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Markov basis for design of experiments with three-level factors

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Abstract

We consider Markov basis arising from fractional factorial designs with three-level factors. Once we have a Markov basis, p values for various conditional tests are estimated by the Markov chain Monte Carlo procedure. For designed experiments with a single count observation for each run, we formulate a generalized linear model and consider a sample space with the same sufficient statistics to the observed data. Each model is characterized by a covariate matrix, which is constructed from the main and the interaction effects we intend to measure. We investigate fractional factorial designs with 3^{p-q} runs noting correspondences to the models for 3^{p-q} contingency tables.

1 Introduction

In the past decade, a new application of computational algebraic techniques to statistics has been developed rapidly. Diaconis and Sturmfels [10] introduced the notion of *Markov basis* and presented a procedure for sampling from discrete conditional distributions by constructing a connected, aperiodic and reversible Markov chain on a given sample space. Since then, many works have been published on the topic of the Markov basis by both algebraists and statisticians. Contributions of the present authors on Markov bases can be found in [2], [3], [4], [5], [6], [7], [8], [14], [21], and [22]. On the other hand series of works by Pistone and his collaborators (e.g., [18], [20], [16], [12], [17]) successfully applied the theory of Gröbner basis to designed experiments. In these works, a design is represented as the variety for a set of polynomial equations.

In view of these two main areas of algebraic statistics, it is of interest to investigate statistical problems which are related to both designed experiments and the Markov basis. In [6] we initiated the study of conditional tests of the main effects and the interaction effects when count data are observed from a designed experiment. In [6] we investigated Markov bases arising from fractional factorial designs with two-level factors. In this paper, extending the results in our previous paper, we consider Markov bases for fractional factorial designs with three-level factors.

We relate the models for the case of fractional factorial designs to various models of contingency tables. In most of the works on Markov bases for contingency tables the models considered are hierarchical models. On the other hand when we map models for fractional factorial designs to models for contingency tables, the resulting models are not necessarily hierarchical. Therefore Markov bases for the case of fractional factorial designs often have different features than Markov bases for hierarchical models. In particular for the fractional factorial designs with three-level factors, we find interesting degree three moves and indispensable fibers with three elements. These are of interest also from algebraic viewpoint.

The construction of this paper is as follows. In Section 2, we illustrate the problem of this paper and describe the testing procedure for evaluating p values of the main and the interaction effects for controllable factors in designed experiments. Similarly to the preceding works on Markov basis for contingency tables, our approach is to construct a connected Markov chain for some conditional sample space. We explain how to define this sample space corresponding to various null hypotheses. In Section 3, we consider the relation between the models for the contingency tables and the models for the designed experiments for fractional factorial designs with three-level factors. Then we state properties of Markov bases for designs which are practically important. In Section 4, we give some discussion.

2 Markov chain Monte Carlo tests for designed experiments

In this section we illustrate the problem of this paper. We consider the Markov chain Monte Carlo procedure for conditional tests of the main and interaction effects of controllable factors for the discrete observation derived from various designed experiments. Our arguments are based on the theory of the generalized linear models ([15]).

2.1 Conditional tests for discrete observations

Suppose that the observations are counts of some events and one observation is obtained from for each run of a designed experiment, which is defined by some *aliasing relation*. (We also consider the case that the observations are the ratio of counts in Section 4.) For example, Table 1 is a $1/8$ fraction of a full factorial design (i.e., a 2^{7-3} fractional factorial

Table 1: Design and number of defects y for the wave-solder experiment

Run	Factor							y
	A	B	C	D	E	F	G	
1	0	0	0	0	0	0	0	69
2	0	0	0	1	1	1	1	31
3	0	0	1	0	0	1	1	55
4	0	0	1	1	1	0	0	149
5	0	1	0	0	1	0	1	46
6	0	1	0	1	0	1	0	43
7	0	1	1	0	1	1	0	118
8	0	1	1	1	0	0	1	30
9	1	0	0	0	1	1	0	43
10	1	0	0	1	0	0	1	45
11	1	0	1	0	1	0	1	71
12	1	0	1	1	0	1	0	380
13	1	1	0	0	0	1	1	37
14	1	1	0	1	1	0	0	36
15	1	1	1	0	0	0	0	212
16	1	1	1	1	1	1	1	52

design) defined from the aliasing relation

$$ABDE = ACDF = BCDG = I. \quad (1)$$

This data set was considered in [6] with some modification from the original data in [9]. The original data was reanalyzed in [13]. The observation y in Table 1 is the number of defects found in wave-soldering process in attaching components to an electronic circuit card. In Chapter 7 of [9], seven factors of a wave-soldering process are considered: (A) prebake condition, (B) flux density, (C) conveyer speed, (D) preheat condition, (E) cooling time, (F) ultrasonic solder agitator and (G) solder temperature. Each factor of Table 1 has two-level, which we write 0 or 1 in this paper. The aim of this experiment is to decide which levels for each factor are desirable to reduce solder defects.

