag{21}$$

Example 7. Consider the case that a set A is given by (14) and the result of experiments is given by Table 1.

x	$y(x)$	x	$y(x)$	x	$y(x)$
00000	93	10000	99	20000	87
00112	97	10112	109	20111	86
00221	98	10221	112	20221	90
01011	90	11011	102	21011	85
01120	96	11120	111	21120	82
01202	102	11202	111	21202	94
02022	97	12022	105	22022	84
02101	95	12101	104	22101	88
02210	95	12210	101	22210	83

Table 1. Result of experiments

First, using (16)–(18),

$$\begin{aligned} Y &= 2596, & Y_1(0) &= 863, & Y_1(1) &= 954, & Y_1(2) &= 779, \\ Y_2(0) &= 871, & Y_2(1) &= 873, & Y_2(2) &= 852, & Y_3(0) &= 842, \\ Y_3(1) &= 868, & Y_3(2) &= 886, & Y_4(0) &= 873, & Y_4(1) &= 848, \\ Y_4(2) &= 875, & Y_5(0) &= 847, & Y_5(1) &= 864, & Y_5(2) &= 885, \\ Y_{1,2}(0,0) &= 288, & Y_{1,2}(0,1) &= 288, & Y_{1,2}(0,2) &= 287, & Y_{1,2}(1,0) &= 320, \\ Y_{1,2}(1,1) &= 324, & Y_{1,2}(1,2) &= 310, & Y_{1,2}(2,0) &= 263, & Y_{1,2}(2,1) &= 261, \\ Y_{1,2}(2,2) &= 255, & Y_{1,3}(0,0) &= 280, & Y_{1,3}(0,1) &= 288, & Y_{1,3}(0,2) &= 295, \\ Y_{1,3}(1,0) &= 306, & Y_{1,3}(1,1) &= 324, & Y_{1,3}(1,2) &= 324, & Y_{1,3}(2,0) &= 256, \\ Y_{1,3}(2,1) &= 256, & Y_{1,3}(2,2) &= 267, & Y_{1,4}(0,0) &= 290, & Y_{1,4}(0,1) &= 282, \\ Y_{1,4}(0,2) &= 291, & Y_{1,4}(1,0) &= 314, & Y_{1,4}(1,1) &= 312, & Y_{1,4}(1,2) &= 328, \\ Y_{1,4}(2,0) &= 269, & Y_{1,4}(2,1) &= 254, & Y_{1,4}(2,2) &= 256. \end{aligned}$$

Next, the following values are obtained.

$$\begin{aligned}
 \bar{y} &= 96.15, & \bar{y}_1(0) &= 95.89, & \bar{y}_1(1) &= 106.00, & \bar{y}_1(2) &= 86.56, \\
 \bar{y}_2(0) &= 96.78, & \bar{y}_2(1) &= 97.00, & \bar{y}_2(2) &= 94.67, & \bar{y}_3(0) &= 93.56, \\
 \bar{y}_3(1) &= 96.44, & \bar{y}_3(2) &= 98.44, & \bar{y}_4(0) &= 97.00, & \bar{y}_4(1) &= 94.22, \\
 \bar{y}_4(2) &= 97.22, & \bar{y}_5(0) &= 94.11, & \bar{y}_5(1) &= 96.00, & \bar{y}_5(2) &= 98.33, \\
 \bar{y}_{1,2}(0,0) &= 96.00, & \bar{y}_{1,2}(0,1) &= 96.00, & \bar{y}_{1,2}(0,2) &= 95.67, & \bar{y}_{1,2}(1,0) &= 106.67, \\
 \bar{y}_{1,2}(1,1) &= 108.00, & \bar{y}_{1,2}(1,2) &= 103.33, & \bar{y}_{1,2}(2,0) &= 87.67, & \bar{y}_{1,2}(2,1) &= 87.00, \\
 \bar{y}_{1,2}(2,2) &= 85.00, & \bar{y}_{1,3}(0,0) &= 93.33, & \bar{y}_{1,3}(0,1) &= 96.00, & \bar{y}_{1,3}(0,2) &= 98.33, \\
 \bar{y}_{1,3}(1,0) &= 102.00, & \bar{y}_{1,3}(1,1) &= 108.00, & \bar{y}_{1,3}(1,2) &= 108.00, & \bar{y}_{1,3}(2,0) &= 85.33, \\
 \bar{y}_{1,3}(2,1) &= 85.33, & \bar{y}_{1,3}(2,2) &= 89.00, & \bar{y}_{1,4}(0,0) &= 96.67, & \bar{y}_{1,4}(0,1) &= 94.00, \\
 \bar{y}_{1,4}(0,2) &= 97.00, & \bar{y}_{1,4}(1,0) &= 104.67, & \bar{y}_{1,4}(1,1) &= 104.00, & \bar{y}_{1,4}(1,2) &= 109.33, \\
 \bar{y}_{1,4}(2,0) &= 89.67, & \bar{y}_{1,4}(2,1) &= 84.67, & \bar{y}_{1,4}(2,2) &= 85.33.
 \end{aligned}$$

