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SUMMARY

In this paper we define an invariant Markov basis for a connected Markov chain over the set of contingency tables with fixed marginals and derive some characterizations of minimality of the invariant basis. We also give a necessary and sufficient condition for uniqueness of invariant minimal Markov basis. The invariance here refers to permutation of indices of each axis of the contingency tables. If the categories of each axis do not have any order relations among them, it is natural to consider the action of the symmetric group on each axis of the contingency table. A general algebraic algorithm for obtaining a Markov basis was given by Diaconis and Sturmfels (1998). Their algorithm is based on computing Gröbner basis of a well-specified polynomial ideal. However the reduced Gröbner basis depends on the particular term order and is not symmetric. Therefore it is of interest to consider properties of invariant Markov basis. We study minimality of invariant Markov basis using techniques of Takemura and Aoki (2003).

Keywords: exact tests, hierarchical models, Markov chain Monte Carlo, orbit, symmetric group, transformation group.

1 Introduction

In performing exact conditional tests in discrete exponential families given sufficient statistics, the p values are usually calculated by large sample approximations. However when the sample size is small compared to the size of the sample space, the large sample approximation may not be sufficiently accurate. When the sample size and the sample space are relatively small, enumeration of the sample space may be feasible with some ingenious enumeration schemes. For the case of two-way contingency tables with fixed row and column sums, Mehta and Patel (1983) proposed a network algorithm, which incorporates appropriate trimming in the enumeration. Aoki (2002, 2003) extended this trimming for Fisher's exact test in two-way contingency tables and for the conditional tests of the Hardy-Weinberg proportions (triangular two-way contingency tables). However, the problem of computing p values by enumeration for k-way contingency tables, $k > 2$, seems to be largely open in the literature.

As another approach, a Markov chain Monte Carlo approach is extensively used in various settings of contingency tables, for example, Besag and Clifford (1989) for performing significance tests for the Ising model; Smith *et al.* (1996) for tests of independence, quasi-independence and quasi-symmetry for square contingency tables; Aoki and Takemura (2002) for tests of quasi-independence for two-way contingency tables containing some structural zeros; Guo and Thompson (1992) for tests of the Hardy-Weinberg proportions; Diaconis and Saloff-Coste (1995) for two-way contingency tables; Hernek (1998), Dyer and Greenhill (2000) for $2 \times J$ contingency tables; Forster *et al.* (1996) for 2^k contingency tables. Most of these literatures deal with various two-way settings.

Diaconis and Sturmfels (1998) proposed a general algorithm for generating random samples from a conditional distribution given sufficient statistics for general discrete exponential family of distributions. They suggests computing a Markov basis by finding a Gröbner basis of a well-specified polynomial ideal. Their approach is extremely appealing because, in principle, it can be used for the problems of any dimension. Despite its generality, however, the power of their procedure is limited for the following two reasons; the computational feasibility and outputs of redundant basis elements. The first one stems from the computational complexity of computing Gröbner bases. Although intensive research is being conducted for improving the efficiency of Gröbner bases computation (e.g. Sturmfels, 1995; Boffi and Rossi, 2001), it is still difficult to obtain a Gröbner basis by standard packages even for problems of moderate sizes. The second one, which we especially consider in this paper, stems from the lack of minimality and symmetry of a reduced Gröbner basis. Gröbner basis is in general not symmetric because it depends on the particular term order.

In this paper, we consider the symmetry of the basis. We treat the permutation of indices of each axis of contingency tables as an action of a direct product of symmetric groups to the basis elements and define an invariant Markov basis. Logically important point is that if a unique minimal Markov basis exists then it is also the unique invariant Markov basis. On the other hand, if a minimal Markov basis is not unique, an invariant minimal Markov basis is important, since a minimal Markov basis is usually not symmetric (see Takemura and Aoki, 2003).

In Takemura and Aoki (2003), we derived some characterizations of a minimal Markov basis and gave a necessary and sufficient condition for uniqueness of a minimal Markov basis. We combine this approach with the theory of transformation groups to study minimality of invariant Markov bases and give some characterizations of invariant Markov basis and its minimality. We also give a necessary and sufficient condition for uniqueness of invariant minimal Markov basis.

The construction of this paper is as follows. Definitions and notations of contingency tables, Markov basis and invariance are given in Section 2. Structures of an invariant minimal Markov basis are derived in Section 3. Examples of all hierarchical $2 \times 2 \times 2 \times 2$ models are studied in Section 4.

2 Preliminaries

In this section, we give necessary notations and definitions on Markov basis in Section 2.1 and group actions on contingency tables in Section 2.2.

2.1 Contingency tables and Markov basis

Consider an $I_1 \times \cdots \times I_k$ k-way contingency table $\boldsymbol{x}$. We denote a cell of the contingency table by $\boldsymbol{i} = (i_1, \ldots, i_k)$ or $\boldsymbol{i} = (i_1 \ldots i_k)$. The set of cells is denoted by

$$\mathcal{I} = \mathcal{I}^1 \times \cdots \times \mathcal{I}^k,$$

where $\mathcal{I}^\ell = \{1, \ldots, I_\ell\}$, $\ell = 1, \ldots, k$. We write $\boldsymbol{x} = \{x(\boldsymbol{i})\}_{\boldsymbol{i}\in\mathcal{I}}$ where $x(\boldsymbol{i})$ is a frequency of cell $\boldsymbol{i}$. Let X denote the set of all k-way contingency tables given by

$$X = \{\boldsymbol{x} = \{x(\boldsymbol{i})\}_{\boldsymbol{i}\in\mathcal{I}} \mid x(\boldsymbol{i}) \in \{0, 1, 2, \ldots\} \text{ for } \boldsymbol{i} \in \mathcal{I}\} \ .$$

We define the *degree* of $\boldsymbol{x} \in X$ as $\deg(\boldsymbol{x}) = \sum_{\boldsymbol{i}\in\mathcal{I}} x(\boldsymbol{i})$, which is the total frequency of $\boldsymbol{x}$. X is partitioned as

$$X = \bigcup_{n=0}^{\infty} X_n, \quad X_n = \{\boldsymbol{x} \in X \mid \deg(\boldsymbol{x}) = n\} \ .$$

Let $K = \{1, \ldots, k\}$ and let D denote a subset of K. The *D-marginal* $\boldsymbol{x}_D = \{x_D(\boldsymbol{i}_D)\}_{\boldsymbol{i}_D\in\mathcal{I}_D}$ of $\boldsymbol{x}$ is the contingency table with *marginal cells* $\boldsymbol{i}_D \in \prod_{\ell\in D} \mathcal{I}^\ell$ and entries given by

$$x_D(\boldsymbol{i}_D) = \sum_{\boldsymbol{j}_{K\setminus D}\in\mathcal{I}_{K\setminus D}} x(\boldsymbol{i}_D, \boldsymbol{j}_{K\setminus D}) \ .$$

Note that $\boldsymbol{x}_D$ is an m-way contingency table if $D = \{i_1, \ldots, i_m\}$.

Let $D_1, \ldots, D_r \subset K$. Throughout this paper we assume that $D_1 \cup \cdots \cup D_r = K$ and there does not exist $i \neq j$ such that $D_i \subseteq D_j$. Note that $\{D_1, \ldots, D_r\}$ corresponds to the generating class of a hierarchical log-linear model for the contingency table. The set of D-marginal frequencies

$$\boldsymbol{t} = \boldsymbol{t}(\boldsymbol{x}) = (\boldsymbol{x}_{D_1}, \ldots, \boldsymbol{x}_{D_r})$$

is the sufficient statistic under the hierarchical log-linear model. Note that if the cells and the elements of the sufficient statistic are ordered appropriately, we can write $\boldsymbol{t}$ in matrix form as $\boldsymbol{t} = A\boldsymbol{x}$ as in Section 2.1 of Takemura and Aoki (2003).

We define the *reference set* of all the contingency tables having the same $(D_1, \ldots, D_r)$-marginals as

$$\mathcal{F}_{\boldsymbol{t}} = \mathcal{F}_{\boldsymbol{t}}(D_1, \ldots, D_r) = \{\boldsymbol{x} \in X \mid \boldsymbol{t}(\boldsymbol{x}) = \boldsymbol{t}\} \ .$$

Since all contingency tables in the same reference set $\mathcal{F}_{\boldsymbol{t}}$ have the same degree, we define the degree of $\boldsymbol{t}$ by $\deg(\boldsymbol{t}) = \deg(\boldsymbol{x})$, $\boldsymbol{x} \in \mathcal{F}_{\boldsymbol{t}}$. Then the set T of possible values of the sufficient statistic $\boldsymbol{t}$, i.e., $T = \{\boldsymbol{t}(\boldsymbol{x}) \mid \boldsymbol{x} \in X\}$, is partitioned as

$$T = \bigcup_{n=0}^{\infty} T_n, \quad T_n = \{\boldsymbol{t} \mid \deg(\boldsymbol{t}) = n\} \ .$$

Let $Z \supset X$ be the set of k-way arrays $\boldsymbol{z} = \{z(\boldsymbol{i})\}_{\boldsymbol{i}\in\mathcal{I}}$ containing integer entries

$$Z = \{\boldsymbol{z} = \{z(\boldsymbol{i})\}_{\boldsymbol{i}\in\mathcal{I}} \mid z(\boldsymbol{i}) \in \{\ldots, -1, 0, 1, \ldots\} \text{ for } \boldsymbol{i} \in \mathcal{I}\} \ .$$

Similarly to the D-marginal $\boldsymbol{x}_D$ of $\boldsymbol{x}$, the D-marginal of $\boldsymbol{z}$ is defined and denoted by $\boldsymbol{z}_D$. An array $\boldsymbol{z} \in Z$ is a *move* for $D_1, \ldots, D_r$ if $\boldsymbol{z}_{D_j} = \boldsymbol{0}$ for $j = 1, \ldots, r$. Here $\boldsymbol{0}$ denotes the zero array. Let $M(D_1, \ldots, D_r)$ denote the set of all moves for $D_1, \ldots, D_r$ given by

$$M(D_1, \ldots, D_r) = \{\boldsymbol{z} \in Z \mid \boldsymbol{z}_{D_j} = \boldsymbol{0}, \quad j = 1, \ldots, r\} \subset Z \ .$$

For a move $\boldsymbol{z}$ for $D_1, \ldots, D_r$, the positive part $\boldsymbol{z}^+ = \{z^+(\boldsymbol{i})\}_{\boldsymbol{i} \in \mathcal{I}}$ and the negative part $\boldsymbol{z}^- = \{z^-(\boldsymbol{i})\}_{\boldsymbol{i} \in \mathcal{I}}$ are defined by

$$z^+(\boldsymbol{i}) = \max(z(\boldsymbol{i}), 0), \quad z^-(\boldsymbol{i}) = \max(-z(\boldsymbol{i}), 0),$$

respectively. Then $\boldsymbol{z} = \boldsymbol{z}^+ - \boldsymbol{z}^-$ and $\boldsymbol{z}^+, \boldsymbol{z}^- \in X$. Moreover, $\boldsymbol{z}^+$ and $\boldsymbol{z}^-$ have the same sufficient statistic, i.e., $\boldsymbol{t}(\boldsymbol{z}^+) = \boldsymbol{t}(\boldsymbol{z}^-)$, and are in the same reference set :

$$\boldsymbol{z}^+, \boldsymbol{z}^- \in \mathcal{F}_{\boldsymbol{t}(\boldsymbol{z}^+)}(D_1, \ldots, D_r) = \mathcal{F}_{\boldsymbol{t}(\boldsymbol{z}^-)}(D_1, \ldots, D_r).$$

Note that if $\boldsymbol{z}$ is a move, then $-\boldsymbol{z}$ is also a move with $(-\boldsymbol{z})^+ = \boldsymbol{z}^-$ and $(-\boldsymbol{z})^- = \boldsymbol{z}^+$. Furthermore non-zero elements of $\boldsymbol{z}^+$ and $\boldsymbol{z}^-$ do not share a common cell. We define a *degree* of $\boldsymbol{z} \in M(D_1, \ldots, D_r)$ as $\deg(\boldsymbol{z}) = \deg(\boldsymbol{z}^+) = \deg(\boldsymbol{z}^-)$. We also define a set of moves with degree less than or equal to n as

$$M_n(D_1, \ldots, D_r) = \{\boldsymbol{z} \in M(D_1, \ldots, D_r) \mid \deg(\boldsymbol{z}) \leq n\}. \tag{1}$$

We occasionally write simply M_n for convenience.

Let $\mathcal{B} \subset M(D_1, \ldots, D_r)$ be a set of moves for $D_1, \ldots, D_r$. Let $\boldsymbol{x}, \boldsymbol{x}' \in \mathcal{F}_{\boldsymbol{t}}(D_1, \ldots, D_r)$. We say that $\boldsymbol{x}'$ is *accessible* from $\boldsymbol{x}$ by $\mathcal{B}$ if there exists a sequence of moves $\boldsymbol{z}_1, \ldots, \boldsymbol{z}_A \in \mathcal{B}$ and $\varepsilon_s \in \{-1, 1\}, \ s = 1, \ldots, A$, such that

$$\begin{aligned} \boldsymbol{x}' &= \boldsymbol{x} + \sum_{s=1}^{A} \varepsilon_s \boldsymbol{z}_s, \\ \boldsymbol{x} + \sum_{s=1}^{a} \varepsilon_s \boldsymbol{z}_s &\in \mathcal{F}_{\boldsymbol{t}}(D_1, \ldots, D_r) \text{ for } 1 \leq a \leq A \ , \end{aligned} \tag{2}$$

i.e., we can apply moves from $\mathcal{B}$ to $\boldsymbol{x}$ one by one and go from $\boldsymbol{x}$ to $\boldsymbol{x}'$, without causing negative cell frequencies on the way. It should be noted that accessibility by $\mathcal{B}$ is an equivalence relation and each reference set is partitioned into disjoint equivalence classes by $\mathcal{B}$. We call these equivalence classes $\mathcal{B}$-*equivalence classes* of the reference set. If $\boldsymbol{x}$ and $\boldsymbol{x}'$ are elements from two different $\mathcal{B}$-equivalence classes of the same reference set, we say that a move $\boldsymbol{z} = \boldsymbol{x} - \boldsymbol{x}'$ *connects* these two equivalence classes (see Section 2 of Takemura and Aoki, 2003).

Here we define a *Markov basis*.

Definition 1 *A finite set $\mathcal{B} \subset M(D_1, \ldots, D_r)$ is a Markov basis for $D_1, \ldots, D_r$ if for all $\boldsymbol{t} \in T$, $\mathcal{F}_{\boldsymbol{t}}(D_1, \ldots, D_r)$ itself constitutes one $\mathcal{B}$-equivalence class.*

Logically important point here is the existence of a finite Markov basis for any $D_1, \ldots, D_r$, which is guaranteed by the Hilbert basis theorem (see Section 3.1 of Diaconis and Sturmfels, 1998). In this definition, if $\mathcal{B}$ is a Markov basis and $\boldsymbol{z}, -\boldsymbol{z} \in \mathcal{B}$, then $\mathcal{B} \setminus \{\boldsymbol{z}\}$ and $\mathcal{B} \setminus \{-\boldsymbol{z}\}$

are also Markov bases, respectively. Moreover, if we replace any element $\boldsymbol{z}$ of a Markov basis $\mathcal{B}$ with $-\boldsymbol{z}$, the remaining set is still a Markov basis. In other words, there is a freedom of the signs of the elements of a Markov basis. In this paper, we identify an element $\boldsymbol{z}$ of a Markov basis with its sign change $-\boldsymbol{z}$ for convenience.

A Markov basis $\mathcal{B}$ is *minimal* if no proper subset of $\mathcal{B}$ is a Markov basis. A minimal Markov basis always exists, because from any Markov basis, we can remove redundant elements one by one, until none of the remaining elements can be removed any further. However, a minimal Markov basis is not always unique. Takemura and Aoki (2003) gives some characterizations of a minimal Markov basis. An important fact is that for $\boldsymbol{t} \in T$ such that $\mathcal{F}_{\boldsymbol{t}}(D_1, \ldots, D_r) = \{\boldsymbol{x}, \boldsymbol{x}'\}$ is a two-elements set, a move $\boldsymbol{z} = \boldsymbol{x} - \boldsymbol{x}'$ belongs to each Markov basis for $D_1, \ldots, D_r$ (see Lemma 2.3 of Takemura and Aoki, 2003). We call such a move an *indispensable move*. Furthermore, the unique minimal Markov basis exists if and only if the set of indispensable moves forms a Markov basis. In this case, the set of indispensable moves is the unique minimal Markov basis (see Corollary 2.2 of Takemura and Aoki, 2003).

Our moves contain many zero cells. Furthermore often the non-zero cells of a move contain either 1 or -1. Therefore a move can be concisely denoted by locations of its non-zero cells. We express a move $\boldsymbol{z}$ of degree n as

$$\boldsymbol{z} = [\{\boldsymbol{i}_1, \ldots, \boldsymbol{i}_n\} \parallel \{\boldsymbol{j}_1, \ldots, \boldsymbol{j}_n\}],$$

where $\boldsymbol{i}_1, \ldots, \boldsymbol{i}_n$ are the cells of positive frequencies of $\boldsymbol{z}$ and $\boldsymbol{j}_1, \ldots, \boldsymbol{j}_n$ are the cells of negative frequencies of $\boldsymbol{z}$. In the case $z(\boldsymbol{i}) > 1$, $\boldsymbol{i}$ is repeated $z(\boldsymbol{i})$ times. Similarly $\boldsymbol{j}$ is repeated $-z(\boldsymbol{j})$ times if $z(\boldsymbol{j}) < -1$. We use similar notation for contingency tables as well. $\boldsymbol{x} \in X_n$ is simply denoted as

$$\boldsymbol{x} = [\{\boldsymbol{i}_1, \ldots, \boldsymbol{i}_n\}] = [\boldsymbol{i}_1, \ldots, \boldsymbol{i}_n] \ .$$

2.2 Symmetric group and its action

Here we define an action of a direct product of symmetric groups on cells. From the action on cells, further actions are induced on contingency tables, marginal cells, marginal frequencies and moves.

First we give a brief list of definitions and notations of group action. Let a group G act on a set $\mathcal{X}$. $G(x) = \{gx \mid g \in G\}$ is the orbit through x. For a subset A of $\mathcal{X}$, $G(A) = \{gx \mid x \in A,\ g \in G\}$. $\mathcal{X}/G$ denotes the orbit space, i.e. the set of orbits. $G_x = \{g \mid gx = x\}$ denotes the isotropy subgroup of x in G. If G acts on $\mathcal{X}$, the action of G on the set of functions f on $\mathcal{X}$ is induced by $gf(x) = f(g^{-1}x)$. Let $h : \mathcal{X} \to \mathcal{Y}$ be a surjection. If $h(x) = h(x') \Rightarrow h(gx') = h(gx), \forall g \in G$, then the action of G on $\mathcal{Y}$ is induced by defining $gy = h(gx)$, where $y = h(x)$. Throughout the rest of this paper, the number of elements of a finite set A is denoted by $|A|$.

In our problem G is the direct product of symmetric groups, which acts on the index set $\mathcal{I}$. Let G^ℓ denote the symmetric group of order I_ℓ for $\ell = 1, \ldots, k$ and let

$$G = G^1 \times G^2 \times \cdots \times G^k$$

be the direct product. We write an element of $g \in G$ as

$$g = g_1 \times \cdots \times g_k = \begin{pmatrix} 1 & \cdots & I_1 \\ \sigma_1(1) & \cdots & \sigma_1(I_1) \end{pmatrix} \times \cdots \times \begin{pmatrix} 1 & \cdots & I_k \\ \sigma_k(1) & \cdots & \sigma_k(I_k) \end{pmatrix} .$$

G acts on $\mathcal{I}$ by

$$\begin{aligned}\boldsymbol{i}' &= g\boldsymbol{i}\\ &= (g_1 i_1, \ldots, g_k i_k)\\ &= (\sigma_1(i_1), \ldots, \sigma_k(i_k)) \ .\end{aligned}$$

Then the action of G on X is induced by

$$\begin{aligned}\boldsymbol{x}' &= g\boldsymbol{x}\\ &= \{x(g^{-1}\boldsymbol{i})\}_{\boldsymbol{i}\in\mathcal{I}}.\end{aligned}$$

G also acts on the marginal cells by

$$\begin{aligned}\boldsymbol{i}'_D &= g\boldsymbol{i}_D\\ &= (g_{s_1} i_{s_1}, \ldots, g_{s_m} i_{s_m})\\ &= (\sigma_{s_1}(i_{s_1}), \ldots, \sigma_{s_m}(i_{s_m})),\end{aligned}$$

where $D = \{s_1, \ldots, s_m\}$. Hence G acts on marginal tables by

$$\begin{aligned}\boldsymbol{x}'_D &= g\boldsymbol{x}_D\\ &= \{x_D(g^{-1}\boldsymbol{i}_D)\}_{\boldsymbol{i}_D\in\mathcal{I}_D}.\end{aligned}$$

Considering this action simultaneously for $D_1, \ldots, D_r$, the action of G on the sufficient statistic $\boldsymbol{t} = (\boldsymbol{x}_{D_1}, \ldots, \boldsymbol{x}_{D_r})$ is defined by

$$g\boldsymbol{t} = (g\boldsymbol{x}_{D_1}, \ldots, g\boldsymbol{x}_{D_r}).$$

An important point here is that the action of G on $\boldsymbol{t}$ is induced from the action of G on $\boldsymbol{x}$, because the the calculation of D-marginals and the action of G on X are commutative. Although this is intuitively clear, we state this as a lemma and give a proof.