Extending the above setting, in this paper, we consider three-level designs with count observations. For example, Table 2 shows a 3^{4-2} fractional factorial design and the observations. We write the three levels as $\{0, 1, 2\}$. Note that the design in Table 2 is also derived from an aliasing relation,

$$C = AB, D = AB^2. \quad (2)$$

We give a more detailed explanation of these aliasing relations in Section 2.2.

We adopt the theory of the *generalized linear models* ([15]) as follows. For these types of count data, it is natural to consider the Poisson model. Write the observations as

Table 2: Design and observations for a 3^{4-2} fractional factorial design

Run	Factor				y
	A	B	C	D	
1	0	0	0	0	y_1
2	0	1	1	2	y_2
3	0	2	2	1	y_3
4	1	0	1	1	y_4
5	1	1	2	0	y_5
6	1	2	0	2	y_6
7	2	0	2	2	y_7
8	2	1	0	1	y_8
9	2	2	1	0	y_9

$\mathbf{y} = (y_1, \dots, y_k)'$, where k is the number of runs and y_i 's are mutually independently distributed with the mean parameter $\mu_i = E(y_i), i = 1, \dots, k$. We express the mean parameter μ_i as

$$g(\mu_i) = \beta_0 + \beta_1 x_{i1} + \dots + \beta_\nu x_{i\nu},$$

where $g(\cdot)$ is the link function and $x_{i1}, \dots, x_{i\nu}$ are the ν covariates defined in Section 2.2. The sufficient statistic is written as $\sum_{i=1}^k x_{ij} y_i$. The canonical link for the Poisson distribution is $g(\mu_i) = \log \mu_i$. For later use, we write the ν -dimensional parameter β and the covariate matrix X as

$$\beta = (\beta_0, \beta_1, \dots, \beta_{\nu-1})' \quad (3)$$

and

$$X = \begin{pmatrix} 1 & x_{11} & \cdots & x_{1\nu-1} \\ \vdots & \vdots & \cdots & \vdots \\ 1 & x_{k1} & \cdots & x_{k\nu-1} \end{pmatrix} = (\mathbf{1}_k \quad \mathbf{x}_1 \quad \cdots \quad \mathbf{x}_{\nu-1}),$$

where $\mathbf{1}_k = (1, \dots, 1)'$ is the k -dimensional column vector consisting of 1's. Then the likelihood function is written as

$$\begin{aligned} \prod_{i=1}^k \frac{\mu_i^{y_i}}{y_i!} e^{-\mu_i} &= \left(\prod_{i=1}^k \frac{e^{-\mu_i}}{y_i!} \right) \exp \left(\sum_{i=1}^k y_i \log \mu_i \right) \\ &= \left(\prod_{i=1}^k \frac{e^{-\mu_i}}{y_i!} \right) \exp \left(\beta_0 \mathbf{1}_k' \mathbf{y} + \sum_{j=1}^{\nu-1} \beta_j \mathbf{x}_j' \mathbf{y} \right) \\ &= \left(\prod_{i=1}^k \frac{e^{-\mu_i}}{y_i!} \right) \exp(\beta' X' \mathbf{y}), \end{aligned}$$

which implies that the sufficient statistic for β is $X' \mathbf{y} = (\mathbf{1}_k' \mathbf{y}, \mathbf{x}_1' \mathbf{y}, \dots, \mathbf{x}_{\nu-1}' \mathbf{y})$.