Last, by using (19)–(21),

$$\begin{aligned}
 \hat{\mu} &= 96.15, & \hat{\alpha}_1(0) &= -0.26, & \hat{\alpha}_1(1) &= 9.85, & \hat{\alpha}_1(2) &= -9.59, \\
 \hat{\alpha}_2(0) &= 0.63, & \hat{\alpha}_2(1) &= 0.85, & \hat{\alpha}_2(2) &= -1.48, & \hat{\alpha}_3(0) &= -2.59, \\
 \hat{\alpha}_3(1) &= 0.30, & \hat{\alpha}_3(2) &= 2.30, & \hat{\alpha}_4(0) &= 0.85, & \hat{\alpha}_4(1) &= -1.93, \\
 \hat{\alpha}_4(2) &= 1.07, & \hat{\alpha}_5(0) &= -2.04, & \hat{\alpha}_5(1) &= -0.15, & \hat{\alpha}_5(2) &= 2.19, \\
 \hat{\beta}_{1,2}(0,0) &= -0.52, & \hat{\beta}_{1,2}(0,1) &= -0.74, & \hat{\beta}_{1,2}(0,2) &= 1.26, & \hat{\beta}_{1,2}(1,0) &= 0.04, \\
 \hat{\beta}_{1,2}(1,1) &= 1.15, & \hat{\beta}_{1,2}(1,2) &= -1.19, & \hat{\beta}_{1,2}(2,0) &= 0.48, & \hat{\beta}_{1,2}(2,1) &= -0.41, \\
 \hat{\beta}_{1,2}(2,2) &= -0.07, & \hat{\beta}_{1,3}(0,0) &= 0.04, & \hat{\beta}_{1,3}(0,1) &= -0.19, & \hat{\beta}_{1,3}(0,2) &= 0.15, \\
 \hat{\beta}_{1,3}(1,0) &= -1.41, & \hat{\beta}_{1,3}(1,1) &= 1.70, & \hat{\beta}_{1,3}(1,2) &= -0.30, & \hat{\beta}_{1,3}(2,0) &= 1.37, \\
 \hat{\beta}_{1,3}(2,1) &= -1.52, & \hat{\beta}_{1,3}(2,2) &= 0.15, & \hat{\beta}_{1,4}(0,0) &= -0.07, & \hat{\beta}_{1,4}(0,1) &= 0.04, \\
 \hat{\beta}_{1,4}(0,2) &= 0.04, & \hat{\beta}_{1,4}(1,0) &= -2.19, & \hat{\beta}_{1,4}(1,1) &= -0.07, & \hat{\beta}_{1,4}(1,2) &= 2.26, \\
 \hat{\beta}_{1,4}(2,0) &= 2.26, & \hat{\beta}_{1,4}(2,1) &= 0.04, & \hat{\beta}_{1,4}(2,2) &= -2.30.
 \end{aligned}$$

□

Although there are software packages that can be used to estimate the effects on the basis of (19)–(21), as yet no software can be used for an arbitrary monotonic set A . Therefore, it is often necessary to implement the procedure for estimating the effects, which requires a considerable amount of time.