Lemma 1 *$(g\boldsymbol{x})_D = g\boldsymbol{x}_D$ for all $g \in G$ and $\boldsymbol{x} \in X$.*

Proof. Write $\tilde{\boldsymbol{x}} = g\boldsymbol{x}$. From the definitions, it follows that

$$\begin{aligned}\tilde{x}_D(\boldsymbol{i}_D) &= \sum_{\boldsymbol{j}_{K\setminus D}\in\mathcal{I}_{K\setminus D}} \tilde{x}(\boldsymbol{i}_D, \boldsymbol{j}_{K\setminus D})\\ &= \sum_{\boldsymbol{j}_{K\setminus D}\in\mathcal{I}_{K\setminus D}} x(g^{-1}(\boldsymbol{i}_D, \boldsymbol{j}_{K\setminus D}))\\ &= \sum_{\boldsymbol{j}_{K\setminus D}\in\mathcal{I}_{K\setminus D}} x(g^{-1}\boldsymbol{i}_D, g^{-1}\boldsymbol{j}_{K\setminus D})\\ &= x_D(g^{-1}\boldsymbol{i}_D)\\ &= (g\boldsymbol{x}_D)(\boldsymbol{i}_D) \ .\end{aligned}$$

Q.E.D.

By this lemma, if $\boldsymbol{x}_{D_i} = \boldsymbol{y}_{D_i}$, $i = 1, \ldots, r$, then $(g\boldsymbol{x})_{D_i} = (g\boldsymbol{y})_{D_i}$, $i = 1, \ldots, r$, $\forall g \in G$. In terms of the sufficient statistic this can be equivalently written as $\boldsymbol{t}(\boldsymbol{x}) = \boldsymbol{t}(\boldsymbol{y}) \Rightarrow \boldsymbol{t}(g\boldsymbol{x}) = \boldsymbol{t}(g\boldsymbol{y})$, $\forall g \in G$. Therefore the action of G on T is induced from the action of G on X. Also it is important to note that the isotropy subgroup $G_{\boldsymbol{t}}$ of $\boldsymbol{t}$ acts on the reference set $\mathcal{F}_{\boldsymbol{t}}$.

So far we have only considered non-negative frequencies. However clearly the above consideration can also be applied to the set Z of integer arrays. In particular, Lemma 1 holds for the action of G on Z, i.e., taking marginals of integer arrays commutes with the action of G. Therefore if $\boldsymbol{z}$ is a move, then $g\boldsymbol{z}$ is a move as well. Therefore

$$G(M(D_1,\ldots,D_r)) = M(D_1,\ldots,D_r).$$

and G acts on $M(D_1,\ldots,D_r)$. More concretely, in terms of the positive part and the negative part we can write

$$\begin{aligned}\boldsymbol{z}' &= g\boldsymbol{z}\\ &= g\boldsymbol{z}^+ - g\boldsymbol{z}^- \ .\end{aligned}$$

We also define that a move $\boldsymbol{z} = \boldsymbol{z}^+ - \boldsymbol{z}^-$ is *symmetric* if $\boldsymbol{z}^+ = g\boldsymbol{z}^-$ for some $g \in G$. Conversely, a move $\boldsymbol{z}$ is *asymmetric* if $G(\boldsymbol{z}^+) \neq G(\boldsymbol{z}^-)$.

Now we can define an invariant set of moves. $\mathcal{B} \subset M(D_1,\ldots,D_r)$ is *G-invariant* if $G(\mathcal{B}) = \mathcal{B}$. Note that here we are identifying a move $\boldsymbol{z} \in \mathcal{B}$ with its sign change $-\boldsymbol{z}$. Therefore $\mathcal{B}$ is G-invariant if and only if

$$\forall g \in G, \forall \boldsymbol{z} \in \mathcal{B} \implies g\boldsymbol{z} \in \mathcal{B} \text{ or } -g\boldsymbol{z} \in \mathcal{B} \ .$$

In other words, $\mathcal{B}$ is G-invariant if and only if it is a union of orbits $\mathcal{B} = \bigcup_{\boldsymbol{z}\in A} G(\boldsymbol{z})$ for some subset $A \subset M(D_1,\ldots,D_r)$ of moves.

A finite set $\mathcal{B} \subset M(D_1,\ldots,D_r)$ is an *invariant Markov basis* for $D_1,\ldots,D_r$ if it is a Markov basis and it is G-invariant. An invariant Markov basis is minimal if no proper G-invariant subset of $\mathcal{B}$ is a Markov basis. A minimal invariant Markov basis always exists, because from any invariant Markov basis, we can remove orbits one by one, until none of the remaining orbits can be removed any further.

3 Characterizations of an invariant Markov basis and its uniqueness

In this section, we first study the relationships between the orbits and $M_{n-1}(D_1,...,D_r)$-equivalence classes of X_n and then derive some characterizations of an invariant minimal Markov basis and its uniqueness.

3.1 Some properties of orbits of contingency tables and marginal frequencies

Here we derive some basic properties of orbits of G acting on X and T. First we note that $\deg(\boldsymbol{x}) = \deg(g\boldsymbol{x})$, $\forall g \in G$, and hence $G(X_n) = X_n$. Therefore we consider the action of G on each X_n separately. Similarly we consider the action of G on each T_n separately.

Consider a particular sufficient statistic $\boldsymbol{t} \in T_n$. Let $G(\boldsymbol{t}) \in T_n/G$ be the orbit through $\boldsymbol{t}$. Let

$$\mathcal{F}_{G(\boldsymbol{t})} = \bigcup_{\boldsymbol{t}'\in G(\boldsymbol{t})} F_{\boldsymbol{t}'}$$

denote the union of reference sets over the orbit $G(\boldsymbol{t})$ through $\boldsymbol{t}$. Let $\boldsymbol{x} \in \mathcal{F}_{\boldsymbol{t}}$. Because $\boldsymbol{t}(g\boldsymbol{x}) = g\boldsymbol{t}$, it follows that

$$g\boldsymbol{x} \in \mathcal{F}_{g\boldsymbol{t}} \subset \mathcal{F}_{G(\boldsymbol{t})}.$$

Therefore $G(\mathcal{F}_{G(\boldsymbol{t})}) = \mathcal{F}_{G(\boldsymbol{t})}$. This implies that X_n is partitioned as

$$X_n = \bigcup_{\alpha \in T_n/G} \mathcal{F}_\alpha, \tag{3}$$

where α runs over the set of different orbits and we can consider the action of G on each $\mathcal{F}_{G(\boldsymbol{t})}$ separately.

Example 1 *Consider the case of $k = 3$ and $D_1 = \{1\}, D_2 = \{2\}, D_3 = \{3\}$. This is the complete independence model of the three-way tables. The decomposition (3) of X_1 for this case is trivial since T_1 itself is one G-orbit. We consider the decomposition of X_2. For this case there are eight G-orbits in T_2 as*

$$\begin{array}{l} T_2/G = \{G(\boldsymbol{t}_1), \ldots, G(\boldsymbol{t}_8)\}, \\ \boldsymbol{t}_i = \boldsymbol{t}(\boldsymbol{x}_i),\ i = 1, \ldots, 8, \\ \boldsymbol{x}_1 = [(111), (111)],\ \boldsymbol{x}_2 = [(111), (112)], \\ \boldsymbol{x}_3 = [(111), (121)],\ \boldsymbol{x}_4 = [(111), (211)], \\ \boldsymbol{x}_5 = [(111), (122)],\ \boldsymbol{x}_6 = [(111), (212)], \\ \boldsymbol{x}_7 = [(111), (221)],\ \boldsymbol{x}_8 = [(111), (222)] \end{array} \tag{4}$$

and we have

$$X_2 = \mathcal{F}_{G(\boldsymbol{t}_1)} \cup \cdots \cup \mathcal{F}_{G(\boldsymbol{t}_8)}. \tag{5}$$

The numbers of elements of the orbits $G(\boldsymbol{t}_1), \ldots, G(\boldsymbol{t}_8)$ are calculated as follows.

$$\begin{array}{ll} |G(\boldsymbol{t}_1)| = I_1 I_2 I_3, & |G(\boldsymbol{t}_2)| = I_1 I_2 \binom{I_3}{2}, \\ |G(\boldsymbol{t}_3)| = I_1 \binom{I_2}{2} I_3, & |G(\boldsymbol{t}_4)| = \binom{I_1}{2} I_2 I_3, \\ |G(\boldsymbol{t}_5)| = I_1 \binom{I_2}{2}\binom{I_3}{2}, & |G(\boldsymbol{t}_6)| = \binom{I_1}{2} I_2 \binom{I_3}{2}, \\ |G(\boldsymbol{t}_7)| = \binom{I_1}{2}\binom{I_2}{2} I_3, & |G(\boldsymbol{t}_8)| = \binom{I_1}{2}\binom{I_2}{2}\binom{I_3}{2}. \end{array} \tag{6}$$

Furthermore we have

$$|\mathcal{F}_{\boldsymbol{t}}| = \begin{cases} 1 & \textit{for}\ \ \boldsymbol{t} \in G(\boldsymbol{t}_1) \cup G(\boldsymbol{t}_2) \cup G(\boldsymbol{t}_3) \cup G(\boldsymbol{t}_4), \\ 2 & \textit{for}\ \ \boldsymbol{t} \in G(\boldsymbol{t}_5) \cup G(\boldsymbol{t}_6) \cup G(\boldsymbol{t}_7), \\ 4 & \textit{for}\ \ \boldsymbol{t} \in G(\boldsymbol{t}_8). \end{cases} \tag{7}$$

Consider a particular $\mathcal{F}_{G(\boldsymbol{t})}$. An important observation is that there is a direct product structure in $\mathcal{F}_{G(\boldsymbol{t})}$. Write

$$G(\boldsymbol{t}) = \{\boldsymbol{t}_1, \ldots, \boldsymbol{t}_a\},$$

where $a = a(\boldsymbol{t}) = |G(\boldsymbol{t})|$ is the number of elements of the orbit $G(\boldsymbol{t}) \subset T_n$. Let $b = b(\boldsymbol{t}) = |\mathcal{F}_{G(\boldsymbol{t})}/G|$ be the number of orbits of G acting on $\mathcal{F}_{G(\boldsymbol{t})}$ and let $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_b$ be representative elements of different orbits, i.e., $\mathcal{F}_{G(\boldsymbol{t})} = G(\boldsymbol{x}_1) \cup \cdots \cup G(\boldsymbol{x}_b)$ gives a partition of $\mathcal{F}_{G(\boldsymbol{t})}$. Then we have the following lemma.

Lemma 2 *$\mathcal{F}_{G(\boldsymbol{t})}$ is partitioned as*

$$\mathcal{F}_{G(\boldsymbol{t})} = \bigcup_{i=1}^{a} \bigcup_{j=1}^{b} \mathcal{F}_{\boldsymbol{t}_i} \cap G(\boldsymbol{x}_j), \tag{8}$$

where each $\mathcal{F}_{\boldsymbol{t}_i} \cap G(\boldsymbol{x}_j)$ is non-empty. Furthermore if $\boldsymbol{t}'_i = g\boldsymbol{t}_i$, then $\boldsymbol{x} \in \mathcal{F}_{\boldsymbol{t}_i} \mapsto g\boldsymbol{x} \in \mathcal{F}_{\boldsymbol{t}'_i}$ gives a bijection between $\mathcal{F}_{\boldsymbol{t}_i} \cap G(\boldsymbol{x})$ and $\mathcal{F}_{\boldsymbol{t}'_i} \cap G(\boldsymbol{x})$.

Proof. $\mathcal{F}_{G(\boldsymbol{t})} = \mathcal{F}_{\boldsymbol{t}_1} \cup \cdots \cup \mathcal{F}_{\boldsymbol{t}_a}$ is a partition. Intersecting this partition with $\mathcal{F}_{G(\boldsymbol{t})} = \bigcup_{j=1}^{b} G(\boldsymbol{x}_j)$ gives the partition (8). Let $\boldsymbol{x} \in \mathcal{F}_{\boldsymbol{t}}$. Then the orbit $G(\boldsymbol{x})$ intersects each reference set, i.e. $G(\boldsymbol{x}) \cap \mathcal{F}_{\boldsymbol{t}_i} \neq \emptyset$ for $i = 1, \ldots, a$.

Since every $g \in G$ is a bijection of $\mathcal{F}_{G(\boldsymbol{t})}$ to itself and

$$g(\mathcal{F}_{\boldsymbol{t}} \cap G(\boldsymbol{x})) = \mathcal{F}_{g\boldsymbol{t}} \cap G(\boldsymbol{x}),$$

g gives a bijection between $\mathcal{F}_{\boldsymbol{t}_i} \cap G(\boldsymbol{x})$ and $\mathcal{F}_{\boldsymbol{t}'_i} \cap G(\boldsymbol{x})$. Q.E.D.

In particular for each j, $\mathcal{F}_{\boldsymbol{t}_i} \cap G(\boldsymbol{x}_j)$, $i = 1, \ldots, a$, have the same number of elements

$$|\mathcal{F}_{\boldsymbol{t}_1} \cap G(\boldsymbol{x}_j)| = \cdots = |\mathcal{F}_{\boldsymbol{t}_a} \cap G(\boldsymbol{x}_j)|.$$

In addition, for $\boldsymbol{t}_i, \boldsymbol{t}'_i \in G(\boldsymbol{t})$ such that $\boldsymbol{t}'_i = g\boldsymbol{t}_i$, the map $g : G_{\boldsymbol{t}_i} \to gG_{\boldsymbol{t}_i}g^{-1}$ gives an isomorphism between $G_{\boldsymbol{t}_i}$ and $G_{\boldsymbol{t}'_i} = gG_{\boldsymbol{t}_i}g^{-1}$, where $G_{\boldsymbol{t}_i}$ and $G_{\boldsymbol{t}'_i}$ are the the isotropy subgroup of $\boldsymbol{t}_i$ and $\boldsymbol{t}'_i$ in G, respectively. Therefore there are the following isomorphic structures in $\mathcal{F}_{\boldsymbol{t}_i}$,

$$(G_{\boldsymbol{t}_i}, \mathcal{F}_{\boldsymbol{t}_i}) \simeq (G_{\boldsymbol{t}'_i}, \mathcal{F}_{\boldsymbol{t}'_i}). \tag{9}$$

Example 2 *(Example 1 continued.) In the decomposition (5), we have $|\mathcal{F}_{G(\boldsymbol{t}_i)}/G| = b(\boldsymbol{t}_i) = 1$ and $\mathcal{F}_{G(\boldsymbol{t}_i)} = G(\boldsymbol{x}_i)$ for $i = 1, \ldots, 8$. Therefore the right hand side of (8) is simply $\bigcup_{i=1}^{a} \mathcal{F}_{\boldsymbol{t}_i}$ in this case. To see the isomorphic structure (9), consider $\mathcal{F}_{G(\boldsymbol{t}_8)}$, for example. The isotropy subgroup of $\boldsymbol{t}_8$ is given by*

$$G_{\boldsymbol{t}_8} = \widetilde{G}^1_{12,12} \times \widetilde{G}^2_{12,12} \times \widetilde{G}^3_{12,12},$$

where we define

$$\widetilde{G}^{\ell}_{i_1 i_2, j_1 j_2} = \{g \in G^{\ell} \mid (\sigma_\ell(i_1), \sigma_\ell(i_2)) \in \{(j_1, j_2), (j_2, j_1)\}\},\ i_1 \neq i_2, j_1 \neq j_2.$$

We also define

$$G^{\ell}_{i_1 i_2, j_1 j_2} = \{g \in G^{\ell} \mid (\sigma_\ell(i_1), \sigma_\ell(i_2)) = (j_1, j_2)\} \subset \widetilde{G}^{\ell}_{i_1 i_2, j_1 j_2}$$

for later use. Since G^ℓ is the symmetric group of order I_ℓ, we have $|\widetilde{G}^{\ell}_{i_1 i_2, j_1 j_2}| = 2(I_\ell - 2)!$ and $|G^{\ell}_{i_1 i_2, j_1 j_2}| = (I_\ell - 2)!$. The reference set $\mathcal{F}_{\boldsymbol{t}_8}$ is written as

$$\mathcal{F}_{\boldsymbol{t}_8} = \{[(111), (222)], [(112), (221)], [(121), (212)], [(122), (211)]\}.$$

Consider another element $\boldsymbol{x}' = [(111), (223)] \in \mathcal{F}_{G(\boldsymbol{t}_8)}$ and write $\boldsymbol{t}' = \boldsymbol{t}(\boldsymbol{x}')$. The isotropy subgroup of $\boldsymbol{t}'$ is given by

$$G_{\boldsymbol{t}'} = \widetilde{G}^1_{12,12} \times \widetilde{G}^2_{12,12} \times \widetilde{G}^3_{13,13}$$

and the reference set $\mathcal{F}_{\boldsymbol{t}'}$ *is written as*

$$\mathcal{F}_{\boldsymbol{t}'} = \{[(111),(223)],[(113),(221)],[(121),(213)],[(123),(211)]\}.$$

We see the relations $\boldsymbol{t}' = g\boldsymbol{t}_8$ *and* $gG_{\boldsymbol{t}_8}g^{-1} = G_{\boldsymbol{t}'}$ *for* $g \in \widetilde{G}^1_{12,12} \times \widetilde{G}^2_{12,12} \times \widetilde{G}^3_{12,13}$. *In particular* $\boldsymbol{x}' = g\boldsymbol{x}_8$ *holds if* $g \in G^1_{12,12} \times G^2_{12,12} \times G^3_{12,13} \cup G^1_{12,21} \times G^2_{12,21} \times G^3_{12,31}$.

Next we present examples of $b = 2$ and $b = 3$.