To define a conditional test, we specify the *null model* and the *alternative model* in terms of the parameter β . To avoid confusion, we express the free parameters under the

null model as the ν -dimensional parameter (3) in this paper. Alternative hypotheses are expressed in terms of additional parameters. For example, in the case of various goodness-of-fit tests, the alternative model is the saturated model, i.e., β is k -dimensional. Then the null and the alternative models are written as

$$\begin{aligned} H_0 &: (\beta_\nu, \dots, \beta_{k-1}) = (0, \dots, 0), \\ H_1 &: (\beta_\nu, \dots, \beta_{k-1}) \neq (0, \dots, 0), \end{aligned}$$

respectively. On the other hand, if we consider significance test of a single additional effect (which can be a main effect or an interaction effect) the alternative model is written in the form of

$$H_1 : (\beta_\nu, \dots, \beta_{\nu+m}) \neq (0, \dots, 0), \quad (4)$$

where $m = 1$ for the case of two-level factors considered in [6]. For the case of three-level factors, m is 2, 4, 8, \dots , depending on the degree of freedom for the factors we consider. We explain this point in Section 2.2.

Depending on the hypotheses, we also specify appropriate test statistic $T(\mathbf{y})$. For example, the likelihood ratio statistic or the Pearson goodness-of-fit statistic are frequently used. Once we specify the null model and the test statistic, our purpose is to calculate the p value. Similarly to the context of the analysis of the contingency tables, Markov chain Monte Carlo procedure is a valuable tool, especially when the traditional large-sample approximation is inadequate and the exact calculation of the p value is infeasible. To perform the Markov chain Monte Carlo procedure, the key notion is to calculate a Markov basis over the sample space

$$\mathcal{F}(X'\mathbf{y}^o) = \{\mathbf{y} \mid X'\mathbf{y} = X'\mathbf{y}^o, y_i \text{ is a nonnegative integer for } i = 1, \dots, k\}, \quad (5)$$

where \mathbf{y}^o is the observed count vector. Once a Markov basis is calculated, we can construct a connected, aperiodic and reversible Markov chain over (5). By the Metropolis-Hastings procedure the chain can be modified to have a stationary distribution as the conditional distribution under the null model, which is written as

$$f(\mathbf{y} \mid X'\mathbf{y} = X'\mathbf{y}^o) = C(X'\mathbf{y}^o) \prod_{i=1}^k \frac{1}{y_i!},$$

where $C(X'\mathbf{y}^o)$ is the normalizing constant determined from $X'\mathbf{y}^o$ defined as

$$C(X'\mathbf{y}^o)^{-1} = \sum_{\mathbf{y} \in \mathcal{F}(X'\mathbf{y}^o)} \left(\prod_{i=1}^k \frac{1}{y_i!} \right).$$

For the definition of Markov basis see [10] and for computational details of Markov chains see [19]. In applications, it is most convenient to rely on algebraic computational softwares such as 4ti2 ([1]) to derive a Markov basis.

2.2 How to define the covariate matrix

As we have seen in Section 2.1, it is key formalization to express various models by the covariate matrix X . The matrix X is constructed from the design matrix to reflect the main and the interaction effects of the factors which we intend to measure.

For the case of two-level factors, we have already considered this problem in [6]. In the case of two-level factors, each main effect and interaction effect can be represented as one column of X . This is because each main and interaction effect has one degree of freedom in the two-level case. For example of Table 1, the main effect model of the seven factors, A, B, C, D, E, F, G can be represented as the covariate matrix

$$X = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 & 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 1 & 0 & 1 & 0 & 1 \\ 1 & 1 & 0 & 0 & 1 & 0 & 0 & 1 \\ 1 & 1 & 0 & 0 & 0 & 1 & 1 & 0 \\ 1 & 0 & 1 & 1 & 1 & 0 & 0 & 1 \\ 1 & 0 & 1 & 1 & 0 & 1 & 1 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 0 & 1 & 0 & 1 \\ 1 & 0 & 0 & 1 & 1 & 1 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 & 0 & 1 & 1 \\ 1 & 0 & 0 & 0 & 1 & 1 & 1 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix},$$

where each column of X represents the contrast of the main effect (and the first column represents the total mean effect). If we intend to include, for example, the interaction effect of $A \times B$, the column

$$(1, 1, 1, 1, 0, 0, 0, 0, 0, 0, 0, 0, 1, 1, 1, 1)'$$

is added to X , which represents the contrast of $A \times B$.