3.4 Analysis of variance

When there are many factors, a comprehensive view of whether an interaction in A can be disregarded is needed. The test procedure involves an analysis of variance. For a detailed explanation of analysis of variance, refer to (Toutenburg & Shalabh, 2009).

The statistics needed in analysis of variance are the following. SS_{Mean} is the correction term (the sum of squares due to the mean), SS_{F_l} is the sum of squares due to the effect of F_l , $SS_{F_l \times F_m}$ is the sum of squares due to the interaction effect of $F_l \times F_m$, and SS_{Error} is the sum of squares due to error. These can be computed as follows.

$$SS_{Mean} = \frac{1}{q^k} Y^2, \quad (22)$$

$$SS_{F_l} = \frac{1}{q^{k-1}} \sum_{\varphi=0}^{q-1} Y_l^2(\varphi) - SS_{Mean}, \quad (23)$$

$$SS_{F_l \times F_m} = \frac{1}{q^{k-2}} \sum_{\varphi=0}^{q-1} \sum_{\psi=0}^{q-1} Y_{l,m}^2(\varphi, \psi) - SS_{F_l} - SS_{F_m} - SS_{Mean}, \quad (24)$$

$$SS_{Error} = \sum_{\mathbf{x} \in C^\perp} y^2(\mathbf{x}) - SS_{Mean} - \sum_{l \in MF} SS_{F_l} - \sum_{\{l,m\} \in IF} SS_{F_l \times F_m}. \quad (25)$$

Example 8. Consider the case that a set A is given by (14) and the result of experiments is given by Table 1. Then, using (22)–(25),

$$\begin{aligned} SS_{Mean} &= 249600.6, SS_{F_1} = 1702.3, SS_{F_2} = 29.9, SS_{F_3} = 108.7, \\ SS_{F_4} &= 50.3, SS_{F_5} = 80.5, SS_{F_1 \times F_2} = 16.6, SS_{F_1 \times F_3} = 27.7, \\ SS_{F_1 \times F_4} &= 60.8, SS_{Error} = 16.6. \end{aligned}$$

□

4. Description of experimental design on the basis of an orthonormal system

In this section, we propose the model of experimental design on the basis of an orthonormal system.

4.1 Model on the basis of an orthonormal system in experimental design

We use $y(\mathbf{x})$ to denote the response of an experiment with a level combination \mathbf{x} , and assume the following model:

$$y(\mathbf{x}) = \sum_{\mathbf{a} \in I_A} f_{\mathbf{a}} \chi_{\mathbf{a}}(\mathbf{x}) + \epsilon_{\mathbf{x}}, \quad (26)$$

where $I_A = \{(b_1 a_1, \dots, b_n a_n) | \mathbf{a} \in A, b_i \in GF(q)\}$ and $\epsilon_{\mathbf{x}}$ is a random error with a zero mean and a constant variance.

Then, the model is expressed by using Fourier coefficients instead of the effect of each factor. The effects are represented by the parameters $\{f_{\mathbf{a}} | \mathbf{a} \in I_A\}$. In addition, there are no constraints between the parameters, and the parameters are independent. Hence, it is clear that the model contains no redundant parameters.

Example 9. Consider $q = 3, n = 5$ and $A = \{00000, 10000, 01000, 00100, 00010, 00001, 11000, 10100, 10010\}$. Then, I_A is given by

$$\begin{aligned} I_A = \{ &00000, 10000, 20000, 01000, 02000, 00100, 00200, 00010, 00020, 00001, 00002, 11000, \\ &12000, 21000, 22000, 10100, 10200, 20100, 20200, 10010, 10020, 20010, 20020\}, \end{aligned}$$

and Fourier coefficients

$$f_{00000}, f_{10000}, f_{20000}, f_{01000}, f_{02000}, f_{00100}, f_{00200}, f_{00010}, f_{00020}, f_{00001}, f_{00002}, f_{11000}, f_{12000}, f_{21000}, f_{22000}, f_{10100}, f_{10200}, f_{20100}, f_{20200}, f_{10010}, f_{10020}, f_{20010}, f_{20020}$$

are parameters. The number of parameters is 23, and these parameters are independent. □

4.2 Estimation of Fourier coefficients in experimental design

First, we present the following theorem (Ukita et al., 2010a).