Example 3 *Consider the case of* $k = 4$ *and* $D_1 = \{1,2\}, D_2 = \{1,3\}, D_3 = \{2,3\}, D_4 = \{3,4\}$. *This is an example of reducible models. Consider a particular* $\boldsymbol{t} \in T_4$ *such that*

$$\boldsymbol{t} = (\boldsymbol{x}_{D_1}, \boldsymbol{x}_{D_2}, \boldsymbol{x}_{D_3}, \boldsymbol{x}_{D_4}),$$

where

$$\begin{aligned}
\boldsymbol{x}_{D_1} &= [(i_1i_2),(i_1i_2'),(i_1'i_2),(i_1'i_2')],\\
\boldsymbol{x}_{D_2} &= [(i_1i_3),(i_1i_3'),(i_1'i_3),(i_1'i_3')],\\
\boldsymbol{x}_{D_3} &= [(i_2i_3),(i_2i_3'),(i_2'i_3),(i_2'i_3')],\\
\boldsymbol{x}_{D_4} &= [(i_3i_4),(i_3i_4'),(i_3'i_4),(i_3'i_4')].
\end{aligned}$$

For each $i_m \neq i_m', m = 1,\ldots,4$, *there are eights elements in* $\mathcal{F}_{\boldsymbol{t}}$ *as*

$$\begin{aligned}
\mathcal{F}_{\boldsymbol{t}} &= \{\boldsymbol{x}_1,\ldots,\boldsymbol{x}_8\},\\
\boldsymbol{x}_1 &= [(i_1i_2i_3i_4),(i_1i_2'i_3'i_4),(i_1'i_2i_3'i_4'),(i_1'i_2'i_3i_4')],\\
\boldsymbol{x}_2 &= [(i_1i_2i_3i_4),(i_1i_2'i_3'i_4'),(i_1'i_2i_3'i_4),(i_1'i_2'i_3i_4')],\\
\boldsymbol{x}_3 &= [(i_1i_2i_3i_4'),(i_1i_2'i_3'i_4),(i_1'i_2i_3'i_4'),(i_1'i_2'i_3i_4)],\\
\boldsymbol{x}_4 &= [(i_1i_2i_3i_4'),(i_1i_2'i_3'i_4'),(i_1'i_2i_3'i_4),(i_1'i_2'i_3i_4)],\\
\boldsymbol{x}_5 &= [(i_1i_2i_3'i_4),(i_1i_2'i_3i_4),(i_1'i_2i_3i_4'),(i_1'i_2'i_3'i_4')],\\
\boldsymbol{x}_6 &= [(i_1i_2i_3'i_4),(i_1i_2'i_3i_4'),(i_1'i_2i_3i_4),(i_1'i_2'i_3'i_4')],\\
\boldsymbol{x}_7 &= [(i_1i_2i_3'i_4'),(i_1i_2'i_3i_4),(i_1'i_2i_3i_4'),(i_1'i_2'i_3'i_4)],\\
\boldsymbol{x}_8 &= [(i_1i_2i_3'i_4'),(i_1i_2'i_3i_4'),(i_1'i_2i_3i_4),(i_1'i_2'i_3'i_4)].
\end{aligned}$$

We see that

$$G_{\boldsymbol{t}} = \widetilde{G}^1_{i_1i_1',i_1i_1'} \times \widetilde{G}^2_{i_2i_2',i_2i_2'} \times \widetilde{G}^3_{i_3i_3',i_3i_3'} \times \widetilde{G}^4_{i_4i_4',i_4i_4'} \tag{10}$$

for this case, and each $\mathcal{F}_{\boldsymbol{t}}$ *contains two* $G_{\boldsymbol{t}}$*-orbits, i.e.,*

$$\mathcal{F}_{\boldsymbol{t}} = \{\boldsymbol{x}_1,\boldsymbol{x}_4,\boldsymbol{x}_5,\boldsymbol{x}_8\} \cup \{\boldsymbol{x}_2,\boldsymbol{x}_3,\boldsymbol{x}_6,\boldsymbol{x}_7\} = G_{\boldsymbol{t}}(\boldsymbol{x}_1) \cup G_{\boldsymbol{t}}(\boldsymbol{x}_2).$$

Extending $\boldsymbol{t}$ *to* $G(\boldsymbol{t})$, *we see the direct product structure (8) of* $\mathcal{F}_{G(\boldsymbol{t})}$, *where* $b = |\mathcal{F}_{G(\boldsymbol{t})}/G| = |\mathcal{F}_{\boldsymbol{t}}/G_{\boldsymbol{t}}| = 2$,

$$a = |G(\boldsymbol{t})| = \binom{I_1}{2}\binom{I_2}{2}\binom{I_3}{2}\binom{I_4}{2}$$

and

$$|\mathcal{F}_{\boldsymbol{t}'} \cap G(\boldsymbol{x}_1)| = |\mathcal{F}_{\boldsymbol{t}'} \cap G(\boldsymbol{x}_2)| = 4$$

for each $\boldsymbol{t}' \in G(\boldsymbol{t})$.

Example 4 *Consider the case of $k = 4$ and $D_1 = \{1, 2\}, D_2 = \{1, 3\}, D_3 = \{2, 3\}, D_4 = \{4\}$. Again this is an example of reducible models. Consider a particular $\boldsymbol{t} \in T_4$ such that*

$$\boldsymbol{t} = (\boldsymbol{x}_{D_1}, \boldsymbol{x}_{D_2}, \boldsymbol{x}_{D_3}, \boldsymbol{x}_{D_4}),$$

where $\boldsymbol{x}_{D_1}, \boldsymbol{x}_{D_2}, \boldsymbol{x}_{D_3}$ are the same as in Example 3, and $\boldsymbol{x}_{D_4} = [(i_4), (i_4), (i'_4), (i'_4)]$. For each $i_m \neq i'_m, m = 1, \dots, 4$, there are twelve elements in $\mathcal{F}_{\boldsymbol{t}}$ as

$$\begin{array}{c} \mathcal{F}_{\boldsymbol{t}} = \{\boldsymbol{x}_1, \dots, \boldsymbol{x}_{12}\}, \\ \boldsymbol{x}_9 = [(i_1 i_2 i_3 i_4), (i_1 i'_2 i'_3 i'_4), (i'_1 i_2 i'_3 i'_4), (i'_1 i'_2 i_3 i_4)], \\ \boldsymbol{x}_{10} = [(i_1 i_2 i_3 i'_4), (i_1 i'_2 i'_3 i_4), (i'_1 i_2 i'_3 i_4), (i'_1 i'_2 i_3 i'_4)], \\ \boldsymbol{x}_{11} = [(i_1 i_2 i'_3 i_4), (i_1 i'_2 i_3 i'_4), (i'_1 i_2 i_3 i'_4), (i'_1 i'_2 i'_3 i_4)], \\ \boldsymbol{x}_{12} = [(i_1 i_2 i'_3 i'_4), (i_1 i'_2 i_3 i_4), (i'_1 i_2 i_3 i_4), (i'_1 i'_2 i'_3 i'_4)] \end{array}$$

and $\boldsymbol{x}_1, \dots, \boldsymbol{x}_8$ are the same as in Example 3. We see that $G_{\boldsymbol{t}}$ is defined by (10) again, and each $\mathcal{F}_{\boldsymbol{t}}$ contains three $G_{\boldsymbol{t}}$-orbits, i.e.,

$$\mathcal{F}_{\boldsymbol{t}} = \{\boldsymbol{x}_1, \boldsymbol{x}_4, \boldsymbol{x}_5, \boldsymbol{x}_8\} \cup \{\boldsymbol{x}_2, \boldsymbol{x}_3, \boldsymbol{x}_6, \boldsymbol{x}_7\} \cup \{\boldsymbol{x}_9, \boldsymbol{x}_{10}, \boldsymbol{x}_{11}, \boldsymbol{x}_{12}\} = G_{\boldsymbol{t}}(\boldsymbol{x}_1) \cup G_{\boldsymbol{t}}(\boldsymbol{x}_2) \cup G_{\boldsymbol{t}}(\boldsymbol{x}_9).$$

Extending $\boldsymbol{t}$ to $G(\boldsymbol{t})$, we see the direct product structure (8) of $\mathcal{F}_{G(\boldsymbol{t})}$, where $b = |\mathcal{F}_{G(\boldsymbol{t})}/G| = |\mathcal{F}_{\boldsymbol{t}}/G_{\boldsymbol{t}}| = 3$,

$$a = |G(\boldsymbol{t})| = \binom{I_1}{2}\binom{I_2}{2}\binom{I_3}{2}\binom{I_4}{2}$$

and

$$|\mathcal{F}_{\boldsymbol{t}'} \cap G(\boldsymbol{x}_1)| = |\mathcal{F}_{\boldsymbol{t}'} \cap G(\boldsymbol{x}_2)| = |\mathcal{F}_{\boldsymbol{t}'} \cap G(\boldsymbol{x}_9)| = 4$$

for each $\boldsymbol{t}' \in G(\boldsymbol{t})$.

The following example of $b = 2$ is somewhat complicated but it is important in showing an asymmetric indispensable move.

Example 5 *Consider the case of $k = 3$ and $D_1 = \{1, 2\}, D_2 = \{1, 3\}, D_3 = \{2, 3\}$. This model is considered extensively for $I_1 = I_2 = 3$ in Aoki and Takemura (2003). Here we study the case of $I_1 = 3, I_2 = 5, I_3 = 6$ and a sufficient statistic $\boldsymbol{t} = (\boldsymbol{x}_{D_1}, \boldsymbol{x}_{D_2}, \boldsymbol{x}_{D_3}) \in T_{14}$, where*

$$\begin{array}{l} \boldsymbol{x}_{D_1} = [(11), (13), (14), (15), (22), (23), (24), (25), (31), (32), (33), (34), (35), (35)], \\ \boldsymbol{x}_{D_2} = [(11), (12), (13), (16), (23), (24), (25), (26), (31), (32), (34), (35), (36), (36)], \\ \boldsymbol{x}_{D_3} = [(11), (16), (24), (26), (32), (33), (34), (41), (43), (45), (52), (55), (56), (56)]. \end{array}$$

In this case, $\mathcal{F}_{\boldsymbol{t}} = \{\boldsymbol{x}_1, \boldsymbol{x}_2\}$, where

$$\begin{array}{l} \boldsymbol{x}_1 = [(111), (132), (143), (156), (224), (233), (245), (256), (316), (326), (334), (341), (352), (355)], \\ \boldsymbol{x}_2 = [(116), (133), (141), (152), (226), (234), (243), (255), (311), (324), (332), (345), (356), (356)]. \end{array}$$

Furthermore, there is no $g \in G$ satisfying $\boldsymbol{x}_1 = g\boldsymbol{x}_2$, i.e., $G(\boldsymbol{x}_1) \cap G(\boldsymbol{x}_2) = \emptyset$. (This is obvious since only $\boldsymbol{x}_2$ contains 2 as a cell frequency.) Therefore $\boldsymbol{x}_1 - \boldsymbol{x}_2$ is an asymmetric indispensable move. Extending $\boldsymbol{t}$ to $G(\boldsymbol{t})$, we see that

$$|\mathcal{F}_{\boldsymbol{t}'} \cap G(\boldsymbol{x}_1)| = |\mathcal{F}_{\boldsymbol{t}'} \cap G(\boldsymbol{x}_2)| = 1$$

for each $\boldsymbol{t}' \in G(\boldsymbol{t})$.

3.2 A direct product structure of each reference set

Considering the isomorphic structures of (9), now we can focus our attention on each reference set. Consider a particular reference set $\mathcal{F}_{\boldsymbol{t}}$. Here we can restrict our attention to the action of $G_{\boldsymbol{t}}$ on $\mathcal{F}_{\boldsymbol{t}}$. In characterizing a Markov basis and its minimality, Takemura and Aoki (2003) showed that it is essential to consider $M_{\deg(\boldsymbol{t})-1}(D_1,\ldots,D_r)$-equivalence classes of $\mathcal{F}_{\boldsymbol{t}}$, where $M_{n-1}(D_1,\ldots,D_r)$ is given in (1). Therefore we have to confirm the relation between the action of $G_{\boldsymbol{t}}$ and $M_{n-1}(D_1,\ldots,D_r)$-equivalence classes of $\mathcal{F}_{\boldsymbol{t}}$, $\deg(\boldsymbol{t}) = n$.

Let $K_{\boldsymbol{t}}$ denote the number of $M_{n-1}(D_1,\ldots,D_r)$-equivalence classes of $\mathcal{F}_{\boldsymbol{t}}$ as in Theorem 1 of Takemura and Aoki (2003). In this paper, we write the set of $M_{n-1}(D_1,\ldots,D_r)$-equivalence classes of $\mathcal{F}_{\boldsymbol{t}}$ as $\mathcal{H}_{\boldsymbol{t}}$ for simplicity, i.e.,

$$\mathcal{H}_{\boldsymbol{t}} = \mathcal{F}_{\boldsymbol{t}}/M_{n-1}(D_1,\ldots,D_r) = \{X_1,\ldots,X_{K_{\boldsymbol{t}}}\}, \quad K_{\boldsymbol{t}} = |\mathcal{H}_{\boldsymbol{t}}|,\ \deg(\boldsymbol{t}) = n,$$

in the notation of Takemura and Aoki (2003). In the sequel let $X_\gamma \in \mathcal{H}_{\boldsymbol{t}}$ denote each equivalence class.

Example 6 *(Example 3 continued.) Consider the model considered in Example 3. Now we can restrict our attention to $I_1 = I_2 = I_3 = I_4 = 2$ case, i.e., $i_m = 1, i'_m = 2$ for $m = 1,\ldots,4$ and consider $M_3(D_1,\ldots,D_4)$-equivalence classes of $\mathcal{F}_{\boldsymbol{t}}$. In this case, we see that $|\mathcal{H}_{\boldsymbol{t}}| = 2$ and*

$$\mathcal{H}_{\boldsymbol{t}} = \mathcal{F}_{\boldsymbol{t}}/M_{n-1}(D_1,\ldots,D_r) = \{\{\boldsymbol{x}_1,\boldsymbol{x}_2,\boldsymbol{x}_3,\boldsymbol{x}_4\},\{\boldsymbol{x}_5,\boldsymbol{x}_6,\boldsymbol{x}_7,\boldsymbol{x}_8\}\}$$

since

$$\begin{aligned}\boldsymbol{x}_1 - \boldsymbol{x}_2 &= [(1111),(1221),(2122),(2212)] - [(1111),(1222),(2121),(2212)]\\ &= [\{(1221),(2122)\} \parallel \{(1222),(2121)\}] \in M_2(D_1,\ldots,D_4),\end{aligned}$$

for example.

Example 7 *(Example 4 continued.) Similar result to Example 6 is derived for the model in Example 4. Again we can restrict our attention to $I_1 = I_2 = I_3 = I_4 = 2$ case and consider $M_3(D_1,\ldots,D_4)$-equivalence classes of $\mathcal{F}_{\boldsymbol{t}}$. In this case, we see that $|\mathcal{H}_{\boldsymbol{t}}| = 2$ and*

$$\mathcal{H}_{\boldsymbol{t}} = \mathcal{F}_{\boldsymbol{t}}/M_{n-1}(D_1,\ldots,D_r) = \{\{\boldsymbol{x}_1,\boldsymbol{x}_2,\boldsymbol{x}_3,\boldsymbol{x}_4,\boldsymbol{x}_9,\boldsymbol{x}_{10}\},\{\boldsymbol{x}_5,\boldsymbol{x}_6,\boldsymbol{x}_7,\boldsymbol{x}_8,\boldsymbol{x}_{11},\boldsymbol{x}_{12}\}\}.$$

We now have the following important lemma.

Lemma 3 *If $\boldsymbol{x}'$ is accessible from $\boldsymbol{x}$ by $M_{n-1}(D_1,\ldots,D_r)$, then $g\boldsymbol{x}'$ is accessible from $g\boldsymbol{x}$ by $M_{n-1}(D_1,\ldots,D_r)$.*

Proof. Note that $\deg(\boldsymbol{z}) \le n-1$ if and only if $\deg(g\boldsymbol{z}) \le n-1$. If $\boldsymbol{x}'$ is accessible from $\boldsymbol{x}$, then by (2)

$$\boldsymbol{x}' = \boldsymbol{x} + \sum_{s=1}^{A} \varepsilon_s \boldsymbol{z}_s,$$

$$\boldsymbol{x} + \sum_{s=1}^{a} \varepsilon_s \boldsymbol{z}_s \in \mathcal{F}_{\boldsymbol{t}}(D_1,\ldots,D_r) \text{ for } 1 \le a \le A\ .$$

Applying g to the both sides of the equations we get

$$g\boldsymbol{x}' = g\boldsymbol{x} + \sum_{s=1}^{A} \varepsilon_s g\boldsymbol{z}_s,$$

$$g\boldsymbol{x} + \sum_{s=1}^{a} \varepsilon_s g\boldsymbol{z}_s \in \mathcal{F}_{g\boldsymbol{t}}(D_1, \ldots, D_r) \text{ for } 1 \le a \le A \ .$$

Q.E.D.

This lemma holds for all $g \in G$. In particular, $g\boldsymbol{x} \in \mathcal{F}_{\boldsymbol{t}(\boldsymbol{x})}$ if $g \in G_{\boldsymbol{t}}$. This implies that an action of $G_{\boldsymbol{t}}$ is induced on $\mathcal{H}_{\boldsymbol{t}}$. In fact if $\pi : \boldsymbol{x} \mapsto X_\gamma$ denotes the natural projection of $\boldsymbol{x}$ to its equivalence class, then Lemma 3 states

$$\pi(\boldsymbol{x}) = \pi(\boldsymbol{x}') \Rightarrow \pi(g\boldsymbol{x}) = \pi(g\boldsymbol{x}').$$

Let $\boldsymbol{x} \in X_\gamma$ and $g \in G_{\boldsymbol{t}}$. Then $g\boldsymbol{x}$ belongs to some $M_{n-1}(D_1, \ldots, D_r)$-equivalence class $X_{\gamma'}$. By Lemma 3, this γ' does not depend on the choice of $\boldsymbol{x} \in X_\gamma$ and we may write $\gamma' = g\gamma$. Since by definition a group action is bijective we have the following lemma.

Lemma 4

$$g \in G_{\boldsymbol{t}} : X_\gamma \mapsto X_{\gamma'}$$

is a bijection of $\mathcal{H}_{\boldsymbol{t}}$ to itself.

Combining this result and the isomorphic structure of (9), we see that the structure of $\mathcal{H}_{\boldsymbol{t}'}$ and in particular $|\mathcal{H}_{\boldsymbol{t}'}|$ are common for all $\boldsymbol{t}' \in G(\boldsymbol{t})$.

Now consider the orbit space $\mathcal{H}_{\boldsymbol{t}}/G_{\boldsymbol{t}}$. Write each element of $\mathcal{H}_{\boldsymbol{t}}/G_{\boldsymbol{t}}$ as Γ, and write

$$X_\Gamma = \bigcup_{X_\gamma \in \Gamma} X_\gamma. \tag{11}$$

Then we have the decomposition

$$\mathcal{F}_{\boldsymbol{t}} = \bigcup_{\Gamma \in \mathcal{H}_{\boldsymbol{t}}/G_{\boldsymbol{t}}} X_\Gamma.$$

By definition, X_Γ is $G_{\boldsymbol{t}}$-invariant for each Γ and $G_{\boldsymbol{t}}$ acts on X_Γ. Therefore we consider each X_Γ separately. An important observation is that there is a direct product structure in X_Γ, which is similar to Lemma 2. Let $\Delta = \Delta(\Gamma) = X_\Gamma/G_{\boldsymbol{t}}$ be the $G_{\boldsymbol{t}}$-orbit space of X_Γ and $\boldsymbol{x}_\delta \in X_\Gamma, \delta \in \Delta$, be the representative elements of different orbits. Then we have the following lemma.

Lemma 5 *$\mathcal{F}_{\boldsymbol{t}}$ is partitioned as*

$$\begin{aligned} \mathcal{F}_{\boldsymbol{t}} &= \bigcup_{\Gamma \in \mathcal{H}_{\boldsymbol{t}}/G_{\boldsymbol{t}}} X_\Gamma \\ &= \bigcup_{\Gamma \in \mathcal{H}_{\boldsymbol{t}}/G_{\boldsymbol{t}}} \left(\bigcup_{X_\gamma \in \Gamma} \bigcup_{\delta \in \Delta} X_\gamma \cap G_{\boldsymbol{t}}(\boldsymbol{x}_\delta) \right), \end{aligned} \tag{12}$$

where each $X_\gamma \cap G_{\boldsymbol{t}}(\boldsymbol{x}_\delta)$ is non-empty. Furthermore if $\gamma' = g\gamma, g \in G_{\boldsymbol{t}}$, then $\boldsymbol{x} \in X_\gamma \mapsto g\boldsymbol{x} \in X_{g\gamma}$ gives a bijection between $X_\gamma \cap G_{\boldsymbol{t}}(\boldsymbol{x})$ and $X_{\gamma'} \cap G_{\boldsymbol{t}}(\boldsymbol{x})$.

Proof. Similarly to the proof of Lemma 2, intersecting the partition (11) with $X_\Gamma = \bigcup_{\delta\in\Delta} G_{\boldsymbol{t}}(\boldsymbol{x}_\delta)$ gives the partition (12). For each $\boldsymbol{x} \in X_\Gamma$, the orbit $G_{\boldsymbol{t}}(\boldsymbol{x})$ intersects each equivalence class X_γ, i.e. $G_{\boldsymbol{t}}(\boldsymbol{x}) \cap X_\gamma \neq \emptyset$ for all $X_\gamma \in \Gamma$.

From Lemma 4 and the definition of X_Γ, every $g \in G_{\boldsymbol{t}}$ is a bijection of X_Γ to itself and

$$g(X_\gamma \cap G_{\boldsymbol{t}}(\boldsymbol{x})) = X_{g\gamma} \cap G_{\boldsymbol{t}}(\boldsymbol{x}).$$

Therefore $g \in G_{\boldsymbol{t}}$ gives a bijection between $X_\gamma \cap G_{\boldsymbol{t}}(\boldsymbol{x})$ and $X_{\gamma'} \cap G_{\boldsymbol{t}}(\boldsymbol{x})$. Q.E.D.