In this paper, we consider the case of three-level designs. To explain three-level fractional factorial designs, first we consider 3^p full factorial designs. Since a 3^p full factorial design is a special case of a multi-way layout, we can use the notions of ANOVA model. In this case, each main effect has two degrees of freedom since each factor has three levels. Similarly, each two-factor interaction has $(3 - 1)(3 - 1) = 4$ degrees of freedom, three-factor interaction has $(3 - 1)(3 - 1)(3 - 1) = 8$ degrees of freedom and so on. As is noted in [23], these sum of squares are further decomposed into components, each with two degrees of freedom. Consider, for example, two-factor interaction $A \times B$. We write the levels of the factors A, B, C, ... as $a, b, c, \dots \in \{0, 1, 2\}$ hereafter. Then $A \times B$ interaction

where each pair of columns represents the contrasts of AB and AB^2 , respectively. For the saturated model, there are 27 columns in X , i.e., one column for the total mean effect, $6(= 2 \times 3)$ columns for the contrasts of the main effects of the factors A, B, C , $12(= 4 \times 3)$ columns for the contrasts of the two-factor interaction effects of $A \times B, A \times C, B \times C$ and 8 columns for the contrasts of the three-factor interaction effect of $A \times B \times C$.

Next we consider the fractional factorial designs. Recall a 3^{4-2} fractional factorial design in Table 2 of Section 1. In this design, since each main effect has two degrees of freedom, the model of the main effects for all factors, A, B, C, D , is nothing but the saturated model. To consider the models with interaction effects, we consider the designs of 27 runs. For example, 3^{4-1} fractional factorial design of resolution IV is defined by the aliasing relation $D = ABC$. The relation $D = ABC$ means that the level d of the factor D is determined by the relation

$$d = a + b + c \pmod{3},$$

which can also be equivalently written as

$$a + b + c + 2d = 0, 1, 2 \pmod{3}.$$

Therefore this aliasing relation is also written as $ABCD^2 = I$. By the similar *modulus 3 calculus*, we can derive all the aliasing relations as follows.

$$\begin{aligned}
I &= ABCD^2 \\
A &= BCD^2 = AB^2C^2D & B &= ACD^2 = AB^2CD^2 \\
C &= ABD^2 = ABC^2D^2 & D &= ABC = ABCD \\
AB &= CD^2 = ABC^2D & AB^2 &= AC^2D = BC^2D \\
AC &= BD^2 = AB^2CD & AC^2 &= AB^2D = BC^2D^2 \\
AD &= AB^2C^2 = BCD & AD^2 &= BC = AB^2C^2D^2 \\
BC^2 &= AB^2D^2 = AC^2D^2 & BD &= AB^2C = ACD \\
CD &= ABC^2 = ABD
\end{aligned} \tag{7}$$

From (7), we can clarify the models where all the effects are estimable. For example, the model of the main effects for the factors A, B, C, D and the interaction effects $A \times B$ is estimable, since the two components of $A \times B$, AB and AB^2 , are not confounded to any main effect. Among the model of the main effects and two two-factor interaction effects, the model with $A \times B$ and $A \times C$ is estimable, while the model with $A \times B$ and $C \times D$ is not estimable since the components AB and CD^2 are confounded. In [23], main effects or components of two-factor interaction effects are called *clear* if they are not confounded to any other main effects or components of two-factor interaction effects. Moreover, a two-factor interaction effect, say $A \times B$ is called *clear* if both of its components, AB and AB^2 , are clear. Therefore (7) implies that each of the main effect and the components, $AB^2, AC^2, AD, BC^2, BD, CD$ are clear, while there is no clear two-factor interaction effect.

3 Correspondence to the models for contingency tables

In this section, we investigate relation between fractional factorial designs with 3^{p-q} runs and contingency tables. Since Markov bases have been mainly considered in the context of contingency tables, it is convenient to characterize the relations from the viewpoint of hierarchical models of contingency tables. For the 2^{p-q} fractional factorial designs, we have considered this topic in [6]. In this paper, we show that many interesting indispensable fibers with three elements appear from the three-level designs.

3.1 Models for the full factorial designs

First we consider 3^p full factorial design and prepare a fundamental fact. Our idea is to index observations as $\mathbf{y} = (y_{i_1 \dots i_p})$, $1 \leq i_1, \dots, i_p \leq 3$, instead of $\mathbf{y} = (y_1, \dots, y_k)'$, $k = 3^p$, to investigate the correspondence to the 3^p contingency table. In the case of the 3^2 full factorial design, for example, the contrasts for each factor and the observation are written as follows.