Theorem 1. *Sampling Theorem for Bandlimited Functions over a $GF(q)^n$ Domain*
Assume that $A \subseteq \{0, 1\}^n$ is monotonic and

$$f(x) = \sum_{a \in I_A} f_a \mathcal{X}_a(x), \quad (27)$$

where $I_A = \{(b_1 a_1, \dots, b_n a_n) | a \in A, b_i \in GF(q)\}$. Then, the Fourier coefficients can be computed as follows:

$$f_a = \frac{1}{q^k} \sum_{x \in C^\perp} f(x) \mathcal{X}_a^*(x), \quad (28)$$

where C^\perp is an orthogonal design for A ($|C^\perp| = q^k$). \square

When an experiment is conducted in accordance to the orthogonal design C^\perp , unbiased estimators of f_a in (26) can be obtained by using Theorem 1 and assuming that $E(\epsilon_x) = 0$:

$$\hat{f}_a = \frac{1}{q^k} \sum_{x \in C^\perp} y(x) \mathcal{X}_a^*(x). \quad (29)$$

Then, the Fourier coefficients can be easily estimated by using Fourier transform. There are a number of software packages for Fourier transform, which can be used to calculate (29) for any monotonic set A .

Example 10. Consider the case that a set A is given by (14) and the result of experiments is given by Table 1. Then,

$$\mathcal{X}_a^*(x) = e^{-2\pi i(a_1 x_1 + a_2 x_2 + a_3 x_3 + a_4 x_4 + a_5 x_5)/3}. \quad (30)$$

Using (29), (30) and $e^{2\pi i k} = 1$ for any integer k ,

$$\begin{aligned} \hat{f}_{00000} &= 2596/27, \\ \hat{f}_{10000} &= (863 + 954e^{-2\pi i/3} + 779e^{-4\pi i/3})/27, \\ \hat{f}_{20000} &= (863 + 779e^{-2\pi i/3} + 954e^{-4\pi i/3})/27, \\ \hat{f}_{01000} &= (871 + 873e^{-2\pi i/3} + 852e^{-4\pi i/3})/27, \\ \hat{f}_{02000} &= (871 + 852e^{-2\pi i/3} + 873e^{-4\pi i/3})/27, \\ \hat{f}_{00100} &= (842 + 868e^{-2\pi i/3} + 886e^{-4\pi i/3})/27, \\ \hat{f}_{00200} &= (842 + 886e^{-2\pi i/3} + 868e^{-4\pi i/3})/27, \\ \hat{f}_{00010} &= (873 + 848e^{-2\pi i/3} + 875e^{-4\pi i/3})/27, \\ \hat{f}_{00020} &= (873 + 875e^{-2\pi i/3} + 848e^{-4\pi i/3})/27, \\ \hat{f}_{00001} &= (847 + 864e^{-2\pi i/3} + 885e^{-4\pi i/3})/27, \\ \hat{f}_{00002} &= (847 + 885e^{-2\pi i/3} + 864e^{-4\pi i/3})/27, \\ \hat{f}_{11000} &= (859 + 863e^{-2\pi i/3} + 874e^{-4\pi i/3})/27, \\ \hat{f}_{12000} &= (867 + 868e^{-2\pi i/3} + 861e^{-4\pi i/3})/27, \\ \hat{f}_{21000} &= (867 + 861e^{-2\pi i/3} + 868e^{-4\pi i/3})/27, \\ \hat{f}_{22000} &= (859 + 874e^{-2\pi i/3} + 863e^{-4\pi i/3})/27, \\ \hat{f}_{10100} &= (860 + 861e^{-2\pi i/3} + 875e^{-4\pi i/3})/27, \\ \hat{f}_{10200} &= (871 + 857e^{-2\pi i/3} + 868e^{-4\pi i/3})/27, \end{aligned}$$

$$\begin{aligned}
\hat{f}_{20100} &= (871 + 868e^{-2\pi i/3} + 857e^{-4\pi i/3})/27, \\
\hat{f}_{20200} &= (860 + 875e^{-2\pi i/3} + 861e^{-4\pi i/3})/27, \\
\hat{f}_{10010} &= (872 + 852e^{-2\pi i/3} + 872e^{-4\pi i/3})/27, \\
\hat{f}_{10020} &= (858 + 859e^{-2\pi i/3} + 879e^{-4\pi i/3})/27, \\
\hat{f}_{20010} &= (858 + 879e^{-2\pi i/3} + 859e^{-4\pi i/3})/27, \\
\hat{f}_{20020} &= (872 + 872e^{-2\pi i/3} + 852e^{-4\pi i/3})/27.
\end{aligned}$$