Example 8 *(Examples 3, 6 continued.) Combining the results of Example 3 and Example 6, a direct product structure for this model is obtained. We see that* $|\Gamma| = |\Delta| = 2$ *and* $|X_\gamma \cap G_{\boldsymbol{t}}(\boldsymbol{x})| = 2$ *for each* $X_\gamma \in \Gamma$. *Since* $G_{\boldsymbol{t}}(X_\gamma) = \mathcal{F}_{\boldsymbol{t}}$, $|\mathcal{H}_{\boldsymbol{t}}/G_{\boldsymbol{t}}| = 1$ *for this model.*

Example 9 *(Examples 4, 7 continued.) Similarly, combining the results of Example 4 and Example 7 yields a direct product structure for this model. We see that* $|\Gamma| = 2, |\Delta| = 3$ *and* $|X_\gamma \cap G_{\boldsymbol{t}}(\boldsymbol{x})| = 2$ *for each* $X_\gamma \in \Gamma$. *Since* $G_{\boldsymbol{t}}(X_\gamma) = \mathcal{F}_{\boldsymbol{t}}$, $|\mathcal{H}_{\boldsymbol{t}}/G_{\boldsymbol{t}}| = 1$ *for this model.*

We see that $|\mathcal{H}_{\boldsymbol{t}}/G_{\boldsymbol{t}}| = 1$ in the above two examples. We present an example of $|\mathcal{H}_{\boldsymbol{t}}/G_{\boldsymbol{t}}| = 2$ by considering the asymmetric indispensable move of Example 5.

Example 10 *(Extension of Example 5.) Consider the case of* $k = 6$ *and* $D_1 = \{1,2\}, D_2 = \{1,3\}, D_3 = \{2,3\}, D_4 = \{4,5\}, D_5 = \{4,6\}, D_6 = \{5,6\}$. *This is a direct product model of two three-way models with all two-dimensional marginals fixed. As for the* $1,2,3$ *axes, we consider* $I_1 = 3, I_2 = 5, I_3 = 6$ *and define* $\boldsymbol{x}_{D_1}, \boldsymbol{x}_{D_2}, \boldsymbol{x}_{D_3}$ *in the same way as Example 5. Therefore the possible patterns of* $\boldsymbol{x}_{\{1,2,3\}}$ *are either* $\boldsymbol{x}_1$ *or* $\boldsymbol{x}_2$ *of Example 5. As for the* $4,5,6$ *axes, we consider* $I_1 = 2, I_2 = 7, I_3 = 7$ *and define* $\boldsymbol{x}_{D_4}, \boldsymbol{x}_{D_5}, \boldsymbol{x}_{D_6}$ *as*

$$\boldsymbol{x}_{D_4} = \boldsymbol{x}_{D_5} = [(11),(12),(13),(14),(15),(16),(17),(21),(22),(23),(24),(25),(26),(27)],$$
$$\boldsymbol{x}_{D_6} = [(11),(12),(21),(23),(32),(34),(43),(45),(54),(56),(65),(67),(76),(77)].$$

In this case, again there are two possible patterns of $\boldsymbol{x}_{\{4,5,6\}}$ *as*

$$\boldsymbol{x}'_1 = [(111),(123),(132),(145),(154),(167),(176),(212),(221),(234),(243),(256),(265),(277)],$$
$$\boldsymbol{x}'_2 = [(112),(121),(134),(143),(156),(165),(177),(211),(223),(232),(245),(254),(267),(276)].$$

$\boldsymbol{x}'_1 - \boldsymbol{x}'_2$ *is a symmetric indispensable move in* $(4,5,6)$*-marginal tables.*

For the sufficient statistic $\boldsymbol{t}$ *defined above, consider the structure of* $\mathcal{F}_{\boldsymbol{t}}$. $\mathcal{F}_{\boldsymbol{t}}$ *is written as*

$$\mathcal{F}_{\boldsymbol{t}} = \{\boldsymbol{x} \mid \boldsymbol{x}_{\{1,2,3\}} = \boldsymbol{x}_1 \text{ or } \boldsymbol{x}_2 \text{ and } \boldsymbol{x}_{\{4,5,6\}} = \boldsymbol{x}'_1 \text{ or } \boldsymbol{x}'_2\}.$$

We have $|\mathcal{F}_{\boldsymbol{t}}| = 3 \cdot 14!$ *since*

$$|\{\boldsymbol{x} \mid \boldsymbol{x}_{\{1,2,3\}} = \boldsymbol{x}_1,\ \boldsymbol{x}_{\{4,5,6\}} = \boldsymbol{x}'_1\}| = 14!,$$
$$|\{\boldsymbol{x} \mid \boldsymbol{x}_{\{1,2,3\}} = \boldsymbol{x}_1,\ \boldsymbol{x}_{\{4,5,6\}} = \boldsymbol{x}'_2\}| = 14!,$$
$$|\{\boldsymbol{x} \mid \boldsymbol{x}_{\{1,2,3\}} = \boldsymbol{x}_2,\ \boldsymbol{x}_{\{4,5,6\}} = \boldsymbol{x}'_1\}| = 14!/2,$$
$$|\{\boldsymbol{x} \mid \boldsymbol{x}_{\{1,2,3\}} = \boldsymbol{x}_2,\ \boldsymbol{x}_{\{4,5,6\}} = \boldsymbol{x}'_2\}| = 14!/2.$$

Consider the M_{13}-equivalence classes of $\mathcal{F}_{\boldsymbol{t}}$. Note that the above four sets are M_2-equivalence classes of $\mathcal{F}_{\boldsymbol{t}}$ since each set contains all combinations of permutations of $(1,2,3)$- and $(4,5,6)$-marginal patterns. Furthermore any two elements in the different sets are not accessible each other by M_{13} since $\boldsymbol{x}_1 - \boldsymbol{x}_2$ and $\boldsymbol{x}'_1 - \boldsymbol{x}'_2$ are indispensable moves in $(1,2,3)$- and $(4,5,6)$-marginal tables, respectively. From these considerations, we see that $|\mathcal{H}_{\boldsymbol{t}}| = 4$. Write $\mathcal{H}_{\boldsymbol{t}} = \{X_{11}, X_{12}, X_{21}, X_{22}\}$, where

$$X_{ij} = \{\boldsymbol{x} \mid \boldsymbol{x}_{\{1,2,3\}} = \boldsymbol{x}_i,\ \boldsymbol{x}_{\{4,5,6\}} = \boldsymbol{x}'_j\}.$$

Considering the $G_{\boldsymbol{t}}$-orbit space of $\mathcal{H}_{\boldsymbol{t}}$, we have

$$\mathcal{H}_{\boldsymbol{t}}/G_{\boldsymbol{t}} = \{\{X_{11}, X_{12}\}, \{X_{21}, X_{22}\}\}$$

since $\boldsymbol{x}_1 - \boldsymbol{x}_2$ is an asymmetric move in $(1,2,3)$-marginal tables, whereas $\boldsymbol{x}'_1 - \boldsymbol{x}'_2$ is a symmetric move in $(4,5,6)$-marginal tables. Therefore $|\mathcal{H}_{\boldsymbol{t}}/G_{\boldsymbol{t}}| = 2$ and $|\Gamma| = 2$ for each $\Gamma \in \mathcal{H}_{\boldsymbol{t}}/G_{\boldsymbol{t}}$, and we have the union of direct product structure in (12).

3.3 Structure of an invariant minimal Markov basis and conditions for its uniqueness

Here we investigate the action of G on the moves. Let $\boldsymbol{z} = \boldsymbol{z}^+ - \boldsymbol{z}^- \in M(D_1, \dots, D_r)$ be a move. By the identification

$$\boldsymbol{z} \leftrightarrow (\boldsymbol{z}^+, \boldsymbol{z}^-) \tag{13}$$

we can regard $\boldsymbol{z}$ as an element of $\mathcal{F}_{\boldsymbol{t}} \times \mathcal{F}_{\boldsymbol{t}}$, where $\boldsymbol{t} = \boldsymbol{t}(\boldsymbol{z}^+) = \boldsymbol{t}(\boldsymbol{z}^-)$. Let $M^{\boldsymbol{t}}(D_1, \dots, D_r)$ denote the set of moves $\boldsymbol{z}$ such that $\boldsymbol{t} = \boldsymbol{t}(\boldsymbol{z}^+) = \boldsymbol{t}(\boldsymbol{z}^-)$.

In order to be more precise, we define

$$\mathcal{F}_{\boldsymbol{t},\boldsymbol{t}} = \{(\boldsymbol{x}_1, \boldsymbol{x}_2) \mid \boldsymbol{x}_1, \boldsymbol{x}_2 \in \mathcal{F}_{\boldsymbol{t}},\ \mathrm{supp}(\boldsymbol{x}_1) \cap \mathrm{supp}(\boldsymbol{x}_2) = \emptyset\},$$

where $\mathrm{supp}(\boldsymbol{x})$ denotes the set of positive cells of $\boldsymbol{x}$. Then by the identification (13), $M^{\boldsymbol{t}}(D_1, \dots, D_r)$ and $\mathcal{F}_{\boldsymbol{t},\boldsymbol{t}}$ are in 1-to-1 correspondence. We identify $M^{\boldsymbol{t}}(D_1, \dots, D_r)$ and $\mathcal{F}_{\boldsymbol{t},\boldsymbol{t}}$ hereafter. For $\alpha \in T_n/G$ we define

$$\mathcal{F}_{\alpha,\alpha} = \cup_{\boldsymbol{t}\in\alpha} \mathcal{F}_{\boldsymbol{t},\boldsymbol{t}}.$$

Then $G(\mathcal{F}_{\alpha,\alpha}) = \mathcal{F}_{\alpha,\alpha}$ and we can consider action of G on each $\mathcal{F}_{\alpha,\alpha}$ separately. It is then clear that Lemma 2 holds also for the moves, i.e.

$$\mathcal{F}_{G(\boldsymbol{t}),G(\boldsymbol{t})} = \bigcup_{i=1}^{a} \bigcup_{j=1}^{b'} \mathcal{F}_{\boldsymbol{t}_i,\boldsymbol{t}_i} \cap G(\boldsymbol{z}_j),$$

where $\boldsymbol{z}_1, \dots, \boldsymbol{z}_{b'}$ are representative moves of the orbits $\mathcal{F}_{G(\boldsymbol{t}),G(\boldsymbol{t})}/G$.

Let $\mathcal{B} \subset M(D_1, \dots, D_r)$ be a finite set of moves and define

$$\mathcal{B}_{n,\alpha} = \mathcal{B} \cap \mathcal{F}_{\alpha,\alpha}, \quad \alpha \in T_n/G.$$

Then $\mathcal{B}$ is partitioned as

$$\mathcal{B} = \bigcup_{n} \bigcup_{\alpha\in T_n/G} \mathcal{B}_{n,\alpha}. \tag{14}$$

Since $\mathcal{B}$ is invariant if and only if it is a union of orbits $G(\boldsymbol{z})$, the following lemma holds.

Lemma 6 *$\mathcal{B}$ is invariant if and only if $\mathcal{B}_{n,\alpha}$ is invariant for each n and $\alpha \in T_n/G$.*

This lemma shows that we can restrict our attention to a particular $\mathcal{F}_{\alpha,\alpha}$ in studying the invariance of a Markov basis.

We now use our argument in Takemura and Aoki (2003) to construct an invariant minimal Markov basis. Fix n and $\alpha \in T_n/G$. Takemura and Aoki (2003) shows that the essential ingredient in the construction of a minimal Markov basis is the $M_{n-1}(D_1,\ldots,D_r)$-equivalence classes of $\mathcal{F}_{\boldsymbol{t}}$, $\boldsymbol{t} \in \alpha$.

Let $\mathcal{B}$ be an invariant set of moves and consider the partition (14). Let $\boldsymbol{z} = \boldsymbol{z}^+ - \boldsymbol{z}^- \in \mathcal{B}_{n,\alpha}$ be a move connecting $X_\gamma \in \mathcal{H}_{\boldsymbol{t}}$ and $X_{\gamma'} \in \mathcal{H}_{\boldsymbol{t}}$, i.e., $\boldsymbol{z}^+ \in X_\gamma$ and $\boldsymbol{z}^- \in X_{\gamma'}$. Then $g\boldsymbol{z} = g\boldsymbol{z}^+ - g\boldsymbol{z}^-$ is a move connecting $X_{g\gamma}$ and $X_{g\gamma'}$. Applying g^{-1} the converse is also true. This implies that the way $\mathcal{B}_{n,\alpha} \cap F_{\boldsymbol{t},\boldsymbol{t}}$ connects the $M_{n-1}(D_1,\ldots,D_r)$-equivalence classes $\mathcal{H}_{\boldsymbol{t}}$ is the same for all $\boldsymbol{t} \in \alpha$.

Now we are in a position to state the following theorem

Theorem 1 *Let $\mathcal{B}$ be a G-invariant minimal Markov basis and Let $\mathcal{B} = \bigcup_n \bigcup_{\alpha \in T_n/G} \mathcal{B}_{n,\alpha}$ be the partition in (14). Then each $\mathcal{B}_{n,\alpha} \cap F_{\boldsymbol{t},\boldsymbol{t}}$, $\boldsymbol{t} \in \alpha, \alpha \in T_n/G$, is a minimal invariant set of moves, which connects $M_{\deg(\boldsymbol{t})-1}(D_1,\ldots,D_r)$-equivalence classes of $\mathcal{F}_{\boldsymbol{t}}$*

Conversely, from each $\alpha \in T_n/G$ with $|\mathcal{H}_\alpha| \geq 2$ choose a representative sufficient statistic $\boldsymbol{t} \in \alpha$ and choose a $G_{\boldsymbol{t}}$-invariant minimal set of moves $\mathcal{B}_{\boldsymbol{t}}$ connecting $M_{\deg(\boldsymbol{t})-1}(D_1,\ldots,D_r)$-equivalence classes of $\mathcal{F}_{\boldsymbol{t}}$, where $G_{\boldsymbol{t}} \subset G$ is the isotropy subgroup of $\boldsymbol{t}$, and extend $\mathcal{B}_{\boldsymbol{t}}$ to $G(\mathcal{B}_{\boldsymbol{t}})$. Then

$$\mathcal{B} = \bigcup_n \bigcup_{\substack{\boldsymbol{t} \in T_n/G \\ |\mathcal{H}_{\boldsymbol{t}}| \geq 2}} G(\mathcal{B}_{\boldsymbol{t}})$$

is a G-invariant minimal Markov basis.

This theorem only adds a statement of minimal G-invariance to the structure of a minimal Markov basis considered in Theorem 1 of Takemura and Aoki (2003). The reason that $\mathcal{B}$ is minimal G-invariant is stated above, and the reason that $\mathcal{B}$ is a Markov basis is included in the proof of Theorem 1 of Takemura and Aoki (2003).

In principle this theorem can be used to construct an invariant minimal Markov basis by considering $\displaystyle\bigcup_{\alpha \in T_n/G} \mathcal{B}_{n,\alpha}, n = 1,2,3,\ldots$ step by step. By the Hilbert basis theorem, there exists some n_0 such that for $n \geq n_0$ no new moves need to be added. Then an invariant minimal Markov basis is written as $\displaystyle\bigcup_{n=1}^{n_0} \bigcup_{\alpha \in T_n/G} \mathcal{B}_{n,\alpha}$. Obviously, there is a considerable difficulty in implementing this procedure directly. To see this, we apply Theorem 1 directly to the complete independence model of the three-way contingency tables.

Example 11 *(Examples 1, 2 continued.) Consider the complete independence model of the three-way contingency tables, i.e., $k = 3, D_1 = \{1\}, D_2 = \{2\}, D_3 = \{3\}$. We apply Theorem 1 directly to this case and derive an invariant minimal Markov basis.*

First consider the case $n = 1$. As is stated in Example 1, T_1 itself is one G-orbit. Further, $\mathcal{F}_{\boldsymbol{t}}$ is one element set for each $\boldsymbol{t} \in T_1$ and is itself an M_0-equivalence class. Therefore we can conclude that no degree 1 move is needed for Markov basis.

Next consider the case $n = 2$. As we derived in Example 1, the orbit space T_2/G is written as (4). Considering (7), we need not consider the case $\boldsymbol{t} \in G(\boldsymbol{t}_1) \cup G(\boldsymbol{t}_2) \cup G(\boldsymbol{t}_3) \cup G(\boldsymbol{t}_4)$ since $\mathcal{F}_{\boldsymbol{t}}$ is one element set (and is itself an M_1-equivalence class). We have to consider all $\boldsymbol{t}$ such that $\boldsymbol{t} \in G(\boldsymbol{t}_5) \cup G(\boldsymbol{t}_6) \cup G(\boldsymbol{t}_7) \cup G(\boldsymbol{t}_8)$. Consider the case $\boldsymbol{t} \in G(\boldsymbol{t}_5) \cup G(\boldsymbol{t}_6) \cup G(\boldsymbol{t}_7)$. We know that $|\mathcal{F}_{\boldsymbol{t}}| = 2$ for these $\boldsymbol{t}$. Representative reference sets are written as

$$
\begin{aligned}
\mathcal{F}_{\boldsymbol{t}_5} &= \{\boldsymbol{x}_5, \boldsymbol{x}'_5\},\ \boldsymbol{x}'_5 = [(112),(121)],\\
\mathcal{F}_{\boldsymbol{t}_6} &= \{\boldsymbol{x}_6, \boldsymbol{x}'_6\},\ \boldsymbol{x}'_6 = [(112),(211)],\\
\mathcal{F}_{\boldsymbol{t}_7} &= \{\boldsymbol{x}_7, \boldsymbol{x}'_7\},\ \boldsymbol{x}'_7 = [(121),(211)].
\end{aligned}
$$

Since each element of $\mathcal{F}_{\boldsymbol{t}}$ is itself an M_1-equivalence class of $\mathcal{F}_{\boldsymbol{t}}$, we have to connect these elements to construct a Markov basis. Obviously, the move that connects two elements of $\mathcal{F}_{\boldsymbol{t}}$ has to be the difference of these, and is an indispensable move. It is also shown that such move is $G_{\boldsymbol{t}}$-invariant. Therefore we have

$$
\mathcal{B}_{\boldsymbol{t}_j} = \{\boldsymbol{z}_j\} = \{\boldsymbol{x}_j - \boldsymbol{x}'_j\},\ j = 5, 6, 7 \tag{15}
$$

and $G(\mathcal{B}_{\boldsymbol{t}_5}) \cup G(\mathcal{B}_{\boldsymbol{t}_6}) \cup G(\mathcal{B}_{\boldsymbol{t}_7})$ is included in all G-invariant minimal Markov basis. Finally consider the case $\boldsymbol{t} \in G(\boldsymbol{t}_8)$. The representative reference set is written as

$$
\begin{gathered}
\mathcal{F}_{\boldsymbol{t}_8} = \{\boldsymbol{x}_8, \boldsymbol{x}'_8, \boldsymbol{x}''_8, \boldsymbol{x}'''_8\},\\
\boldsymbol{x}'_8 = [(112),(221)],\ \boldsymbol{x}''_8 = [(121),(212)],\ \boldsymbol{x}'''_8 = [(211),(122)].
\end{gathered}
$$

and each element of $\mathcal{F}_{\boldsymbol{t}_8}$ is itself an M_1-equivalence class. We have to construct a set of moves which is $G_{\boldsymbol{t}_8}$-invariance and connects these four equivalence classes. Here we have the following proposition.

Proposition 1 *$G_{\boldsymbol{t}_8}$-invariant minimal set of moves $\mathcal{B}_{\boldsymbol{t}_8}$ which connects the four elements of $\mathcal{F}_{\boldsymbol{t}_8}$ is either of the following three sets.*

$$
\begin{aligned}
&\{\boldsymbol{x}_8 - \boldsymbol{x}'_8, \boldsymbol{x}''_8 - \boldsymbol{x}'''_8, \boldsymbol{x}_8 - \boldsymbol{x}''_8, \boldsymbol{x}'_8 - \boldsymbol{x}'''_8\},\\
&\{\boldsymbol{x}_8 - \boldsymbol{x}'_8, \boldsymbol{x}''_8 - \boldsymbol{x}'''_8, \boldsymbol{x}_8 - \boldsymbol{x}'''_8, \boldsymbol{x}'_8 - \boldsymbol{x}''_8\},\\
&\{\boldsymbol{x}_8 - \boldsymbol{x}''_8, \boldsymbol{x}'_8 - \boldsymbol{x}'''_8, \boldsymbol{x}_8 - \boldsymbol{x}'''_8, \boldsymbol{x}'_8 - \boldsymbol{x}''_8\}.
\end{aligned} \tag{16}
$$

Proof. *This proposition is directly shown from the fact that the following three sets of moves,*

$$
\{\boldsymbol{x}_8 - \boldsymbol{x}'_8, \boldsymbol{x}''_8 - \boldsymbol{x}'''_8\},\ \{\boldsymbol{x}_8 - \boldsymbol{x}''_8, \boldsymbol{x}'_8 - \boldsymbol{x}'''_8\},\ \{\boldsymbol{x}_8 - \boldsymbol{x}'''_8, \boldsymbol{x}'_8 - \boldsymbol{x}''_8\} \tag{17}
$$

are $G_{\boldsymbol{t}_8}$-orbits in $M(D_1, D_2, D_3)$, respectively. *Q.E.D.*

We consider the action of group $G_{\boldsymbol{t}_8}$ to the reference set $\mathcal{F}_{\boldsymbol{t}_8}$ in detail. We have shown in Example 2 that $G_{\boldsymbol{t}_8} = \widetilde{G}^1_{12,12} \times \widetilde{G}^2_{12,12} \times \widetilde{G}^3_{12,12}$. Let $g^1 \in G^1_{12,12} \times G^2_{12,12} \times G^3_{12,12} \subset G_{\boldsymbol{t}_8}$. Then it follows that $\{e, g^1\}$ is an isotropy subgroup either of $\boldsymbol{x}_8, \boldsymbol{x}'_8, \boldsymbol{x}''_8, \boldsymbol{x}'''_8$. The pair of $(G_{\boldsymbol{t}_8}, \mathcal{F}_{\boldsymbol{t}_8})$ is isomorphic to $(G_{\boldsymbol{t}_8}, G_{\boldsymbol{t}_8}/\{e, g^1\})$, and $G_{\boldsymbol{t}_8}/\{e, g^1\}$ is isomorphic to Klein four-group.