Run	A	B	AB	AB ²	\mathbf{y}
1	0	0	0	0	y_{11}
2	0	1	1	2	y_{12}
3	0	2	2	1	y_{13}
4	1	0	1	1	y_{21}
5	1	1	2	0	y_{22}
6	1	2	0	2	y_{23}
7	2	0	2	2	y_{31}
8	2	1	0	1	y_{32}
9	2	2	1	0	y_{33}

In this case, we see that the sufficient statistic for the parameter for the total mean is expressed as $y_{..}$ and, under given $y_{..}$, the sufficient statistic for the parameter of the main effects of the factors A and B are expressed as $y_{i.}$ and $y_{.j}$, respectively. Moreover, it is seen that adding contrasts for AB and AB² yields the saturated model. Note that this relation also holds for higher dimensional contingency tables, which we summarize in the following. We write the controllable factors as A_1, A_2, A_3, \dots instead of A, B, C... here. We also use the notation of D -marginal in the p -dimensional contingency tables for $D \subset \{1, \dots, p\}$ here. For example, $\{1\}$ -marginal, $\{2\}$ -marginal, $\{3\}$ -marginal of $\mathbf{y} = (y_{ijk})$ are the one-dimensional tables $\{y_{i.}\}$, $\{y_{.j}\}$, $\{y_{..k}\}$, respectively, and $\{1, 2\}$ -marginal, $\{1, 3\}$ -marginal, $\{2, 3\}$ -marginal of $\mathbf{y} = (y_{ijk})$ are the two-dimensional tables $\{y_{ij.}\}$, $\{y_{i.k}\}$, $\{y_{.jk}\}$, respectively. See [11] for the formal definition.

Fact 3.1. *For 3^p full factorial design, write observations as $\mathbf{y} = (y_{i_1 \dots i_p})$. Then the necessary and the sufficient condition that the $\{i_1, \dots, i_n\}$ -marginal n -dimensional table ($n \leq p$) is uniquely determined from $X'\mathbf{y}$ is that the covariate matrix X includes the*

contrasts for all the components of m -factor interaction effects $A_{j_1} \times A_{j_2} \times \cdots \times A_{j_m}$ for all $\{j_1, \dots, j_m\} \subset \{i_1, \dots, i_n\}, m \leq n$.

This fact is easily proved as follows. The saturated model for the 3^n full factorial design is expressed as the contrast for the total mean, $2 \times n$ contrasts for the main effects, $2^m \times \binom{n}{m}$ contrasts for the m -factor interaction effects for $m = 2, \dots, n$, since they are linearly independent and

$$1 + 2n + \sum_{m=2}^n 2^m \binom{n}{m} = (1 + 2)^n = 3^n.$$

3.2 Models for the fractional factorial designs

Fact 3.1 states that hierarchical models for the controllable factors in the 3^p full factorial design corresponds to the hierarchical models for the 3^p contingency table completely. On the other hand, hierarchical models for the controllable factors in the 3^{p-q} fractional factorial design do not correspond to the hierarchical models for the 3^p contingency table in general. This is because X contains only part of the contrasts of interaction elements in the case of fractional factorial designs. Consequently, many interesting structures appear in considering the Markov basis for the fractional factorial designs.

As a simplest example, we first consider a design with 9 runs for three controllable factors, i.e., 3^{3-1} fractional factorial design. Write three controllable factors as A, B, C, and define C = AB. The design is represented as Table 2 by ignoring the factor D. In this design, the covariate matrix for the main effects model of A, B, C is defined as

$$X' = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}.$$

To investigate the structure of the fiber, write the observation as a frequency of the 3×3 contingency table, y_{11}, \dots, y_{33} . Then the fiber is the set of tables with the same row sums $\{y_{i.}\}$, column sums $\{y_{.j}\}$ and the contrast displayed as

$$\begin{bmatrix} 0 & 1 & 2 \\ 1 & 2 & 0 \\ 2 & 0 & 1 \end{bmatrix}.$$

To construct a minimal Markov basis, we see that the moves to connect the following three-elements fiber are sufficient

$$\left\{ \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix}, \begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix} \right\}.$$

Therefore any two moves from the set

$$\left\{ \begin{bmatrix} +1 & -1 & 0 \\ 0 & +1 & -1 \\ -1 & 0 & +1 \end{bmatrix}, \begin{bmatrix} +1 & 0 & -1 \\ -1 & +1 & 0 \\ 0 & -1 & +1 \end{bmatrix}, \begin{bmatrix} 0 & +1 & -1 \\ -1 & 0 & +1 \\ +1 & -1 & 0 \end{bmatrix} \right\}$$

is a minimal Markov basis. In the following, to save the space, we use binomial representation. For example, the above three moves are written as

$$y_{11}y_{22}y_{33} - y_{12}y_{23}y_{31}, y_{11}y_{22}y_{33} - y_{13}y_{21}y_{32}, y_{12}y_{23}y_{31} - y_{13}y_{21}y_{32}.$$