□

In particular, when $q = 2^m$, where m is an integer and $m \geq 1$, it is possible to use the vector-radix fast Fourier transform (FFT), which is a multidimensional implementation of the FFT algorithm, for calculating (29) for all $\mathbf{a} \in I_A$. The complexity of the vector-radix FFT is $O(q^k \log q^k)$. In addition, it can be shown that the Yates' Method (Yates, 1937) for efficient calculation of (19)–(21) in the case of $q = 2$ is equivalent to the vector-radix FFT for calculation of (29).

4.3 The relation between the Fourier coefficients and the effect of each factor

In a description of experimental design on the basis of an orthonormal system, the model is expressed by using Fourier coefficients. Fourier coefficients themselves do not provide a direct representation of the effect of each factor.

On the other hand, since the previous model in experimental design is expressed through the effect of each factor, it is easy to understand how each factor affects the response variable.

In this section, we present three theorems of the relation between the Fourier coefficients and the effect of each factor (Ukita & Matsushima, 2011).

First, we present a theorem of the relation between the Fourier coefficient and the general mean.

Theorem 2. Let $\hat{\mu}$ be the unbiased estimator of the general mean μ in the model of Sect.3.1, and let $\hat{f}_{0\dots 0}$ be that of the Fourier coefficient $f_{0\dots 0}$ in the model of Sect.4.1. Then, the following equation holds:

$$\hat{\mu} = \hat{f}_{0\dots 0}. \quad (31)$$

□

Next, we present a theorem of the relation between the Fourier coefficients and the effect of the main factor.

Theorem 3. Let $\hat{\alpha}_1(\varphi)$ be the unbiased estimator of the effect of the main factor $\alpha_1(\varphi)$ in the model of Sect.3.1, and let $\hat{f}_{0\dots 0a_1 0\dots 0}$ be that of the Fourier coefficient $f_{0\dots 0a_1 0\dots 0}$ in the model of Sect.4.1. Then, the following equation holds:

$$\hat{\alpha}_1(\varphi) = \sum_{\substack{a_1 \in GF(q) \\ a_1 \neq 0}} \mathcal{X}_{a_1}(\varphi) \hat{f}_{0\dots 0a_1 0\dots 0}. \quad (32)$$

□

Last, we present a theorem of the relation between the Fourier coefficients and the effect of the interaction.

Theorem 4. Let $\hat{\beta}_{l,m}(\varphi, \psi)$ be the unbiased estimator of the effect of the interaction $\beta_{l,m}(\varphi, \psi)$ in the model of Sect.3.1, and let $\hat{f}_{0\dots 0a_l 0\dots 0a_m 0\dots 0}$ be that of the Fourier coefficient $f_{0\dots 0a_l 0\dots 0a_m 0\dots 0}$ in the model of Sect.4.1.

Then, the following equation holds:

$$\hat{\beta}_{l,m}(\varphi, \psi) = \sum_{\substack{a_l \in GF(q) \\ a_l \neq 0}} \sum_{\substack{a_m \in GF(q) \\ a_m \neq 0}} \mathcal{X}_{a_l}(\varphi) \mathcal{X}_{a_m}(\psi) \hat{f}_{0\dots 0a_l 0\dots 0a_m 0\dots 0}. \quad (33)$$

□

From these theorems, the effect of each factor can be easily obtained from the computed Fourier coefficients.

Example 11. Let $q = 3$ and $n = 5$. Consider the general mean, the effect of main factor F_1 , and the effect of the interaction of F_1 and F_2 . Then,

$$\mathcal{X}_l(k) = e^{2\pi i k / 3}. \quad (34)$$

First, using (31), $\hat{\mu} = \hat{f}_{00000}$ holds.