Next consider the case $n = 3$. But in this case, it is observed that no move of degree 3 is needed. In fact, no move of degree $n \geq 3$ is needed in this model as shown in Section 3 of Takemura and Aoki (2003). From these considerations, an invariant minimal Markov basis for this model is summarized as follows.

Proposition 2 *A G-invariant minimal Markov basis for the complete independent model of the three-way contingency tables is written as*

$$\mathcal{B} = G(\mathcal{B}_{\boldsymbol{t}_5}) \cup G(\mathcal{B}_{\boldsymbol{t}_6}) \cup G(\mathcal{B}_{\boldsymbol{t}_7}) \cup G(\mathcal{B}_{\boldsymbol{t}_8}),$$

where $\mathcal{B}_{\boldsymbol{t}_5}, \mathcal{B}_{\boldsymbol{t}_6}, \mathcal{B}_{\boldsymbol{t}_7}$ are sets of indispensable moves given in (15) and $\mathcal{B}_{\boldsymbol{t}_8}$ is either of the three sets of dispensable moves in (16).

The number of the G-invariant minimal Markov basis elements is derived as

$$|\mathcal{B}| = \sum_{j=5}^{8} |G(\mathcal{B}_{\boldsymbol{t}_j})| = \sum_{j=5}^{8} |G(\boldsymbol{t}_j)| \cdot |\mathcal{B}_{\boldsymbol{t}_j}| = \sum_{j=5}^{7} |G(\boldsymbol{t}_j)| + 2|G(\boldsymbol{t}_8)|$$

where $|G(\boldsymbol{t}_j)|$ is given in (6).

In this example, we see that an invariant minimal Markov basis for this model is not unique. It should be noted that a minimal Markov basis is not unique either for this model (Takemura and Aoki, 2003). Since the set of the indispensable moves is G-invariant, an invariant minimal Markov basis and a minimal Markov basis differ only in dispensable moves. This is always true and here we also state the following obvious fact.

Lemma 7 *If there exists a unique minimal Markov basis, then it is a unique invariant minimal Markov basis.*

Now we derive a necessary and sufficient condition for the existence of a unique invariant minimal Markov basis. As a direct consequence of Theorem 1, first we give the following corollary to Theorem 1 without a proof.

Corollary 1 *An invariant minimal Markov basis is unique if and only if for each n and $\alpha \in T_n/G$ with $|\mathcal{H}_\alpha| \geq 2$ $\mathcal{B}_{\boldsymbol{t}}, \boldsymbol{t} \in \alpha$, is a unique minimal $G_{\boldsymbol{t}}$-invariant set of moves connecting $M_{\deg(\boldsymbol{t})-1}(D_1, \dots, D_r)$-equivalence classes of $\mathcal{F}_{\boldsymbol{t}}$.*

Therefore we consider $\mathcal{F}_{\boldsymbol{t}}$ for each $\boldsymbol{t}$ separately. Recall that there is an union of direct products structure in $\mathcal{F}_{\boldsymbol{t}}$ as shown in (12). Since each X_Γ is $G_{\boldsymbol{t}}$-invariant, first we summarize the structure of a minimal invariant set of moves connecting different X_Γ's, $\Gamma \in \mathcal{H}_{\boldsymbol{t}}/G_{\boldsymbol{t}}$.

Lemma 8 *$\mathcal{B}$ is a $G_{\boldsymbol{t}}$-invariant minimal set of moves that connects $X_\Gamma, \Gamma \in \mathcal{H}_{\boldsymbol{t}}/G_{\boldsymbol{t}}$ if and only if $\mathcal{B}$ is written as*

$$\mathcal{B} = G_{\boldsymbol{t}}(\boldsymbol{z}_1) \cup \cdots \cup G_{\boldsymbol{t}}(\boldsymbol{z}_{|\mathcal{H}_{\boldsymbol{t}}/G_{\boldsymbol{t}}|-1}), \qquad (18)$$

where the set of the representative moves $\boldsymbol{z}_1, \dots, \boldsymbol{z}_{|\mathcal{H}_{\boldsymbol{t}}/G_{\boldsymbol{t}}|-1}$ connects $X_\Gamma, \Gamma \in \mathcal{H}_{\boldsymbol{t}}/G_{\boldsymbol{t}}$ into a tree.

Proof. Let $\boldsymbol{z} = \boldsymbol{z}^+ - \boldsymbol{z}^-$ is a move that connects X_Γ and $X_{\Gamma'}, \Gamma \neq \Gamma'$, i.e., $\boldsymbol{z}^+ \in X_\Gamma$ and $\boldsymbol{z}^- \in X_{\Gamma'}$. Then $g\boldsymbol{z}$ also connects X_Γ and $X_{\Gamma'}$ for any $g \in G_{\boldsymbol{t}}$, since $g\boldsymbol{z}^+ \in X_\Gamma, g\boldsymbol{z}^- \in X_{\Gamma'}$. Q.E.D.

This lemma implies the following necessarily condition for existing an unique invariant minimal Markov basis.

Corollary 2 *If an invariant minimal Markov basis is unique, then the following conditions hold for all* $\boldsymbol{t}$ *such that* $|\mathcal{H}_{\boldsymbol{t}}| \geq 2$.

- (*i*) $|\mathcal{H}_{\boldsymbol{t}}/G_{\boldsymbol{t}}|$ *is at most* 2.
- (*ii*) *For* $\mathcal{F}_{\boldsymbol{t}}$ *such that* $|\mathcal{H}_{\boldsymbol{t}}/G_{\boldsymbol{t}}| = 2, G_{\boldsymbol{t}}(\boldsymbol{z})$ *is the same for all* $\boldsymbol{z} = \boldsymbol{z}^+ - \boldsymbol{z}^-, \boldsymbol{z}^+ \in X_\gamma, \boldsymbol{z}^- \in X_{\gamma'}$, *where* $\mathcal{F}_{\boldsymbol{t}} = X_\gamma \cup X_{\gamma'}$.

Next we consider the structure of a minimal invariant set of moves connecting the equivalence classes in each X_Γ. Consider a move $\boldsymbol{z} = \boldsymbol{z}^+ - \boldsymbol{z}^-$ connecting different $X_\gamma \in X_\Gamma$, i.e., $\boldsymbol{z}^+ \in X_\gamma, \boldsymbol{z}^- \in X_{\gamma'}, X_\gamma \neq X_{\gamma'}$. Since the action of $G_{\boldsymbol{t}}$ on X_Γ is transitive, without loss of generality we fix X_γ to be a particular equivalence set X_{γ_0} and let $\boldsymbol{z}^+ \in X_{\gamma_0}$ when we consider $G_{\boldsymbol{t}}(\boldsymbol{z})$. For each $\gamma' \neq \gamma_0$, we define an *orbit graph* $\mathcal{G}_{\gamma'} = \mathcal{G}(X_\Gamma, E_{\gamma'})$, where the edge set $E_{\gamma'}$ is defined as

$$E_{\gamma'} = \{(X_{\gamma_1}, X_{\gamma_2}) \mid (g\boldsymbol{z}^+, g\boldsymbol{z}^-) \in (X_{\gamma_1}, X_{\gamma_2}) \text{ for some } g \in G_{\boldsymbol{t}} \text{ where } \boldsymbol{z}^+ \in X_{\gamma_0}, \boldsymbol{z}^- \in X_{\gamma'}\}.$$

It should be noted that $E_{\gamma'}$ (and hence $\mathcal{G}_{\gamma'}$) does not depend on the choice of $\boldsymbol{z}^+ \in X_{\gamma_0}$ and $\boldsymbol{z}^- \in X_{\gamma'}$, whereas the orbits $G_{\boldsymbol{t}}(\boldsymbol{z})$ differ for the different choice of (δ_1, δ_2), where $\boldsymbol{z}^+ \in X_{\gamma_0} \cap G_{\boldsymbol{t}}(\boldsymbol{x}_{\delta_1})$, $\boldsymbol{z}^- \in X_{\gamma'} \cap G_{\boldsymbol{t}}(\boldsymbol{x}_{\delta_2})$ when $|\Delta| = |X_\Gamma/G_{\boldsymbol{t}}| \geq 2$. Furthermore

$$E_{\gamma_1} \cap E_{\gamma_2} = \emptyset \text{ for all } \gamma_1 \neq \gamma_2$$

by definition. We also define that the orbit graph $\mathcal{G}_{\gamma'}$ is *indispensable* if the graph $\mathcal{G}(X_\Gamma, \bigcup_{\gamma \neq \gamma'} E_\gamma)$ is not connected. An important point here is that if the set of indispensable orbit graphs connects all the equivalence classes in X_Γ, then this corresponds to the unique minimal invariant set of moves for X_Γ. Combining this result and Corollary 2, we have the following result.

Theorem 2 *A minimal invariant Markov basis is unique if and only if the following conditions hold for all* $\boldsymbol{t}$ *such that* $|\mathcal{H}_{\boldsymbol{t}}| \geq 2$, *in addition to (i) and (ii) of Corollary 2.*

- (*iii*) $|\Delta| = |X_\Gamma/G_{\boldsymbol{t}}| = 1$ *for all* Γ.
- (*iv*) *The set of indispensable orbit graphs connects all* $X_\gamma \in X_\Gamma$ *for all* Γ.
- (*v*) *For all indispensable orbit graphs of (iv), there is only one orbit* $G_{\boldsymbol{t}}(\boldsymbol{z})$ *that derives it.*

In Section 3 of Takemura and Aoki (2003), minimal Markov bases and their uniqueness are shown for some examples. We see that for some examples a minimal Markov basis is unique, and for other examples it is not unique. Since a unique minimal Markov basis is also the unique invariant minimal Markov basis, logically interesting case is that, an invariant minimal Markov basis is unique, nevertheless a minimal Markov basis is not unique. The Hardy-Weinberg model is such an example, if we define a symmetric group acting to the upper triangular tables appropriately. See Section 3 of Takemura and Aoki (2003). Except for this peculiar example, the only example that we have found so far is a one-way contingency tables.

Example 12 *Consider the case of $k = 1$ and $D = \{1\}$. As is stated in Takemura and Aoki (2003), a minimal Markov basis for this case is not unique, and consists of $I_1 - 1$ degree 1 moves that connect I elements in X_1 into a tree. By Cayley's theorem, there are $I_1^{I_1-2}$ ways of choosing a minimal Markov basis. On the other hand, the set of all degree 1 moves,*

$$\mathcal{B} = \{\boldsymbol{x} - \boldsymbol{x}' \mid \boldsymbol{x}, \boldsymbol{x}' \in X_1, \boldsymbol{x} \neq \boldsymbol{x}'\}$$

is a G-orbit in $M(D)$. Therefore $\mathcal{B}$ is the unique invariant minimal Markov basis. $\mathcal{B}$ consists of $\binom{I_1}{2}$ degree 1 moves.

We show that three examples considered so far do not have unique invariant minimal Markov basis.

Example 13 *(Examples 3, 6, 8 continued.) Consider $\mathcal{B}_{4,\boldsymbol{t}}$ where $\boldsymbol{t} \in T_4/G$ is given in Example 3. In this case, the conditions of Corollary 2 is satisfied since $|\mathcal{H}_{\boldsymbol{t}}/G_{\boldsymbol{t}}| = 1$. However, the ways of connecting two equivalence classes, $\{\boldsymbol{x}_1, \boldsymbol{x}_2, \boldsymbol{x}_3, \boldsymbol{x}_4\}, \{\boldsymbol{x}_5, \boldsymbol{x}_6, \boldsymbol{x}_7, \boldsymbol{x}_8\}$ are not unique. In fact, though the orbit graph (i.e., connected two vertices) is unique and indispensable, there are the following five $G_{\boldsymbol{t}}$-invariant minimal set of moves that derives it.*

$$\begin{array}{l}
\{\boldsymbol{x}_1 - \boldsymbol{x}_5, \boldsymbol{x}_4 - \boldsymbol{x}_8\}, \quad \{\boldsymbol{x}_1 - \boldsymbol{x}_8, \boldsymbol{x}_4 - \boldsymbol{x}_5\}, \\
\{\boldsymbol{x}_2 - \boldsymbol{x}_6, \boldsymbol{x}_3 - \boldsymbol{x}_7\}, \quad \{\boldsymbol{x}_2 - \boldsymbol{x}_7, \boldsymbol{x}_3 - \boldsymbol{x}_6\}, \\
\{\boldsymbol{x}_1 - \boldsymbol{x}_6, \boldsymbol{x}_1 - \boldsymbol{x}_7, \boldsymbol{x}_2 - \boldsymbol{x}_5, \boldsymbol{x}_2 - \boldsymbol{x}_8, \boldsymbol{x}_3 - \boldsymbol{x}_5, \boldsymbol{x}_3 - \boldsymbol{x}_8, \boldsymbol{x}_4 - \boldsymbol{x}_6, \boldsymbol{x}_4 - \boldsymbol{x}_7\}.
\end{array}$$

Example 14 *(Examples 4, 7, 9 continued.) Consider $\mathcal{B}_{4,\boldsymbol{t}}$ where $\boldsymbol{t} \in T_4/G$ is given in Example 4. Similarly to Example 13, the conditions of Corollary 2 is satisfied in this case since $|\mathcal{H}_{\boldsymbol{t}}/G_{\boldsymbol{t}}| = 1$. However, the ways of connecting two equivalence classes, $\{\boldsymbol{x}_1, \boldsymbol{x}_2, \boldsymbol{x}_3, \boldsymbol{x}_4, \boldsymbol{x}_9, \boldsymbol{x}_{10}\}$, $\{\boldsymbol{x}_5, \boldsymbol{x}_6, \boldsymbol{x}_7, \boldsymbol{x}_8, \boldsymbol{x}_{11}, \boldsymbol{x}_{12}\}$ are not unique. In this case, the orbit graph also consists of connected two vertices, and is unique and indispensable. However, there are the following nine $G_{\boldsymbol{t}}$-invariant minimal set of moves that derives it.*

$$\begin{array}{l}
\{\boldsymbol{x}_1 - \boldsymbol{x}_5, \boldsymbol{x}_4 - \boldsymbol{x}_8\}, \quad \{\boldsymbol{x}_1 - \boldsymbol{x}_8, \boldsymbol{x}_4 - \boldsymbol{x}_5\}, \\
\{\boldsymbol{x}_2 - \boldsymbol{x}_6, \boldsymbol{x}_3 - \boldsymbol{x}_7\}, \quad \{\boldsymbol{x}_2 - \boldsymbol{x}_7, \boldsymbol{x}_3 - \boldsymbol{x}_6\}, \\
\{\boldsymbol{x}_9 - \boldsymbol{x}_{11}, \boldsymbol{x}_{10} - \boldsymbol{x}_{12}\}, \quad \{\boldsymbol{x}_9 - \boldsymbol{x}_{12}, \boldsymbol{x}_{10} - \boldsymbol{x}_{11}\}, \\
\{\boldsymbol{x}_1 - \boldsymbol{x}_6, \boldsymbol{x}_1 - \boldsymbol{x}_7, \boldsymbol{x}_2 - \boldsymbol{x}_5, \boldsymbol{x}_2 - \boldsymbol{x}_8, \boldsymbol{x}_3 - \boldsymbol{x}_5, \boldsymbol{x}_3 - \boldsymbol{x}_8, \boldsymbol{x}_4 - \boldsymbol{x}_7, \boldsymbol{x}_4 - \boldsymbol{x}_6\}, \\
\{\boldsymbol{x}_1 - \boldsymbol{x}_{11}, \boldsymbol{x}_1 - \boldsymbol{x}_{12}, \boldsymbol{x}_9 - \boldsymbol{x}_5, \boldsymbol{x}_9 - \boldsymbol{x}_8, \boldsymbol{x}_4 - \boldsymbol{x}_{11}, \boldsymbol{x}_4 - \boldsymbol{x}_{12}, \boldsymbol{x}_{10} - \boldsymbol{x}_5, \boldsymbol{x}_{10} - \boldsymbol{x}_8\}, \\
\{\boldsymbol{x}_2 - \boldsymbol{x}_{11}, \boldsymbol{x}_2 - \boldsymbol{x}_{12}, \boldsymbol{x}_9 - \boldsymbol{x}_6, \boldsymbol{x}_9 - \boldsymbol{x}_7, \boldsymbol{x}_3 - \boldsymbol{x}_{11}, \boldsymbol{x}_3 - \boldsymbol{x}_{12}, \boldsymbol{x}_{10} - \boldsymbol{x}_6, \boldsymbol{x}_{10} - \boldsymbol{x}_7\}.
\end{array}$$

Example 15 *(Examples 1, 2, 11 continued.) We have seen that an invariant minimal Markov basis is not unique for the complete independence model of the three-way contingency tables. In fact, three sets of moves (17) in Proposition 1 correspond to different orbit graphs, respectively. Therefore in this case, each orbit graph is dispensable.*

4 Invariant minimal Markov basis for all hierarchical 2^4 models

In this section, we give a complete list of a minimal and an invariant minimal Markov basis for all hierarchical $2 \times 2 \times 2 \times 2$ models. Though our list is restricted to the case of $2 \times 2 \times 2 \times 2$, if a set of moves whose supports are contained in $2 \times 2 \times 2 \times 2$ array constitutes a Markov basis for a general $I_1 \times I_2 \times I_3 \times I_4$ case, we can derive a minimal and an invariant minimal Markov basis for the general case, by considering the orbits T_n/G. For example, a minimal and an invariant minimal Markov basis for the complete independence model of the three-way contingency tables are derived in Examples 1, 2 and 11. These results are extensions of the results for the $2 \times 2 \times 2$ case, since the moves with supports contained in $2 \times 2 \times 2$ arrays constitute a Markov basis for general case.

To derive the following list, we used several methods. If the model is decomposable, it is known that Markov bases consist of degree 2 moves only (Dobra, 2001). If the model is reducible, an algorithm proposed by Dobra and Sullivant (2002) can be used. We also perform a primitive consideration of the sign patterns, which is similar to Aoki and Takemura (2003).

What the list means is as follows. The models that we consider are hierarchical 2^4 models. There are 20 different models. Figure 1 is the list of independence graphs of these models.