In this paper, we consider three types of fractional factorial designs with 27 runs, which are important for practical applications. We investigate the relations between various models for the fractional factorial designs and the $3 \times 3 \times 3$ contingency table. In the context of the Markov basis for the contingency tables, Markov basis for the $3 \times 3 \times 3$ contingency tables have been investigated by many researchers, especially for the no three-factor interaction model by [3]. In the following, we investigate Markov bases for some models, especially we are concerned about their *minimality*, *unique minimality* and *indispensability* of their elements. These concepts are presented in [21] and [8]. In this paper, we define that a Markov basis is minimal if no proper subset of it is a Markov basis. A minimal Markov basis is unique if there is only one minimal Markov basis except for sign changes of their elements. An element of a Markov basis is represented as a binomial. We call it a move following our previous papers. A move \mathbf{z} is indispensable if \mathbf{z} or $-\mathbf{z}$ belongs to every Markov basis.

3_{IV}^{4-1} fractional factorial design defined from $D = ABC$ In the case of four controllable factors for design with 27 runs, we have a resolution IV design by setting $D = ABC$. As seen in Section 2.2, all main effects are clear, whereas all the two-factor interactions are not clear in this design.

For the main effect model in this design, the sufficient statistic is written as

$$\{y_{i\cdot\cdot}\}, \{y_{\cdot j\cdot}\}, \{y_{\cdot\cdot k}\}$$

and the contrasts of ABC,

$$\begin{aligned} & y_{111} + y_{123} + y_{132} + y_{213} + y_{222} + y_{231} + y_{312} + y_{321} + y_{333}, \\ & y_{112} + y_{121} + y_{133} + y_{211} + y_{223} + y_{232} + y_{313} + y_{322} + y_{331}, \\ & y_{113} + y_{122} + y_{131} + y_{212} + y_{221} + y_{233} + y_{311} + y_{323} + y_{332}. \end{aligned}$$

By calculation by 4ti2, we see that the minimal Markov basis for this model consists of 54 degree 2 moves and 24 degree 3 moves. All the elements of the same degrees are on the same orbit (see [5],[7]). The elements of degree 2 connect three-elements fibers such as

$$\{y_{112}y_{221}, y_{121}y_{212}, y_{122}y_{211}\} \tag{8}$$

into a tree, and the elements of degree 3 connect three-elements fibers such as

$$\{y_{111}y_{122}y_{133}, y_{112}y_{123}y_{131}, y_{113}y_{121}y_{132}\} \quad (9)$$

into a tree. For the fiber (8), for example, two moves such as

$$y_{121}y_{212} - y_{112}y_{221}, y_{122}y_{211} - y_{112}y_{221}$$

are needed for a Markov basis. See [21] for detail on the structure of a minimal Markov basis.

Considering the aliasing relations given by (7), we can consider models with interaction effects. We see by performing 4ti2 that the structures of the minimal Markov bases for each model are given as follows.

- For the model of the main effects and the interaction effect $A \times B$, 27 indispensable moves of degree 2 such as $y_{113}y_{321} - y_{111}y_{323}$ and 54 dispensable moves of degree 3 constitute a minimal Markov basis. The degree 3 elements are on two orbits, one connects 9 three-elements fibers such as (9) and the other connects 18 three-elements fibers such as $\{y_{111}y_{133}y_{212}, y_{112}y_{131}y_{213}, y_{113}y_{132}y_{211}\}$.
- For the model of the main effects and the interaction effects $A \times B, A \times C$, 6 dispensable moves of degree 3, 81 indispensable moves of degree 4 such as

$$y_{112}y_{121}y_{213}y_{221} - y_{111}y_{122}y_{211}y_{223}$$

and 171 indispensable moves of degree 6, 63 moves such as

$$y_{112}y_{121}y_{133}y_{213}y_{222}y_{231} - y_{111}y_{123}y_{132}y_{211}y_{223}y_{232}$$

and 108 moves such as

$$y_{112}y_{121}y_{213}y_{231}y_{311}y_{323} - y_{111}y_{122}y_{211}y_{233}y_{313}y_{321},$$

constitute a minimal Markov basis. The degree 3 elements connect three-elements fibers such as (9).