Next, using (32) and (34), the following equations

$$\begin{aligned} \hat{\alpha}_1(0) &= \hat{f}_{10000} + \hat{f}_{20000}, \\ \hat{\alpha}_1(1) &= e^{2\pi i / 3} \hat{f}_{10000} + e^{4\pi i / 3} \hat{f}_{20000}, \\ \hat{\alpha}_1(2) &= e^{4\pi i / 3} \hat{f}_{10000} + e^{2\pi i / 3} \hat{f}_{20000}, \end{aligned}$$

hold. Hence, it is clear that the effects of main factor F_1 (3 parameters) can be obtained from the computed Fourier coefficients (2 parameters).

Last, using (33) and (34), the following equations

$$\begin{aligned} \hat{\beta}_{1,2}(0,0) &= \hat{f}_{11000} + \hat{f}_{12000} + \hat{f}_{21000} + \hat{f}_{22000}, \\ \hat{\beta}_{1,2}(0,1) &= e^{2\pi i / 3} \hat{f}_{11000} + e^{4\pi i / 3} \hat{f}_{12000} + e^{2\pi i / 3} \hat{f}_{21000} + e^{4\pi i / 3} \hat{f}_{22000}, \\ \hat{\beta}_{1,2}(0,2) &= e^{4\pi i / 3} \hat{f}_{11000} + e^{2\pi i / 3} \hat{f}_{12000} + e^{4\pi i / 3} \hat{f}_{21000} + e^{2\pi i / 3} \hat{f}_{22000}, \\ \hat{\beta}_{1,2}(1,0) &= e^{2\pi i / 3} \hat{f}_{11000} + e^{2\pi i / 3} \hat{f}_{12000} + e^{4\pi i / 3} \hat{f}_{21000} + e^{4\pi i / 3} \hat{f}_{22000}, \\ \hat{\beta}_{1,2}(1,1) &= e^{4\pi i / 3} \hat{f}_{11000} + \hat{f}_{12000} + \hat{f}_{21000} + e^{2\pi i / 3} \hat{f}_{22000}, \\ \hat{\beta}_{1,2}(1,2) &= \hat{f}_{11000} + e^{4\pi i / 3} \hat{f}_{12000} + e^{2\pi i / 3} \hat{f}_{21000} + \hat{f}_{22000}, \\ \hat{\beta}_{1,2}(2,0) &= e^{4\pi i / 3} \hat{f}_{11000} + e^{4\pi i / 3} \hat{f}_{12000} + e^{2\pi i / 3} \hat{f}_{21000} + e^{2\pi i / 3} \hat{f}_{22000}, \\ \hat{\beta}_{1,2}(2,1) &= \hat{f}_{11000} + e^{2\pi i / 3} \hat{f}_{12000} + e^{4\pi i / 3} \hat{f}_{21000} + \hat{f}_{22000}, \\ \hat{\beta}_{1,2}(2,2) &= e^{2\pi i / 3} \hat{f}_{11000} + \hat{f}_{12000} + \hat{f}_{21000} + e^{4\pi i / 3} \hat{f}_{22000}, \end{aligned}$$

hold. Hence, it is clear that the effects of the interaction of F_1 and F_2 (9 parameters) can be obtained from the computed Fourier coefficients (4 parameters). □

From these theorems, the effect of each factor can be easily obtained from the Fourier coefficients. Therefore, it is possible to implement easily the estimation procedures as well as to understand how each factor affects the response variable in a model based on an orthonormal system.

4.4 Analysis of variance in experimental design

On the other hand, it is already shown that the analysis of variance can also be performed in the model of experimental design on the basis of an orthonormal system (Ukita et al., 2010b). We present three theorems with respect to the sum of squares needed in analysis of variance.