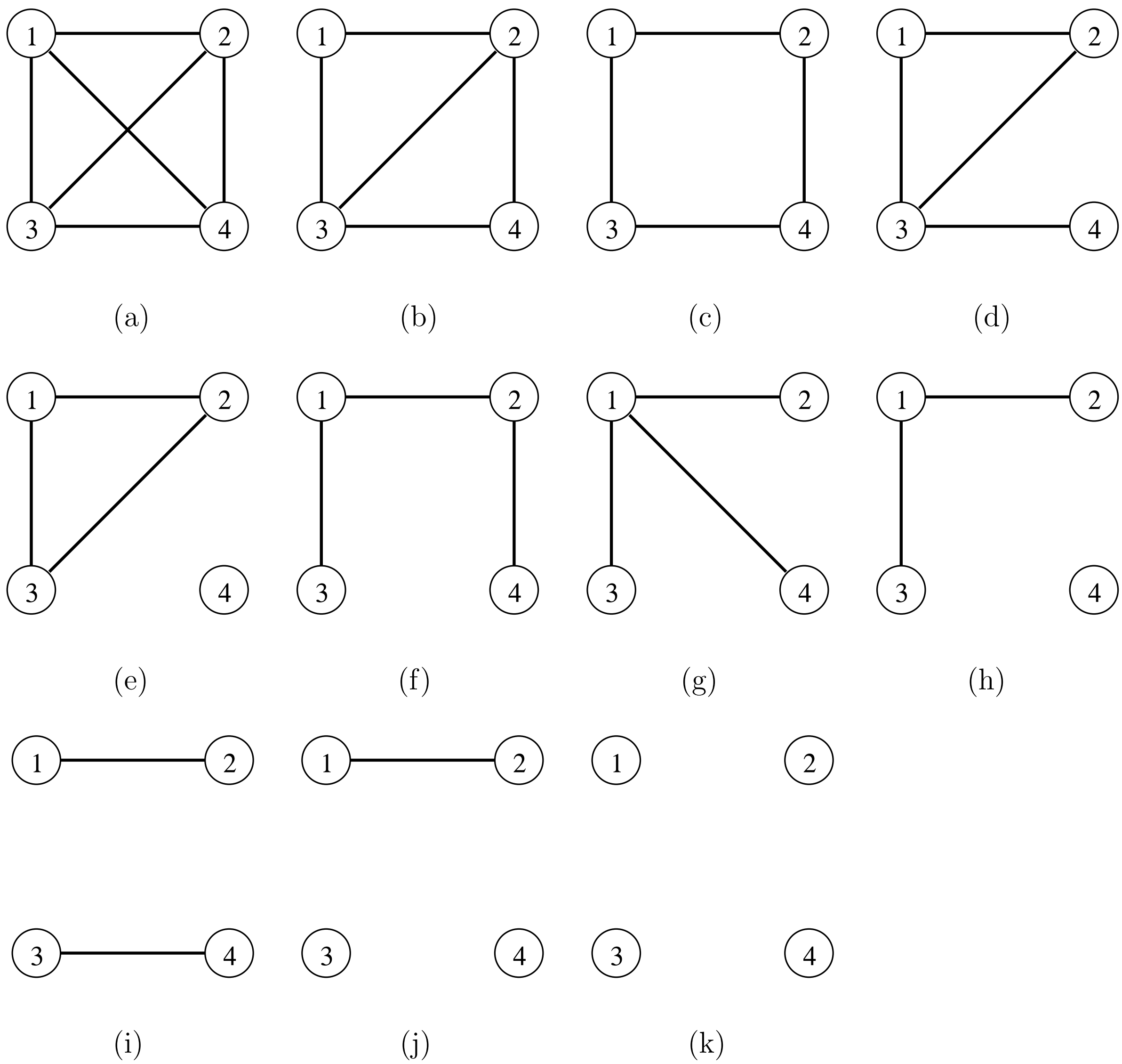

Figure 1: Independence graphs for four-way contingency tables

We specify each model by their generating set. For example, a model 123/24/34 means $D_1 = \{1,2,3\}, D_2 = \{2,4\}, D_3 = \{3,4\}$. The **degree of freedom** is a number of independent cells in 2^4 tables under the models. For each model, we give a minimal and an invariant minimal Markov basis. As stated in Theorem 1, an invariant minimal Markov basis is written as

$$\mathcal{B} = \bigcup_{n=1}^{n_0} \bigcup_{\substack{\boldsymbol{t} \in T_n/G \\ |\mathcal{H}_{\boldsymbol{t}}| \geq 2}} G(\mathcal{B}_{\boldsymbol{t}}).$$

In our models, n_0 is at most 8. We give a list of $\mathcal{B}_{\boldsymbol{t}}$ for all $\boldsymbol{t} \in T_n/G, |\mathcal{H}_{\boldsymbol{t}}| \geq 2$. To specify each move, we use symbols $\boldsymbol{x}$ and $\boldsymbol{y}$ to denote representative elements $\boldsymbol{x} \in X_4$ and $\boldsymbol{y} \in X_2$ in this section. Though some of these representative elements are already used in Examples in the previous section, we newly number these elements to avoid confusion. We give sets of **indispensable moves**, i.e., $\mathcal{B}_{\boldsymbol{t}}$ such that $|\mathcal{H}_{\boldsymbol{t}}| = 2$, with their representative elements. For example, there are 6 indispensable moves of degree 4 with representative elements $\boldsymbol{x}_1, \boldsymbol{x}_2, \boldsymbol{x}_3$ for the model 123/124/34. This means that, for $i = 1,2,3$, each reference set with the same sufficient statistic $\boldsymbol{t}(\boldsymbol{x}_i)$ has two elements, i.e., $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{x}_i)} = \{\boldsymbol{x}_{i,1}, \boldsymbol{x}_{i,2}\}$, and the representative move is written as $\mathcal{B}_{\boldsymbol{t}(\boldsymbol{x}_i)} = \{\boldsymbol{x}_{i,1} - \boldsymbol{x}_{i,2}\}$. A complete list of the indispensable moves is given by extending each $\mathcal{B}_{\boldsymbol{t}(\boldsymbol{x}_i)}$ to $G(\mathcal{B}_{\boldsymbol{t}(\boldsymbol{x}_i)})$, i.e.,

$$G(\mathcal{B}_{\boldsymbol{t}(\boldsymbol{x}_1)}) \cup G(\mathcal{B}_{\boldsymbol{t}(\boldsymbol{x}_2)}) \cup G(\mathcal{B}_{\boldsymbol{t}(\boldsymbol{x}_3)}),$$

and there are

$$6 = \sum_{i=1}^{3} |G(\mathcal{B}_{\boldsymbol{t}(\boldsymbol{x}_i)})| = \sum_{i=1}^{3} |\mathcal{B}_{\boldsymbol{t}(\boldsymbol{x}_i)}| \cdot |G(\boldsymbol{t}(\boldsymbol{x}_i))| = \sum_{i=1}^{3} |G(\boldsymbol{t}(\boldsymbol{x}_i))|$$

elements of indispensable moves. In our examples, $|G(\boldsymbol{t})|$ is equal for each n such that $\boldsymbol{t} \in T_n$ when $|\mathcal{H}_{\boldsymbol{t}}| = 2$ and given as

$$|G(\boldsymbol{t})| = \begin{cases} 1, & \boldsymbol{t} \in T_8, \\ 8, & \boldsymbol{t} \in T_6, \\ 2, & \boldsymbol{t} \in T_4, \\ 4, & \boldsymbol{t} \in T_2. \end{cases}$$

Uniqueness of a minimal Markov basis is also shown. As we have stated, if the set of indispensable moves constitutes a Markov basis, this is a unique (invariant) minimal Markov basis. On the other hand, if a minimal Markov basis is not unique, uniqueness of an invariant minimal Markov basis is important. In all of 2^4 hierarchical models, however, we found that an invariant minimal Markov basis is also not unique when a minimal Markov basis is not unique. We discuss this point in Section 5. When a minimal basis is not unique, there is at least one reference set which itself does not constitute one $\mathcal{B}$-equivalence class, where $\mathcal{B}$ is the set of indispensable moves. Furthermore, if $\mathcal{F}_{\boldsymbol{t}}$ is such a reference set, all the reference sets in $\mathcal{F}_{G(\boldsymbol{t})}$ have the isomorphic structures as stated in Lemma 2. We give this **isomorphic structures of reference sets** with representative elements, $|G(\boldsymbol{t})|, |\mathcal{F}_{G(\boldsymbol{t})}/G|$ and $|\mathcal{F}_{\boldsymbol{t}}|$. Then we give a **direct product structure for each reference set** $\mathcal{F}_{\boldsymbol{t}} \in \mathcal{F}_{G(\boldsymbol{t})}$ as shown in Lemma 5, with $|\Delta|$ and $|\Lambda|$. We omit $|\mathcal{H}_{\boldsymbol{t}}/G_{\boldsymbol{t}}|$ since for all our models $|\mathcal{H}_{\boldsymbol{t}}/G_{\boldsymbol{t}}| = 1$. Finally we give a **minimal basis**, **orbit graphs** and an **invariant minimal basis for each reference set**. As for a minimal basis, we only show the number of different set of dispensable moves and number of its elements, which are calculated from the number of equivalence classes and the number of their elements. As is stated in Takemura and Aoki (2003), if a reference set consists of t equivalence classes and each equivalence class has u elements, there are $u^{t^{t-2}}$ different set of $t-1$ moves for this reference set in a minimal basis. On the other hand, for an invariant minimal basis, we show the orbit graphs and the orbits of moves that derive them. Table 1 shows the numbers of elements in each minimal basis and invariant minimal basis.

4.1 Models with the independence graph (a)

- Model 1234 (saturated, graphical model)
  degree of freedom: 0

- Model 123/124/134/234
  degree of freedom: 1
  indispensable move: 1 move of degree 8 with representative element

  $$[(1111)(1122)(1212)(1221)(2112)(2121)(2211)(2222)].$$

  uniqueness: unique minimal basis exists.

- Model 123/124/134
  degree of freedom: 2
  indispensable moves: 2 moves of degree 4 with representative element

  $$\boldsymbol{x}_1 = [(1111)(1122)(1212)(1221)].$$

  uniqueness: unique minimal basis exists.

- Model 123/124/34
  degree of freedom: 3
  indispensable moves: 6 moves of degree 4 with representative elements

  $$\boldsymbol{x}_1,\ \boldsymbol{x}_2 = [(1111)(1122)(2112)(2121)],\ \boldsymbol{x}_3 = [(1111)(1122)(2212)(2221)].$$

  uniqueness: unique minimal basis exists.

- Model 123/14/24/34
  degree of freedom: 4
  indispensable moves: 12 moves of degree 4 with representative elements

  $$\boldsymbol{x}_1,\ \boldsymbol{x}_2,\ \boldsymbol{x}_3,\ \boldsymbol{x}_4 = [(1111)(1212)(2112)(2211)],$$
  $$\boldsymbol{x}_5 = [(1111)(1212)(2122)(2221)],\ \boldsymbol{x}_6 = [(1111)(1222)(2112)(2221)]$$

  and 8 moves of degree 6 with representative element

  $$[(1111)(1111)(1122)(1212)(2112)(2221)].$$

  uniqueness: unique minimal basis exists.

Table 1: List of minimal basis and invariant minimal basis for 2^4 hierarchical models

graph	generating set	number of basis
(a)	1234	$\emptyset$
	123/124/134/234	unique minimal basis (1 move of deg 8)
	123/124/134	unique minimal basis (2 moves of deg 4)
	123/124/34	unique minimal basis (6 moves of deg 4)
	123/14/24/34	unique minimal basis (12 moves of deg 4 and 8 moves of deg 6)
	12/13/14/23/24/34	unique minimal basis (20 moves of deg 4 and 40 moves of deg 6)
(b)	123/234	unique minimal basis (4 moves of deg 2)
	123/24/34	unique minimal basis (4 moves of deg 2 and 16 moves of deg 4)
	12/13/23/24/34	indispensable moves: 4 moves of deg 2 and 28 moves of deg 4 dispensable moves of a minimal basis: 16 kinds of 3 moves of deg 4 dispensable moves of an invariant minimal basis: 3 kinds of 4 moves of deg 4
(c)	12/13/24/34	unique minimal basis (8 moves of deg 2 and 8 moves of deg 4)
(d)	123/34	unique minimal basis (12 moves of deg 2)
	12/13/23/34	indispensable moves: 12 moves of deg 2 and 4 moves of deg 4 dispensable moves of a minimal basis: 4096 kinds of 5 moves of deg 4 dispensable moves of an invariant minimal basis: 8 kinds of 10 moves of deg 4 or 2 kinds of 16 moves of deg 4
(e)	123/4	unique minimal basis (28 moves of deg 2)
	12/13/23/4	indispensable moves: 28 moves of deg 2 and 2 moves of deg 4 dispensable moves of a minimal basis: 9216 kinds of 3 moves of deg 4 dispensable moves of an invariant minimal basis: 24 kinds of 10 moves of deg 4 or 12 kinds of 16 moves of deg 4
(f)	12/13/24	unique minimal basis (20 moves of deg 2)
(g)	12/13/14	indispensable moves: 12 moves of deg 2 dispensable moves of a minimal basis: 256 kinds of 6 moves of deg 2 dispensable moves of an invariant minimal basis: 3 kinds of 8 moves of deg 2
(h)	12/13/4	indispensable moves: 28 moves of deg 2 dispensable moves of a minimal basis: 256 kinds of 6 moves of deg 2 dispensable moves of an invariant minimal basis: 3 kinds of 8 moves of deg 2
(i)	12/34	unique minimal basis (36 moves of deg 2)
(j)	12/3/4	indispensable moves: 28 moves of deg 2 dispensable moves of a minimal basis: $16^6 = 16777216$ kinds of 18 moves of deg 2 dispensable moves of an invariant minimal basis: 27 kinds of 24 moves of deg 2
(k)	1/2/3/4	indispensable moves: 24 moves of deg 2 dispensable moves of a minimal basis: $16^8 \times 8^6 = 1.1259 \times 10^{15}$ kinds of 31 moves of deg 2 dispensable moves of an invariant minimal basis: 2268 kinds of 44 moves of deg 2

- Model 12/13/14/23/24/34
  degree of freedom: 5
  indispensable moves: 20 moves of degree 4 with representative elements

  $$\begin{aligned}&\boldsymbol{x}_1,\ \boldsymbol{x}_2,\ \boldsymbol{x}_3,\ \boldsymbol{x}_4,\ \boldsymbol{x}_5,\ \boldsymbol{x}_6,\\ &\boldsymbol{x}_7 = [(1111)(1221)(2121)(2211)],\ \boldsymbol{x}_8 = [(1111)(1221)(2122)(2212)],\\ &\boldsymbol{x}_9 = [(1111)(1222)(2121)(2212)],\ \boldsymbol{x}_{10} = [(1111)(1222)(2122)(2211)]\end{aligned}$$

  and 40 moves of degree 6 with representative elements

  $$\begin{aligned}&[(1111)(1111)(1122)(1212)(2112)(2221)],\\ &[(1111)(1111)(1222)(2122)(2212)(2221)],\\ &[(1111)(1111)(1122)(1221)(2121)(2212)],\\ &[(1111)(1111)(1212)(1221)(2122)(2211)],\\ &[(1111)(1111)(1222)(2112)(2121)(2211)].\end{aligned}$$

  uniqueness: unique minimal basis exists.

4.2 Models with the independence graph (b)

- Model 123/234 (graphical, decomposable model)
  degree of freedom: 4
  indispensable moves: 4 moves of degree 2 with representative element

  $$\boldsymbol{y}_1 = [(1111)(2112)].$$

  uniqueness: unique minimal basis exists.

- Model 123/24/34
  degree of freedom: 5
  indispensable moves: 4 moves of degree 2 with representative element $\boldsymbol{y}_1$,
  and 16 moves of degree 4 with representative elements

  $$\begin{aligned}&\boldsymbol{x}_1,\ \boldsymbol{x}_3,\\ &\boldsymbol{x}_{11} = [(1111)(1122)(1212)(2221)],\ \boldsymbol{x}_{12} = [(1111)(1122)(1221)(2212)],\\ &\boldsymbol{x}_{13} = [(1111)(1212)(1221)(2122)],\ \boldsymbol{x}_{14} = [(1111)(1212)(2122)(2221)],\\ &\boldsymbol{x}_{15} = [(1111)(1221)(2122)(2212)],\ \boldsymbol{x}_{16} = [(1111)(2122)(2212)(2221)].\end{aligned}$$

  uniqueness: unique minimal basis exists.

- Model 12/13/23/24/34
  degree of freedom: 6
  indispensable moves: 4 moves of degree 2 with representative element $\boldsymbol{y}_1$,
  and 28 moves of degree 4 with representative elements

  $$\begin{aligned}&\boldsymbol{x}_1,\ \boldsymbol{x}_3,\ \boldsymbol{x}_7,\ \boldsymbol{x}_9,\ \boldsymbol{x}_{11},\ \boldsymbol{x}_{12},\ \boldsymbol{x}_{13},\ \boldsymbol{x}_{14},\ \boldsymbol{x}_{16},\\ &\boldsymbol{x}_{17} = [(1111)(1221)(2121)(2212)],\ \boldsymbol{x}_{18} = [(1111)(1221)(2122)(2211)],\\ &\boldsymbol{x}_{19} = [(1112)(1221)(2122)(2212)],\ \boldsymbol{x}_{20} = [(1111)(1222)(2122)(2212)],\\ &\boldsymbol{x}_{21} = [(1111)(1222)(2122)(2211)].\end{aligned}$$

uniqueness: unique minimal basis does not exist.
isomorphic structures of reference set:

$$\mathcal{F}_{\boldsymbol{t}(\boldsymbol{x}_8)} = G(\boldsymbol{x}_8),\ |G(\boldsymbol{t}(\boldsymbol{x}_8))| = 1,\ |\mathcal{F}_{\boldsymbol{t}(\boldsymbol{x}_8)}| = 4.$$

direct product structure for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{x}_8)}$:

$$\begin{gathered}\mathcal{F}_{\boldsymbol{t}(\boldsymbol{x}_8)} = X_{\gamma_1} \cup X_{\gamma_2} \cup X_{\gamma_3} \cup X_{\gamma_4} = G(\boldsymbol{x}_8),\\ X_{\gamma_1} = \{\boldsymbol{x}_8\},\ X_{\gamma_2} = \{\boldsymbol{x}_{8,2}\},\ X_{\gamma_3} = \{\boldsymbol{x}_{8,3}\},\ X_{\gamma_4} = \{\boldsymbol{x}_{8,4}\},\\ |\Gamma| = 4,\ |\Lambda| = 1,\\ |X_{\gamma_1} \cap G(\boldsymbol{x}_8)| = |\{\boldsymbol{x}_8\}| = 1,\\ \boldsymbol{x}_{8,2} = [(1121)(1211)(2112)(2222)],\\ \boldsymbol{x}_{8,3} = [(1112)(1222)(2121)(2211)],\\ \boldsymbol{x}_{8,4} = [(1122)(1212)(2111)(2221)].\end{gathered}$$

minimal basis for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{x}_8)}$: 16 kinds of 3 moves.
orbit graphs for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{x}_8)}$: 3 kinds of dispensable orbit graphs,

$$\begin{aligned}E_{\gamma_2} &= \{(X_{\gamma_1}, X_{\gamma_2}), (X_{\gamma_3}, X_{\gamma_4})\},\\ E_{\gamma_3} &= \{(X_{\gamma_1}, X_{\gamma_3}), (X_{\gamma_2}, X_{\gamma_4})\},\\ E_{\gamma_4} &= \{(X_{\gamma_1}, X_{\gamma_4}), (X_{\gamma_2}, X_{\gamma_3})\},\end{aligned}$$

which correspond to

$$\begin{aligned}\mathcal{B}_{\gamma_2} &= \{\boldsymbol{x}_8 - \boldsymbol{x}_{8,2}, \boldsymbol{x}_{8,3} - \boldsymbol{x}_{8,4}\},\\ \mathcal{B}_{\gamma_3} &= \{\boldsymbol{x}_8 - \boldsymbol{x}_{8,3}, \boldsymbol{x}_{8,2} - \boldsymbol{x}_{8,4}\},\\ \mathcal{B}_{\gamma_4} &= \{\boldsymbol{x}_8 - \boldsymbol{x}_{8,4}, \boldsymbol{x}_{8,2} - \boldsymbol{x}_{8,3}\},\end{aligned}$$

respectively.
invariant minimal basis for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{x}_8)}$: 3 kinds of 4 moves,

$$\{\mathcal{B}_{\gamma_2}, \mathcal{B}_{\gamma_3}\},\ \{\mathcal{B}_{\gamma_2}, \mathcal{B}_{\gamma_4}\},\ \{\mathcal{B}_{\gamma_3}, \mathcal{B}_{\gamma_4}\}.$$

4.3 Models with the independence graph (c)

- Model 12/13/24/34 (graphical model)
  degree of freedom: 7
  indispensable moves: 8 moves of degree 2 with representative elements

  $$\boldsymbol{y}_1,\ \boldsymbol{y}_2 = [(1111)(1221)],$$

  and 8 moves of degree 4 with representative elements $\boldsymbol{x}_3, \boldsymbol{x}_5, \boldsymbol{x}_9, \boldsymbol{x}_{10}$.
  uniqueness: unique minimal basis exists.

4.4 Models with the independence graph (d)

- Model 123/34 (graphical, decomposable model)
  degree of freedom: 6
  indispensable moves: 12 moves of degree 2 with representative elements

  $$\boldsymbol{y}_1,\ \boldsymbol{y}_3 = [(1111)(1212)],\ \boldsymbol{y}_4 = [(1111)(2212)].$$

  uniqueness: unique minimal basis exists.