- For the model of the main effects and the interaction effects $A \times B, A \times C, B \times C$, 27 indispensable moves of degree 6 such as

$$y_{113}y_{121}y_{132}y_{211}y_{222}y_{233} - y_{111}y_{122}y_{133}y_{213}y_{221}y_{232}$$

and 27 indispensable moves of degree 8 such as

$$y_{111}^2y_{122}y_{133}y_{212}y_{221}y_{313}y_{331} - y_{112}y_{113}y_{121}y_{131}y_{211}y_{222}y_{311}y_{333}$$

constitute a unique minimal Markov basis.

- For the model of the main effect and the interaction effects $A \times B, A \times C, A \times D$, 6 dispensable moves of degree 3 constitute a minimal Markov basis, which connect three-elements fibers such as (9).

3_{III}^{5-2} **fractional factorial design defined from** $D = AB, E = AB^2C$ In the case of five controllable factors for designs with 27 runs, the contrasts for the two main factors are allocated by two aliasing relations.

In this paper, we consider two designs from Table 5A.2 of [23]. First we consider the 3_{III}^{5-2} fractional factorial design defined from $D = AB, E = AB^2C$.

For this design, we can consider the following nine distinct hierarchical models (except for the saturated model). Minimal Markov bases for these models are calculated by 4ti2 as follows.

- For the model of the main effects of A, B, C, D, E, 27 indispensable moves of degree 2 such as $y_{112}y_{221} - y_{111}y_{222}$, 56 dispensable moves of degree 3, 54 indispensable moves of degree 4 such as

$$y_{112}y_{121}y_{231}y_{312} - y_{111}y_{131}y_{212}y_{322}$$

and 9 indispensable moves of degree 6 such as

$$y_{122}y_{131}y_{211}y_{232}y_{312}y_{321} - y_{111}y_{112}y_{222}^2y_{321}^2$$

constitute a minimal Markov basis. The degree 3 elements are in 3 orbits, which connects three types of three-elements fibers, i.e.,

$$\begin{aligned} &18 \text{ moves for 9 fibers such as } \{y_{111}y_{123}y_{132}, y_{113}y_{122}y_{131}, y_{112}y_{121}y_{133}\}, \\ &36 \text{ moves for 18 fibers such as } \{y_{111}y_{123}y_{212}, y_{113}y_{122}y_{211}, y_{112}y_{121}y_{213}\} \text{ and} \\ &2 \text{ moves for the fiber } \{y_{112}y_{223}y_{331}, y_{131}y_{212}y_{323}, y_{121}y_{232}y_{313}\}. \end{aligned}$$

- For the model of the main effects and the interaction effect $A \times C$, 18 dispensable moves of degree 3, 162 indispensable moves of degree 4 such as

$$y_{112}y_{121}y_{213}y_{221} - y_{111}y_{122}y_{211}y_{223},$$

135 indispensable moves of degree 5 such as

$$\begin{aligned} &81 \text{ moves of the form } y_{112}y_{113}y_{121}y_{221}y_{331} - y_{111}y_{122}y_{123}y_{231}y_{311} \text{ and} \\ &54 \text{ moves of the form } y_{112}^2y_{121}y_{221}y_{331} - y_{111}y_{122}y_{132}y_{211}y_{321} \end{aligned}$$

and 54 indispensable moves of degree 6 such as

$$y_{111}y_{122}y_{133}y_{211}y_{222}y_{233} - y_{112}y_{123}y_{131}y_{213}y_{221}y_{232} \quad (10)$$

constitute a minimal Markov basis. The degree 3 elements connect three-elements fibers such as

$$\{y_{111}y_{123}y_{132}, y_{112}y_{121}y_{133}, y_{113}y_{122}y_{131}\} \quad (11)$$

- For the model of the main effects and the interaction effect $C \times E$, 27 indispensable moves of degree 2 such as $y_{112}y_{221} - y_{111}y_{222}$ constitute a unique minimal Markov basis.

- For the model of the main effects and the interaction effects $A \times C, A \times E$, 6 indispensable moves of degree 3 and 81 indispensable moves of degree 6 such as

$$y_{122}y_{131}y_{211}y_{232}y_{312}y_{321} - y_{111}y_{112}y_{221}y_{222}y_{331}y_{332}$$

constitute a minimal Markov basis. The degree 3 elements connect three-elements fibers such as (11).