Theorem 5. Let SS_{Mean} be the sum of squares due to the mean in Sect.3.4, and let $\hat{f}_{0\dots 0}$ be the unbiased estimator of the Fourier coefficient $f_{0\dots 0}$ in the model of Sect.4.1. Then,

$$q^k |\hat{f}_{0\dots 0}|^2 = SS_{Mean}, \quad (35)$$

where

$$\hat{f}_{0\dots 0} = \frac{1}{q^k} \sum_{\mathbf{x} \in C^\perp} y(\mathbf{x}) \mathcal{X}_{0\dots 0}^*(\mathbf{x}). \quad (36)$$

□

Theorem 6. Let SS_{F_l} be the sum of squares due to the effect of F_l in Sect.3.4, and let $\hat{f}_{0\dots 0a_l 0\dots 0}$ be the unbiased estimator of the Fourier coefficient $f_{0\dots 0a_l 0\dots 0}$ in the model of Sect.4.1. Then,

$$\sum_{\substack{a_l \in GF(q) \\ a_l \neq 0}} q^k |\hat{f}_{0\dots 0a_l 0\dots 0}|^2 = SS_{F_l}, \quad l = 1, 2, \dots, n, \quad (37)$$

where

$$\hat{f}_{0\dots 0a_l 0\dots 0} = \frac{1}{q^k} \sum_{\mathbf{x} \in C^\perp} y(\mathbf{x}) \mathcal{X}_{0\dots 0a_l 0\dots 0}^*(\mathbf{x}). \quad (38)$$

□

Theorem 7. Let $SS_{F_l \times F_m}$ be the sum of squares due to the interaction effect of $F_l \times F_m$ in Sect.3.4, and let $\hat{f}_{0\dots 0a_l 0\dots 0a_m 0\dots 0}$ be the unbiased estimator of the Fourier coefficient $f_{0\dots 0a_l 0\dots 0a_m 0\dots 0}$ in the model of Sect.4.1. Then,

$$\sum_{a_l \neq 0} \sum_{a_m \neq 0} q^k |\hat{f}_{0\dots 0a_l 0\dots 0a_m 0\dots 0}|^2 = SS_{F_l \times F_m}, \quad l, m = 1, 2, \dots, n, (l < m), \quad (39)$$

where the sums are taken over $a_l, a_m \in GF(q)$ and

$$\hat{f}_{0\dots 0a_l 0\dots 0a_m 0\dots 0} = \frac{1}{q^k} \sum_{\mathbf{x} \in C^\perp} y(\mathbf{x}) \mathcal{X}_{0\dots 0a_l 0\dots 0a_m 0\dots 0}^*(\mathbf{x}). \quad (40)$$

□

By these theorems, SS_{Mean} , SS_{F_l} and $SS_{F_l \times F_m}$ can be obtained in the proposed description of experimental design. In addition, using the Parseval-Plancherel formula and these theorems, SS_{Error} can be computed as follows.

$$SS_{Error} = \sum_{\mathbf{x} \in C^\perp} y^2(\mathbf{x}) - SS_{Mean} - \sum_{l \in MF} SS_{F_l} - \sum_{\{l, m\} \in IF} SS_{F_l \times F_m}. \quad (41)$$

Example 12. Consider the case that a set A is given by (14) and the result of experiments is given by Table 1. Then, using the result of Example 10, $\sum_{k=0}^2 e^{2\pi i k/3} = 0$ and $e^{2\pi i} = 1$,

$$|\hat{f}_{00000}|^2 = \hat{f}_{00000} \hat{f}_{00000}^* = (2596/27)(2596/27) = 9244.466, \quad (42)$$

$$\begin{aligned} |\hat{f}_{10000}|^2 &= \hat{f}_{10000} \hat{f}_{10000}^* \\ &= (863 + 954e^{-2\pi i/3} + 779e^{-4\pi i/3})(863 + 954e^{2\pi i/3} + 779e^{4\pi i/3})/27^2 \\ &= (863^2 + 954^2 + 779^2 - 863 \cdot 954 - 863 \cdot 779 - 954 \cdot 779)/27^2 \\ &= 31.52401. \end{aligned} \quad (43)$$