- Model 12/13/23/34
  degree of freedom: 7
  indispensable moves: 12 moves of degree 2 with representative elements $\boldsymbol{y}_1, \boldsymbol{y}_3, \boldsymbol{y}_4$, and 4 moves of degree 4 with representative elements $\boldsymbol{x}_7, \boldsymbol{x}_{10}$.
  uniqueness: unique minimal basis does not exist.
  isomorphic structures of reference sets:

$$\begin{gathered}\mathcal{F}_{G(\boldsymbol{t}(\boldsymbol{x}_{17}))} = \mathcal{F}_{\boldsymbol{t}(\boldsymbol{x}_{17})} \cup \mathcal{F}_{\boldsymbol{t}(\boldsymbol{x}_{18})} \cup \mathcal{F}_{\boldsymbol{t}(\boldsymbol{x}_{19})} \cup \mathcal{F}_{\boldsymbol{t}(\boldsymbol{x}_{20})} = G(\boldsymbol{x}_{17}),\\ |G(\boldsymbol{t}(\boldsymbol{x}_{17}))| = 4,\ |\mathcal{F}_{G(\boldsymbol{t}(\boldsymbol{x}_{17}))}/G| = 1,\ |\mathcal{F}_{\boldsymbol{t}(\boldsymbol{x}_{17})}| = 4,\end{gathered}$$

$$\begin{gathered}\mathcal{F}_{\boldsymbol{t}(\boldsymbol{x}_8)} = G(\boldsymbol{x}_8) \cup G(\boldsymbol{x}_9),\\ |G(\boldsymbol{t}(\boldsymbol{x}_8))| = 1,\ |\mathcal{F}_{G(\boldsymbol{t}(\boldsymbol{x}_8))}/G| = 2,\ |\mathcal{F}_{\boldsymbol{t}(\boldsymbol{x}_8)}| = 8.\end{gathered}$$

  direct product structure for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{x}_{17})}$:

$$\begin{gathered}\mathcal{F}_{\boldsymbol{t}(\boldsymbol{x}_{17})} = X_{\gamma_1} \cup X_{\gamma_2} = G_{\boldsymbol{t}(\boldsymbol{x}_{17})}(\boldsymbol{x}_{17}),\\ X_{\gamma_1} = \{\boldsymbol{x}_{17}, \boldsymbol{x}_{20,3}\},\ X_{\gamma_2} = \{\boldsymbol{x}_{18,2}, \boldsymbol{x}_{19,4}\},\\ |\Gamma| = 2,\ |\Lambda| = 1,\\ |X_{\gamma_1} \cap G_{\boldsymbol{t}(\boldsymbol{x}_{17})}(\boldsymbol{x}_{17})| = |\{\boldsymbol{x}_{17}, \boldsymbol{x}_{20,3}\}| = 2,\\ \boldsymbol{x}_{18,2} = [(1121)(1211)(2112)(2221)],\\ \boldsymbol{x}_{19,4} = [(1121)(1212)(2111)(2221)],\\ \boldsymbol{x}_{20,3} = [(1112)(1221)(2121)(2211)].\end{gathered}$$

  direct product structure for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{x}_8)}$:

$$\begin{gathered}\mathcal{F}_{\boldsymbol{t}(\boldsymbol{x}_8)} = X_{\gamma_1} \cup X_{\gamma_2} = G_{\boldsymbol{t}(\boldsymbol{x}_8)}(\boldsymbol{x}_8) \cup G_{\boldsymbol{t}(\boldsymbol{x}_8)}(\boldsymbol{x}_9),\\ X_{\gamma_1} = \{\boldsymbol{x}_8, \boldsymbol{x}_{8,3}, \boldsymbol{x}_9, \boldsymbol{x}_{9,3}\},\ X_{\gamma_2} = \{\boldsymbol{x}_{8,2}, \boldsymbol{x}_{8,4}, \boldsymbol{x}_{9,2}, \boldsymbol{x}_{9,4}\},\\ |\Gamma| = 2,\ |\Lambda| = 2,\\ |X_{\gamma_1} \cap G_{\boldsymbol{t}(\boldsymbol{x}_8)}(\boldsymbol{x}_8)| = |\{\boldsymbol{x}_8, \boldsymbol{x}_{8,3}\}| = 2,\\ \boldsymbol{x}_{9,2} = [(1121)(1212)(2111)(2222)],\\ \boldsymbol{x}_{9,3} = [(1112)(1221)(2122)(2211)],\\ \boldsymbol{x}_{9,4} = [(1122)(1211)(2112)(2221)].\end{gathered}$$

  minimal basis for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{x}_{17})}$: 4 kinds of 1 move.
  minimal basis for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{x}_8)}$: 16 kinds of 1 move.
  orbit graph for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{x}_{17})}$: unique indispensable orbit graph,

$$\{(X_{\gamma_1}, X_{\gamma_2})\}$$

  which either of

$$\begin{gathered}\mathcal{B}_1 = \{\boldsymbol{x}_{17} - \boldsymbol{x}_{18,2}, \boldsymbol{x}_{20,3} - \boldsymbol{x}_{19,4}\},\\ \mathcal{B}_2 = \{\boldsymbol{x}_{17} - \boldsymbol{x}_{19,4}, \boldsymbol{x}_{20,3} - \boldsymbol{x}_{18,2}\}\end{gathered}$$

  derives.
  invariant minimal basis for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{x}_{17})}$: 2 kinds of 2 moves, $\mathcal{B}_1$ or $\mathcal{B}_2$.
  orbit graph for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{x}_8)}$: unique indispensable orbit graph,

$$\{(X_{\gamma_1}, X_{\gamma_2})\}$$

which either of

$$\mathcal{B}_1 = \{\boldsymbol{x}_8 - \boldsymbol{x}_{8,2}, \boldsymbol{x}_{8,3} - \boldsymbol{x}_{8,4}\},\ \mathcal{B}_2 = \{\boldsymbol{x}_8 - \boldsymbol{x}_{8,4}, \boldsymbol{x}_{8,2} - \boldsymbol{x}_{8,3}\},$$
$$\mathcal{B}_3 = \{\boldsymbol{x}_9 - \boldsymbol{x}_{9,2}, \boldsymbol{x}_{9,3} - \boldsymbol{x}_{9,4}\},\ \mathcal{B}_4 = \{\boldsymbol{x}_9 - \boldsymbol{x}_{9,4}, \boldsymbol{x}_{9,2} - \boldsymbol{x}_{9,3}\},$$
$$\mathcal{B}_5 = \{\boldsymbol{x}_8 - \boldsymbol{x}_{9,2}, \boldsymbol{x}_8 - \boldsymbol{x}_{9,4}, \boldsymbol{x}_9 - \boldsymbol{x}_{8,2}, \boldsymbol{x}_9 - \boldsymbol{x}_{8,4}, \boldsymbol{x}_{9,3} - \boldsymbol{x}_{8,2}, \boldsymbol{x}_{9,3} - \boldsymbol{x}_{8,4}, \boldsymbol{x}_{8,3} - \boldsymbol{x}_{9,2}, \boldsymbol{x}_{8,3} - \boldsymbol{x}_{9,4}\}$$

derives.
invariant minimal basis for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{x}_8)}$: 5 kinds, i.e., 4 kinds of 2 moves, $\mathcal{B}_1, \ldots, \mathcal{B}_4$, or 1 kind of 8 moves, $\mathcal{B}_5$.

4.5 Models with the independence graph (e)

- Model 123/4 (graphical, decomposable model)
degree of freedom: 7
indispensable moves: 28 moves of degree 2 with representative elements

$$\begin{aligned}&\boldsymbol{y}_1,\ \boldsymbol{y}_3,\ \boldsymbol{y}_4,\\ &\boldsymbol{y}_5 = [(1111)(1122)],\ \boldsymbol{y}_6 = [(1111)(1222)],\\ &\boldsymbol{y}_7 = [(1111)(2122)],\ \boldsymbol{y}_8 = [(1111)(2222)].\end{aligned}$$

uniqueness: unique minimal basis exists.

- Model 12/13/23/4
degree of freedom: 8
indispensable moves: 28 moves of degree 2 with representative elements

$$\boldsymbol{y}_1, \boldsymbol{y}_3, \boldsymbol{y}_4, \boldsymbol{y}_5, \boldsymbol{y}_6, \boldsymbol{y}_7, \boldsymbol{y}_8,$$

and 2 moves of degree 4 with representative element $\boldsymbol{x}_7$.
uniqueness: unique minimal basis does not exist.
isomorphic structures of reference sets:

$$\mathcal{F}_{G(\boldsymbol{t}(\boldsymbol{x}_{17}))} = \mathcal{F}_{\boldsymbol{t}(\boldsymbol{x}_{17})} \cup \mathcal{F}_{\boldsymbol{t}(\boldsymbol{x}_{19})} = G(\boldsymbol{x}_{17}),$$
$$|G(\boldsymbol{t}(\boldsymbol{x}_{17}))| = 2,\ |\mathcal{F}_{G(\boldsymbol{t}(\boldsymbol{x}_{17}))}/G| = 1,\ |\mathcal{F}_{\boldsymbol{t}(\boldsymbol{x}_{17})}| = 8,$$

$$\mathcal{F}_{\boldsymbol{t}(\boldsymbol{x}_8)} = G(\boldsymbol{x}_8) \cup G(\boldsymbol{x}_9) \cup G(\boldsymbol{x}_{10}),$$
$$|G(\boldsymbol{t}(\boldsymbol{x}_8))| = 1,\ |\mathcal{F}_{G(\boldsymbol{t}(\boldsymbol{x}_8))}/G| = 3,\ |\mathcal{F}_{\boldsymbol{t}(\boldsymbol{x}_8)}| = 12.$$

direct product structure for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{x}_{17})}$:

$$\mathcal{F}_{\boldsymbol{t}(\boldsymbol{x}_{17})} = X_{\gamma_1} \cup X_{\gamma_2} = G_{\boldsymbol{t}(\boldsymbol{x}_{17})}(\boldsymbol{x}_{17}),$$
$$X_{\gamma_1} = \{\boldsymbol{x}_{17}, \boldsymbol{x}_{18}, \boldsymbol{x}_{19,3}, \boldsymbol{x}_{20,3}\},\ X_{\gamma_2} = \{\boldsymbol{x}_{17,2}, \boldsymbol{x}_{18,2}, \boldsymbol{x}_{19,4}, \boldsymbol{x}_{20,4}\},$$
$$|\Gamma| = 2,\ |\Lambda| = 1,$$
$$|X_{\gamma_1} \cap G_{\boldsymbol{t}(\boldsymbol{x}_{17})}(\boldsymbol{x}_{17})| = |\{\boldsymbol{x}_{17}, \boldsymbol{x}_{18}, \boldsymbol{x}_{19,3}, \boldsymbol{x}_{20,3}\}| = 4,$$
$$\boldsymbol{x}_{17,2} = [(1121)(1211)(2111)(2222)],$$
$$\boldsymbol{x}_{19,3} = [(1111)(1222)(2121)(2211)],$$
$$\boldsymbol{x}_{20,4} = [(1122)(1211)(2111)(2221)].$$

direct product structure for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{x}_8)}$:

$$\begin{gathered}\mathcal{F}_{\boldsymbol{t}(\boldsymbol{x}_8)} = X_{\gamma_1} \cup X_{\gamma_2} = G_{\boldsymbol{t}(\boldsymbol{x}_8)}(\boldsymbol{x}_8) \cup G_{\boldsymbol{t}(\boldsymbol{x}_8)}(\boldsymbol{x}_9) \cup G_{\boldsymbol{t}(\boldsymbol{x}_8)}(\boldsymbol{x}_{10}),\\ X_{\gamma_1} = \{\boldsymbol{x}_8, \boldsymbol{x}_{8,3}, \boldsymbol{x}_9, \boldsymbol{x}_{9,3}, \boldsymbol{x}_{10}, \boldsymbol{x}_{10,3}\},\\ X_{\gamma_2} = \{\boldsymbol{x}_{8,2}, \boldsymbol{x}_{8,4}, \boldsymbol{x}_{9,2}, \boldsymbol{x}_{9,4}, \boldsymbol{x}_{10,2}, \boldsymbol{x}_{10,4}\},\\ |\Gamma| = 2,\ |\Lambda| = 3,\\ |X_{\gamma_1} \cap G_{\boldsymbol{t}(\boldsymbol{x}_8)}(\boldsymbol{x}_8)| = |\{\boldsymbol{x}_8, \boldsymbol{x}_{8,3}\}| = 2,\\ \boldsymbol{x}_{10,2} = [(1122)(1211)(2111)(2222)],\\ \boldsymbol{x}_{10,3} = [(1112)(1221)(2121)(2212)],\\ \boldsymbol{x}_{10,4} = [(1121)(1212)(2112)(2221)].\end{gathered}$$

minimal basis for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{x}_{17})}$: 16 kinds of 1 move.
minimal basis for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{x}_8)}$: 36 kinds of 1 move.
orbit graph for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{x}_{17})}$: unique indispensable orbit graph,

$$\{(X_{\gamma_1}, X_{\gamma_2})\}$$

which either of

$$\begin{aligned}\mathcal{B}_1 &= \{\boldsymbol{x}_{20,3} - \boldsymbol{x}_{20,4}, \boldsymbol{x}_{19,3} - \boldsymbol{x}_{19,4}, \boldsymbol{x}_{18} - \boldsymbol{x}_{18,2}, \boldsymbol{x}_{17} - \boldsymbol{x}_{17,2}\},\\ \mathcal{B}_2 &= \{\boldsymbol{x}_{20,3} - \boldsymbol{x}_{18,2}, \boldsymbol{x}_{19,3} - \boldsymbol{x}_{17,2}, \boldsymbol{x}_{18} - \boldsymbol{x}_{20,4}, \boldsymbol{x}_{17} - \boldsymbol{x}_{19,4}\},\\ \mathcal{B}_3 &= \{\boldsymbol{x}_{20,3} - \boldsymbol{x}_{19,4}, \boldsymbol{x}_{19,3} - \boldsymbol{x}_{20,4}, \boldsymbol{x}_{18} - \boldsymbol{x}_{17,2}, \boldsymbol{x}_{17} - \boldsymbol{x}_{18,2}\},\\ \mathcal{B}_4 &= \{\boldsymbol{x}_{20,3} - \boldsymbol{x}_{17,2}, \boldsymbol{x}_{19,3} - \boldsymbol{x}_{18,2}, \boldsymbol{x}_{18} - \boldsymbol{x}_{19,4}, \boldsymbol{x}_{17} - \boldsymbol{x}_{20,4}\}\end{aligned}$$

derives.
invariant minimal basis for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{x}_{17})}$: 4 kinds of 4 moves, $\mathcal{B}_1, \ldots, \mathcal{B}_4$.
orbit graph for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{x}_8)}$: unique indispensable orbit graph,

$$\{(X_{\gamma_1}, X_{\gamma_2})\}$$

which either of

$$\begin{gathered}\mathcal{B}_1 = \{\boldsymbol{x}_8 - \boldsymbol{x}_{8,2}, \boldsymbol{x}_{8,3} - \boldsymbol{x}_{8,4}\},\ \mathcal{B}_2 = \{\boldsymbol{x}_8 - \boldsymbol{x}_{8,4}, \boldsymbol{x}_{8,3} - \boldsymbol{x}_{8,2}\},\\ \mathcal{B}_3 = \{\boldsymbol{x}_9 - \boldsymbol{x}_{9,2}, \boldsymbol{x}_{9,3} - \boldsymbol{x}_{9,4}\},\ \mathcal{B}_4 = \{\boldsymbol{x}_9 - \boldsymbol{x}_{9,4}, \boldsymbol{x}_{9,3} - \boldsymbol{x}_{9,2}\},\\ \mathcal{B}_5 = \{\boldsymbol{x}_{10} - \boldsymbol{x}_{10,2}, \boldsymbol{x}_{10,3} - \boldsymbol{x}_{10,4}\},\ \mathcal{B}_6 = \{\boldsymbol{x}_{10} - \boldsymbol{x}_{10,4}, \boldsymbol{x}_{10,3} - \boldsymbol{x}_{10,2}\},\\ \mathcal{B}_7 = \{\boldsymbol{x}_8 - \boldsymbol{x}_{9,2}, \boldsymbol{x}_8 - \boldsymbol{x}_{9,4}, \boldsymbol{x}_{8,3} - \boldsymbol{x}_{9,2}, \boldsymbol{x}_{8,3} - \boldsymbol{x}_{9,4},\\ \boldsymbol{x}_9 - \boldsymbol{x}_{8,2}, \boldsymbol{x}_9 - \boldsymbol{x}_{8,4}, \boldsymbol{x}_{9,3} - \boldsymbol{x}_{8,2}, \boldsymbol{x}_{9,3} - \boldsymbol{x}_{8,4}\},\\ \mathcal{B}_8 = \{\boldsymbol{x}_8 - \boldsymbol{x}_{10,2}, \boldsymbol{x}_8 - \boldsymbol{x}_{10,4}, \boldsymbol{x}_{8,3} - \boldsymbol{x}_{10,2}, \boldsymbol{x}_{8,3} - \boldsymbol{x}_{10,4},\\ \boldsymbol{x}_{10} - \boldsymbol{x}_{8,2}, \boldsymbol{x}_{10} - \boldsymbol{x}_{8,4}, \boldsymbol{x}_{10,3} - \boldsymbol{x}_{8,2}, \boldsymbol{x}_{10,3} - \boldsymbol{x}_{8,4}\},\\ \mathcal{B}_9 = \{\boldsymbol{x}_9 - \boldsymbol{x}_{10,2}, \boldsymbol{x}_9 - \boldsymbol{x}_{10,4}, \boldsymbol{x}_{9,3} - \boldsymbol{x}_{10,2}, \boldsymbol{x}_{9,3} - \boldsymbol{x}_{10,4},\\ \boldsymbol{x}_{10} - \boldsymbol{x}_{9,2}, \boldsymbol{x}_{10} - \boldsymbol{x}_{9,4}, \boldsymbol{x}_{10,3} - \boldsymbol{x}_{9,2}, \boldsymbol{x}_{10,3} - \boldsymbol{x}_{9,4}\}\end{gathered}$$

derives.
invariant minimal basis for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{x}_8)}$: 9 kinds, i.e., 6 kinds of 2 moves, $\mathcal{B}_1, \ldots, \mathcal{B}_6$, or 3 kinds of 8 moves, $\mathcal{B}_7, \ldots, \mathcal{B}_9$.

4.6 Models with the independence graph (f)

- Model 123/4 (graphical, decomposable model)
  degree of freedom: 8
  indispensable moves: 20 moves of degree 2 with representative elements $\boldsymbol{y}_1, \boldsymbol{y}_2, \boldsymbol{y}_5, \boldsymbol{y}_6, \boldsymbol{y}_7$.
  uniqueness: unique minimal basis exists.

4.7 Models with the independence graph (g)

- Model 12/13/14 (graphical, decomposable model)
  degree of freedom: 8
  indispensable moves: 12 moves of degree 2 with representative elements $\boldsymbol{y}_2, \boldsymbol{y}_3, \boldsymbol{y}_5$.
  uniqueness: unique minimal basis does not exist.
  isomorphic structures of reference sets:

$$\mathcal{F}_{G(\boldsymbol{t}(\boldsymbol{y}_6))} = \mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_6)} \cup \mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}'_6)} = G(\boldsymbol{y}_6),$$
$$|G(\boldsymbol{t}(\boldsymbol{y}_6))| = 2,\ |\mathcal{F}_{G(\boldsymbol{t}(\boldsymbol{y}_6))}/G| = 1,\ |\mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_6)}| = 4,$$
$$\boldsymbol{y}'_6 = [(2111)(2222)].$$

  direct product structure for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_6)}$:

$$\mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_6)} = X_{\gamma_1} \cup X_{\gamma_2} \cup X_{\gamma_3} \cup X_{\gamma_4} = G_{\boldsymbol{t}(\boldsymbol{y}_6)}(\boldsymbol{y}_6),$$
$$X_{\gamma_1} = \{\boldsymbol{y}_6\},\ X_{\gamma_2} = \{\boldsymbol{y}_{6,2}\},\ X_{\gamma_3} = \{\boldsymbol{y}_{6,3}\},\ X_{\gamma_4} = \{\boldsymbol{y}_{6,4}\},$$
$$|\Gamma| = 4,\ |\Lambda| = 1,$$
$$|X_{\gamma_1} \cap G_{\boldsymbol{t}(\boldsymbol{y}_6)}(\boldsymbol{y}_6)| = |\{\boldsymbol{y}_6\}| = 1,$$
$$\boldsymbol{y}_{6,2} = [(1112)(1221)],$$
$$\boldsymbol{y}_{6,3} = [(1121)(1212)],$$
$$\boldsymbol{y}_{6,4} = [(1122)(1211)].$$

  minimal basis for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_6)}$: 16 kinds of 3 moves.
  orbit graphs for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_6)}$: 3 kinds of dispensable orbit graphs,

$$E_{\gamma_2} = \{(X_{\gamma_1}, X_{\gamma_2}), (X_{\gamma_3}, X_{\gamma_4})\},$$
$$E_{\gamma_3} = \{(X_{\gamma_1}, X_{\gamma_3}), (X_{\gamma_2}, X_{\gamma_4})\},$$
$$E_{\gamma_4} = \{(X_{\gamma_1}, X_{\gamma_4}), (X_{\gamma_2}, X_{\gamma_3})\},$$

  which correspond to

$$\mathcal{B}_{\gamma_2} = \{\boldsymbol{y}_6 - \boldsymbol{y}_{6,2}, \boldsymbol{y}_{6,3} - \boldsymbol{y}_{6,4}\},$$
$$\mathcal{B}_{\gamma_3} = \{\boldsymbol{y}_6 - \boldsymbol{y}_{6,3}, \boldsymbol{y}_{6,2} - \boldsymbol{y}_{6,4}\},$$
$$\mathcal{B}_{\gamma_4} = \{\boldsymbol{y}_6 - \boldsymbol{y}_{6,4}, \boldsymbol{y}_{6,2} - \boldsymbol{y}_{6,3}\},$$

  respectively.
  invariant minimal basis for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_6)}$: 3 kinds of 4 moves,

$$\{\mathcal{B}_{\gamma_2}, \mathcal{B}_{\gamma_3}\},\ \{\mathcal{B}_{\gamma_2}, \mathcal{B}_{\gamma_4}\},\ \{\mathcal{B}_{\gamma_3}, \mathcal{B}_{\gamma_4}\}.$$

4.8 Models with the independence graph (h)

- Model 12/13/4 (graphical, decomposable model)
  degree of freedom: 9
  indispensable moves: 28 moves of degree 2 with representative elements

$$\boldsymbol{y}_1, \boldsymbol{y}_2, \boldsymbol{y}_3, \boldsymbol{y}_4, \boldsymbol{y}_5, \boldsymbol{y}_7, \boldsymbol{y}_8.$$

  uniqueness: unique minimal basis does not exist.
  isomorphic structures of reference sets:

$$\mathcal{F}_{G(\boldsymbol{t}(\boldsymbol{y}_6))} = \mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_6)} \cup \mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}'_6)} = G(\boldsymbol{y}_6),$$
$$|G(\boldsymbol{t}(\boldsymbol{y}_6))| = 2,\ |\mathcal{F}_{G(\boldsymbol{t}(\boldsymbol{y}_6))}/G| = 1,\ |\mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_6)}| = 4.$$

direct product structure for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_6)}$: same as model 12/13/14.
minimal basis for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_6)}$: 16 kinds of 3 moves.
orbit graphs for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_6)}$: 3 kinds of dispensable orbit graphs (same as model 12/13/14).
invariant minimal basis for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_6)}$: 3 kinds of 4 moves (same as model 12/13/14).