- For the model of the main effects and the interaction effects $A \times C, B \times C$, 27 indispensable moves of degree 4 such as

$$y_{112}y_{121}y_{232}y_{311} - y_{111}y_{132}y_{212}y_{321}$$

and 54 indispensable moves of degree 6 such as

$$y_{112}y_{121}y_{133}y_{211}y_{223}y_{232} - y_{111}y_{123}y_{132}y_{212}y_{221}y_{233}$$

constitute a unique minimal Markov basis.

- For the model of the main effects and the interaction effects $A \times C, C \times E$, 27 indispensable moves of degree 4 such as

$$y_{111}y_{132}y_{211}y_{222} - y_{112}y_{131}y_{212}y_{221}$$

and 54 indispensable moves of degree 6 such as (10) constitute a unique minimal Markov basis.

- For the model of the main effects and the interaction effects $A \times C, A \times E, C \times E$, 9 indispensable moves of degree 6 such as

$$y_{113}y_{122}y_{131}y_{212}y_{221}y_{233} - y_{111}y_{123}y_{132}y_{211}y_{223}y_{232}$$

constitute a unique minimal Markov basis.

- For the model of the main effects and the interaction effects $A \times C, B \times C, C \times D$, 9 indispensable moves of degree 6 such as

$$y_{122}y_{131}y_{211}y_{232}y_{312}y_{321} - y_{111}y_{112}y_{221}y_{222}y_{331}y_{332}$$

constitute a unique minimal Markov basis.

- For the model of the main effects and the interaction effects $A \times C, B \times C, C \times E$, 9 indispensable moves of degree 6 such as

$$y_{112}y_{121}y_{211}y_{232}y_{322}y_{331} - y_{111}y_{122}y_{212}y_{231}y_{321}y_{332}$$

constitute a unique minimal Markov basis.

3_{III}^{5-2} **fractional factorial design defined from** $D = AB, E = AB^2$ Next we consider 3_{III}^{5-2} fractional factorial design defined from $D = AB, E = AB^2$. For this design, we can consider the following four distinct hierarchical models (except for the saturated model). Minimal Markov bases for these models are calculated by 4ti2 as follows.

- For the model of the main effects of A, B, C, D, E , 108 indispensable moves of degree 2 such as $y_{112}y_{121} - y_{111}y_{122}$ constitute a unique minimal Markov basis.
- For the model of the main effects and the interaction effect $A \times C$, 27 indispensable moves of degree 2 such as $y_{112}y_{121} - y_{111}y_{122}$ constitute a unique minimal Markov basis.
- For the model of the main effects and the interaction effects $A \times C, B \times C$, 27 indispensable moves of degree 4 such as

$$y_{112}y_{121}y_{211}y_{222} - y_{111}y_{122}y_{212}y_{221}$$

and 54 indispensable moves of degree 6 such as

$$y_{112}y_{121}y_{133}y_{211}y_{223}y_{232} - y_{111}y_{123}y_{132}y_{212}y_{221}y_{233}$$

constitute a unique minimal Markov basis.

- For the model of the main effects and the interaction effects $A \times C, B \times C, C \times D$, 9 indispensable moves of degree 6 such as

$$y_{111}y_{132}y_{212}y_{221}y_{322}y_{331} - y_{112}y_{131}y_{211}y_{222}y_{321}y_{332}$$

constitute a unique minimal Markov basis.

4 Discussion

In this paper, we investigate a Markov basis arising from the fractional factorial designs with three-level factors. As noted in Section 1, the notion of a Markov basis is one of the fundamental key words in the first work of the computational algebraic statistics. Moreover, the designed experiment is also one of the areas in statistics where the theory of the Gröbner basis found applications. Since we give another application of the theory of the Gröbner basis to the designed experiments, this paper relates to both of the works by Diaconis and Sturmfels ([10]) and Pistone and Wynn ([18]).

Though we suppose that the observations are counts in Section 2, our arguments can also be applied to the case that the observations are the ratio of counts. In this case, we consider the logistic link function instead of the logit link, and investigate the relation between 3^{p-q} fractional factorial designs to the 3^{p-q+1} contingency tables. See [6] for the two-level case.

One of the interesting observations of this paper is that many three-elements fibers arise in considering minimal Markov bases. In fact, in the examples considered in Section

3.2, all the dispensable moves of minimal Markov bases are needed for connecting three-elements fibers, where each element of the fibers does not share supports in each other. This shows that the every positive and the negative part of the dispensable moves is a indispensable. See notion of the *indispensable monomial* in [8].

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