Similarly,

$$\begin{aligned} |\hat{f}_{20000}|^2 &= 31.52401, \\ |\hat{f}_{01000}|^2 &= |\hat{f}_{02000}|^2 = 0.552812, \quad |\hat{f}_{00100}|^2 = |\hat{f}_{00200}|^2 = 2.013717, \\ |\hat{f}_{00010}|^2 &= |\hat{f}_{00020}|^2 = 0.931413, \quad |\hat{f}_{00001}|^2 = |\hat{f}_{00002}|^2 = 1.491084, \\ |\hat{f}_{11000}|^2 &= |\hat{f}_{22000}|^2 = 0.248285, \quad |\hat{f}_{12000}|^2 = |\hat{f}_{21000}|^2 = 0.058985, \\ |\hat{f}_{10100}|^2 &= |\hat{f}_{20200}|^2 = 0.289438, \quad |\hat{f}_{10200}|^2 = |\hat{f}_{20100}|^2 = 0.223594, \\ |\hat{f}_{10010}|^2 &= |\hat{f}_{20020}|^2 = 0.548697, \quad |\hat{f}_{10020}|^2 = |\hat{f}_{20010}|^2 = 0.577503. \end{aligned}$$

Hence, using Theorem 5–7 and (41),

$$\begin{aligned} SS_{Mean} &= 27|\hat{f}_{00000}|^2 = 249600.6, \\ SS_{F_1} &= 27(|\hat{f}_{10000}|^2 + |\hat{f}_{20000}|^2) = 1702.3, \\ SS_{F_2} &= 27(|\hat{f}_{01000}|^2 + |\hat{f}_{02000}|^2) = 29.9, \\ SS_{F_3} &= 27(|\hat{f}_{00100}|^2 + |\hat{f}_{00200}|^2) = 108.7, \\ SS_{F_4} &= 27(|\hat{f}_{00010}|^2 + |\hat{f}_{00020}|^2) = 50.3, \\ SS_{F_5} &= 27(|\hat{f}_{00001}|^2 + |\hat{f}_{00002}|^2) = 80.5, \\ SS_{F_1 \times F_2} &= 27(|\hat{f}_{11000}|^2 + |\hat{f}_{12000}|^2 + |\hat{f}_{21000}|^2 + |\hat{f}_{22000}|^2) = 16.6, \\ SS_{F_1 \times F_3} &= 27(|\hat{f}_{10100}|^2 + |\hat{f}_{10200}|^2 + |\hat{f}_{20100}|^2 + |\hat{f}_{20200}|^2) = 27.7, \\ SS_{F_1 \times F_4} &= 27(|\hat{f}_{10010}|^2 + |\hat{f}_{10020}|^2 + |\hat{f}_{20010}|^2 + |\hat{f}_{20020}|^2) = 60.8, \\ SS_{Error} &= 16.6. \end{aligned}$$

□

Therefore, the analysis of variance can be executed in the proposed description of experimental design.

Hence, it is clear that two main procedures in the experimental design, that is, the estimation of the effects and the analysis of variance can be executed in a description of experimental design on the basis of an orthonormal system.

5. Conclusion

In this chapter, we have proposed that the model of experimental design be expressed as an orthonormal system, and shown that the model contains no redundant parameters. Then, the model is expressed by using Fourier coefficients instead of the effect of each factor. As there is an abundance of software for calculating the Fourier transform, such a system allows for a straightforward implementation of the procedures for estimating the Fourier coefficients by using Fourier transform. In addition, the effect of each factor can be easily obtained from the Fourier coefficients. Therefore, it is possible to implement easily the estimation procedures

as well as to understand how each factor affects the response variable in a model based on an orthonormal system. Moreover, it is already shown that the analysis of variance can also be performed in a model based on an orthonormal system. Hence, it is clear that two main procedures in the experimental design, that is, the estimation of the effects and the analysis of variance can be executed in a description of experimental design on the basis of an orthonormal system.

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In this book the reader will find a collection of chapters authored/co-authored by a large number of experts around the world, covering the broad field of digital signal processing. This book intends to provide highlights of the current research in the digital signal processing area, showing the recent advances in this field. This work is mainly destined to researchers in the digital signal processing and related areas but it is also accessible to anyone with a scientific background desiring to have an up-to-date overview of this domain. Each chapter is self-contained and can be read independently of the others. These nineteenth chapters present methodological advances and recent applications of digital signal processing in various domains as communications, filtering, medicine, astronomy, and image processing.

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