4.9 Models with the independence graph (i)

- Model 12/34 (graphical, decomposable model)
  degree of freedom: 9
  indispensable moves: 36 moves of degree 2 with representative elements

$$\begin{array}{l} \boldsymbol{y}_1,\ \boldsymbol{y}_2,\ \boldsymbol{y}_3,\ \boldsymbol{y}_4,\ \boldsymbol{y}_6,\ \boldsymbol{y}_7,\ \boldsymbol{y}_8, \\ \boldsymbol{y}_9 = [(1111)(2121)],\ \boldsymbol{y}_{10} = [(1111)(2221)]. \end{array}$$

  uniqueness: unique minimal basis exists.

4.10 Models with the independence graph (j)

- Model 12/3/4 (graphical, decomposable model)
  degree of freedom: 10
  indispensable moves: 28 moves of degree 2 with representative elements

$$\boldsymbol{y}_1, \boldsymbol{y}_2, \boldsymbol{y}_3, \boldsymbol{y}_4, \boldsymbol{y}_5, \boldsymbol{y}_9, \boldsymbol{y}_{10}.$$

  uniqueness: unique minimal basis does not exist.
  isomorphic structures of reference sets:

$$\begin{gathered} \mathcal{F}_{G(\boldsymbol{t}(\boldsymbol{y}_6))} = \mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_6)} \cup \mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_6')} = G(\boldsymbol{y}_6), \\ |G(\boldsymbol{t}(\boldsymbol{y}_6))| = 2,\ |\mathcal{F}_{G(\boldsymbol{t}(\boldsymbol{y}_6))}/G| = 1,\ |\mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_6)}| = 4, \\ \mathcal{F}_{G(\boldsymbol{t}(\boldsymbol{y}_7))} = \mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_7)} \cup \mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_7')} = G(\boldsymbol{y}_7), \\ |G(\boldsymbol{t}(\boldsymbol{y}_7))| = 2,\ |\mathcal{F}_{G(\boldsymbol{t}(\boldsymbol{y}_7))}/G| = 1,\ |\mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_7)}| = 4, \\ \boldsymbol{y}_7' = [(1211)(2222)], \\ \mathcal{F}_{G(\boldsymbol{t}(\boldsymbol{y}_8))} = \mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_8)} \cup \mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_8')} = G(\boldsymbol{y}_8), \\ |G(\boldsymbol{t}(\boldsymbol{y}_8))| = 2,\ |\mathcal{F}_{G(\boldsymbol{t}(\boldsymbol{y}_8))}/G| = 1,\ |\mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_8)}| = 4, \\ \boldsymbol{y}_8' = [(1211)(2122)]. \end{gathered}$$

  direct product structure for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_6)}$: same as model 12/13/14.
  direct product structure for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_7)}$:

$$\begin{gathered} \mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_7)} = X_{\gamma_1} \cup X_{\gamma_2} \cup X_{\gamma_3} \cup X_{\gamma_4} = G_{\boldsymbol{t}(\boldsymbol{y}_7)}(\boldsymbol{y}_7), \\ X_{\gamma_1} = \{\boldsymbol{y}_7\},\ X_{\gamma_2} = \{\boldsymbol{y}_{7,2}\},\ X_{\gamma_3} = \{\boldsymbol{y}_{7,3}\},\ X_{\gamma_4} = \{\boldsymbol{y}_{7,4}\}, \\ |\Gamma| = 4,\ |\Lambda| = 1, \\ |X_{\gamma_1} \cap G_{\boldsymbol{t}(\boldsymbol{y}_7)}(\boldsymbol{y}_7)| = |\{\boldsymbol{y}_7\}| = 1, \\ \boldsymbol{y}_{7,2} = [(1112)(2121)], \\ \boldsymbol{y}_{7,3} = [(1121)(2112)], \\ \boldsymbol{y}_{7,4} = [(1122)(2111)]. \end{gathered}$$

direct product structure for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_8)}$:

$$\mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_8)} = X_{\gamma_1} \cup X_{\gamma_2} \cup X_{\gamma_3} \cup X_{\gamma_4} = G_{\boldsymbol{t}(\boldsymbol{y}_8)}(\boldsymbol{y}_8),$$
$$X_{\gamma_1} = \{\boldsymbol{y}_8\},\ X_{\gamma_2} = \{\boldsymbol{y}_{8,2}\},\ X_{\gamma_3} = \{\boldsymbol{y}_{8,3}\},\ X_{\gamma_4} = \{\boldsymbol{y}_{8,4}\},$$
$$|\Gamma| = 4,\ |\Lambda| = 1,$$
$$|X_{\gamma_1} \cap G_{\boldsymbol{t}(\boldsymbol{y}_8)}(\boldsymbol{y}_8)| = |\{\boldsymbol{y}_8\}| = 1,$$
$$\boldsymbol{y}_{8,2} = [(1112)(2221)],$$
$$\boldsymbol{y}_{8,3} = [(1121)(2212)],$$
$$\boldsymbol{y}_{8,4} = [(1122)(2211)].$$

minimal basis for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_6)}, \mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_7)}, \mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_8)}$: 16 kinds of 3 moves, respectively.
orbit graphs for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_6)}, \mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_7)}, \mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_8)}$: 3 kinds of dispensable orbit graphs, respectively (same as model 12/13/14).
invariant minimal basis for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_6)}, \mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_7)}, \mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_8)}$: 3 kinds of 4 moves, respectively (same as model 12/13/14).

4.11 Models with the independence graph (k)

- Model 12/3/4 (graphical, decomposable model)
  degree of freedom: 11
  indispensable moves: 24 moves of degree 2 with representative elements

$$\boldsymbol{y}_1,\ \boldsymbol{y}_2,\ \boldsymbol{y}_3,\ \boldsymbol{y}_5,\ \boldsymbol{y}_9,\ \boldsymbol{y}_{11} = [(1111)(2211)].$$

  uniqueness: unique minimal basis does not exist.
  isomorphic structures of reference sets:

$$\mathcal{F}_{G(\boldsymbol{t}(\boldsymbol{y}_4))} = \mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_4)} \cup \mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}'_4)} = G(\boldsymbol{y}_4),$$
$$|G(\boldsymbol{t}(\boldsymbol{y}_4))| = 2,\ |\mathcal{F}_{G(\boldsymbol{t}(\boldsymbol{y}_4))}/G| = 1,\ |\mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_4)}| = 4,$$
$$\boldsymbol{y}'_4 = [(1121)(2222)],$$
$$\mathcal{F}_{G(\boldsymbol{t}(\boldsymbol{y}_6))} = \mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_6)} \cup \mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}'_6)} = G(\boldsymbol{y}_6),$$
$$|G(\boldsymbol{t}(\boldsymbol{y}_6))| = 2,\ |\mathcal{F}_{G(\boldsymbol{t}(\boldsymbol{y}_6))}/G| = 1,\ |\mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_6)}| = 4,$$
$$\mathcal{F}_{G(\boldsymbol{t}(\boldsymbol{y}_7))} = \mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_7)} \cup \mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}'_7)} = G(\boldsymbol{y}_7),$$
$$|G(\boldsymbol{t}(\boldsymbol{y}_7))| = 2,\ |\mathcal{F}_{G(\boldsymbol{t}(\boldsymbol{y}_7))}/G| = 1,\ |\mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_7)}| = 4,$$
$$\mathcal{F}_{G(\boldsymbol{t}(\boldsymbol{y}_{10}))} = \mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_{10})} \cup \mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}'_{10})} = G(\boldsymbol{y}_{10}),$$
$$|G(\boldsymbol{t}(\boldsymbol{y}_{10}))| = 2,\ |\mathcal{F}_{G(\boldsymbol{t}(\boldsymbol{y}_{10}))}/G| = 1,\ |\mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_{10})}| = 4,$$
$$\boldsymbol{y}'_{10} = [(1112)(2222)],$$

$$\mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_8)} = G(\boldsymbol{y}_8),$$
$$|G(\boldsymbol{t}(\boldsymbol{y}_8))| = 1,\ |\mathcal{F}_{G(\boldsymbol{t}(\boldsymbol{y}_8))}/G| = 1,\ |\mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_8)}| = 8.$$

  direct product structure for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_4)}$:

$$\mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_4)} = X_{\gamma_1} \cup X_{\gamma_2} \cup X_{\gamma_3} \cup X_{\gamma_4} = G_{\boldsymbol{t}(\boldsymbol{y}_4)}(\boldsymbol{y}_4),$$
$$X_{\gamma_1} = \{\boldsymbol{y}_4\},\ X_{\gamma_2} = \{\boldsymbol{y}_{4,2}\},\ X_{\gamma_3} = \{\boldsymbol{y}_{4,3}\},\ X_{\gamma_4} = \{\boldsymbol{y}_{4,4}\},$$
$$|\Gamma| = 4,\ |\Lambda| = 1,$$
$$|X_{\gamma_1} \cap G_{\boldsymbol{t}(\boldsymbol{y}_4)}(\boldsymbol{y}_4)| = |\{\boldsymbol{y}_4\}| = 1,$$
$$\boldsymbol{y}_{4,2} = [(1112)(2211)],$$
$$\boldsymbol{y}_{4,3} = [(1211)(2112)],$$
$$\boldsymbol{y}_{4,4} = [(1212)(2111)].$$

direct product structure for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_6)}$: same as model 12/13/14.
direct product structure for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_7)}$: same as model 12/3/4.
direct product structure for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_{10})}$:

$$\begin{gathered}
\mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_{10})} = X_{\gamma_1} \cup X_{\gamma_2} \cup X_{\gamma_3} \cup X_{\gamma_4} = G_{\boldsymbol{t}(\boldsymbol{y}_{10})}(\boldsymbol{y}_{10}), \\
X_{\gamma_1} = \{\boldsymbol{y}_{10}\},\ X_{\gamma_2} = \{\boldsymbol{y}_{10,2}\},\ X_{\gamma_3} = \{\boldsymbol{y}_{10,3}\},\ X_{\gamma_4} = \{\boldsymbol{y}_{10,4}\}, \\
|\Gamma| = 4,\ |\Lambda| = 1, \\
|X_{\gamma_1} \cap G_{\boldsymbol{t}(\boldsymbol{y}_{10})}(\boldsymbol{y}_{10})| = |\{\boldsymbol{y}_{10}\}| = 1, \\
\boldsymbol{y}_{10,2} = [(1121)(2211)], \\
\boldsymbol{y}_{10,3} = [(1211)(2121)], \\
\boldsymbol{y}_{10,4} = [(1221)(2111)].
\end{gathered}$$

direct product structure for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_8)}$:

$$\begin{gathered}
\mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_8)} = X_{\gamma_1} \cup X_{\gamma_2} \cup X_{\gamma_3} \cup X_{\gamma_4} \cup X_{\gamma_5} \cup X_{\gamma_6} \cup X_{\gamma_7} \cup X_{\gamma_8} = G_{\boldsymbol{t}(\boldsymbol{y}_8)}(\boldsymbol{y}_8), \\
X_{\gamma_1} = \{\boldsymbol{y}_8\},\ X_{\gamma_2} = \{\boldsymbol{y}_{8,2}\},\ X_{\gamma_3} = \{\boldsymbol{y}_{8,3}\},\ X_{\gamma_4} = \{\boldsymbol{y}_{8,4}\}, \\
X_{\gamma_5} = \{\boldsymbol{y}_{8,5}\},\ X_{\gamma_6} = \{\boldsymbol{y}_{8,6}\},\ X_{\gamma_7} = \{\boldsymbol{y}_{8,7}\},\ X_{\gamma_8} = \{\boldsymbol{y}_{8,8}\}, \\
|\Gamma| = 8,\ |\Lambda| = 1, \\
|X_{\gamma_1} \cap G_{\boldsymbol{t}(\boldsymbol{y}_8)}(\boldsymbol{y}_8)| = |\{\boldsymbol{y}_8\}| = 1, \\
\boldsymbol{y}_{8,2} = [(1112)(2221)], \\
\boldsymbol{y}_{8,3} = [(1121)(2212)], \\
\boldsymbol{y}_{8,4} = [(1122)(2211)], \\
\boldsymbol{y}_{8,5} = [(1211)(2122)], \\
\boldsymbol{y}_{8,6} = [(1212)(2121)], \\
\boldsymbol{y}_{8,7} = [(1221)(2112)], \\
\boldsymbol{y}_{8,8} = [(1222)(2111)].
\end{gathered}$$

minimal basis for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_4)}, \mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_6)}, \mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_7)}, \mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_{10})}$: 16 kinds of 3 moves, respectively.
minimal basis for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_8)}$: $8^{8-2} = 262144$ kinds of 7 moves.
orbit graphs for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_4)}, \mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_6)}, \mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_7)}, \mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_{10})}$: 3 kinds of dispensable orbit graphs, respectively (same as model 12/13/14).
invariant minimal basis for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_4)}, \mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_6)}, \mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_7)}, \mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_{10})}$: 3 kinds of 4 moves, respectively (same as model 12/13/14).
orbit graphs for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_8)}$: 7 kinds of dispensable orbit graphs,

$$\begin{aligned}
E_{\gamma_2} &= \{(X_{\gamma_1}, X_{\gamma_2}), (X_{\gamma_3}, X_{\gamma_4}), (X_{\gamma_5}, X_{\gamma_6}), (X_{\gamma_7}, X_{\gamma_8})\}, \\
E_{\gamma_3} &= \{(X_{\gamma_1}, X_{\gamma_3}), (X_{\gamma_2}, X_{\gamma_4}), (X_{\gamma_5}, X_{\gamma_7}), (X_{\gamma_6}, X_{\gamma_8})\}, \\
E_{\gamma_4} &= \{(X_{\gamma_1}, X_{\gamma_4}), (X_{\gamma_2}, X_{\gamma_3}), (X_{\gamma_5}, X_{\gamma_8}), (X_{\gamma_6}, X_{\gamma_7})\}, \\
E_{\gamma_5} &= \{(X_{\gamma_1}, X_{\gamma_5}), (X_{\gamma_2}, X_{\gamma_6}), (X_{\gamma_3}, X_{\gamma_7}), (X_{\gamma_4}, X_{\gamma_8})\}, \\
E_{\gamma_6} &= \{(X_{\gamma_1}, X_{\gamma_6}), (X_{\gamma_2}, X_{\gamma_5}), (X_{\gamma_3}, X_{\gamma_8}), (X_{\gamma_4}, X_{\gamma_7})\}, \\
E_{\gamma_7} &= \{(X_{\gamma_1}, X_{\gamma_7}), (X_{\gamma_2}, X_{\gamma_8}), (X_{\gamma_3}, X_{\gamma_5}), (X_{\gamma_4}, X_{\gamma_6})\}, \\
E_{\gamma_8} &= \{(X_{\gamma_1}, X_{\gamma_8}), (X_{\gamma_2}, X_{\gamma_7}), (X_{\gamma_3}, X_{\gamma_6}), (X_{\gamma_4}, X_{\gamma_5})\},
\end{aligned}$$

which correspond to $\mathcal{B}_{\gamma_2}, \ldots, \mathcal{B}_{\gamma_8}$, respectively.
invariant minimal basis for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_8)}$: 7 kinds of 12 moves,

$$\begin{gathered}
\{\mathcal{B}_{\gamma_2}, \mathcal{B}_{\gamma_3}, \mathcal{B}_{\gamma_4}\},\ \{\mathcal{B}_{\gamma_2}, \mathcal{B}_{\gamma_5}, \mathcal{B}_{\gamma_6}\},\ \{\mathcal{B}_{\gamma_2}, \mathcal{B}_{\gamma_7}, \mathcal{B}_{\gamma_8}\},\ \{\mathcal{B}_{\gamma_3}, \mathcal{B}_{\gamma_5}, \mathcal{B}_{\gamma_7}\}, \\
\{\mathcal{B}_{\gamma_3}, \mathcal{B}_{\gamma_6}, \mathcal{B}_{\gamma_8}\},\ \{\mathcal{B}_{\gamma_4}, \mathcal{B}_{\gamma_5}, \mathcal{B}_{\gamma_8}\},\ \{\mathcal{B}_{\gamma_4}, \mathcal{B}_{\gamma_6}, \mathcal{B}_{\gamma_7}\}.
\end{gathered}$$

5 Discussion

In this paper we define an invariant minimal Markov basis and derive its basic characteristics. Of course, we can construct an invariant Markov basis from any Markov basis as the union of all orbits of the basis elements. However, even if we start with a minimal Markov basis, the union of all orbits of the basis elements is not necessarily an invariant minimal basis. For example, consider again the complete independence model of the three-way case of Example 11. A set of moves

$$\{\boldsymbol{x}_8 - \boldsymbol{x}_8',\ \boldsymbol{x}_8 - \boldsymbol{x}_8'',\ \boldsymbol{x}_8 - \boldsymbol{x}_8'''\}$$

connects the four elements $\boldsymbol{x}_8, \boldsymbol{x}_8', \boldsymbol{x}_8'', \boldsymbol{x}_8'''$ into a tree, and thus is a minimal basis elements for $\{\boldsymbol{x}_8, \boldsymbol{x}_8', \boldsymbol{x}_8'', \boldsymbol{x}_8'''\}$. However, it is seen that the union of the orbits of these three moves contains 6 moves, and hence not minimal invariant. From these considerations, structure of an invariant minimal Markov basis is important.

Theorem 1 states how to construct an invariant minimal Markov basis. This theorem is an extension of Theorem 1 of Takemura and Aoki (2003). To construct a minimal Markov basis, we can add basis elements step by step from low degree, by considering all reference sets as stated in Theorem 1 of Takemura and Aoki (2003). On the other hand, to construct an invariant minimal Markov basis, we have to add the orbit of moves step by step from low degree. Similar to the construction of a minimal Markov basis, it is difficult to construct an invariant minimal Markov basis by applying Theorem 1 directly. But if a minimal Markov basis is available, we can construct an invariant minimal Markov basis relatively easily, by considering all the reference sets one by one, which is covered by the dispensable moves in the minimal Markov basis. The results of Section 4 is obtained in such a way.

It seems also difficult to give a simple necessary and sufficient conditions on $D_1, \ldots, D_r$ such that an invariant minimal Markov basis is unique. It is of interest to derive conditions such that an invariant minimal Markov basis is unique even if a minimal Markov basis is not unique. As stated in Section 3, such an example we have found so far is the obvious one-way contingency table, except for the peculiar case of the Hardy-Weinberg model.

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